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Full Length Article

Numerical Modeling of Transport and Transformation of Synthetic Wastewater in Irrigated Soils using HYDRUS-1D

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Abstract

Irrigation with wastewater poses risks to deterioration of the hydraulic soil properties and contamination of groundwater. In order to study these concerns, synthetic wastewater was poured on one-dimensional aerobic sand columns and the results were analyzed. A randomized complete block design under unsaturated, steady-state flux conditions (1 cm h^{-1}) was performed with soil columns treated with synthetic wastewater. Glucose, NH_4Cl and phosphate were provided as the carbon, nitrogen and phosphorus source, respectively. Four irrigation treatments with different levels of Chemical Oxygen Demand (COD) were applied. Soil water content, electrical conductivity, water potential and hydraulic conductivities were monitored. A numerical model, Hydrus-1D, was used to inversely estimate water and solute transport parameters such as water content, dispersivity and degradation constant. In all treatments the hydraulic transport properties remained constant. Conversely, the first-order kinetics degradation constant decreased in an identical way for all COD-treatments. With the time the efficiency of the degradation of synthetic wastewater dropped, shown as decreasing degradation kinetic constant. It is also concluded that if a primary treatment removes the solids from wastewater, which is essential for drip irrigation, domestic wastewater, similar to our synthetic water and without toxic or pathogen elements, poses little risks to contaminate groundwater. © 2013 Friends Science Publishers

Keywords: HYDRUS-1D; Solute transport; Irrigation; Synthetic wastewater; Chemical oxygen demand

Introduction

Irrigation with wastewater has become a common practice in developed and under-development countries (AATSE, 2004; Jimenez and Asano, 2008). A major concern about using wastewater for irrigation is that the hydraulic properties of the soil are influenced by wastewater. Another concern is that the wastewater could penetrate and pollute the phreatic water table. Accurate assessment of parameter and predictive uncertainty of water and solute transport is essential to optimally manage soils and subsurface aquifers and to address chemical pollution in these resources. The variety and complexity of the physical, chemical and biological interactions between the solute and the soil or subsurface aquifer medium often make it very difficult to describe and predict solute transport behavior in these types of porous media. The modeling of solute transport requires a thorough understanding of the main processes involved.

The hydraulic properties of unsaturated soil are assessed by parameter optimization methods, which became popular in mid 1980s (e.g., Kool *et al*., 1985), initially in conjunction with mostly one- and multi-step outflow experiments. Different studies have shown that inverse optimization of hydraulic and solute transport properties are suitable techniques in saturated and unsaturated zone area (Ritter *et al.*, 2005; Šimůnek *et al*., 2009; Wöhling and Vrugt, 2007; Chou and Wyseure, 2009; Scharnagl *et al.*, 2011; Nasir *et al.*, 2012).

Description of solute transport behaviour by use of suitable models is crucial to understand the fate of solute. One of the most interesting application transport model for describing the contaminant transport in the porous media is the convection–dispersion equation (CDE) (Bear, 1972). Most mechanistic transport models for solutes in porous materials are based on the convection-dispersion equation (CDE).

This study aimed at evaluating the changes of unsaturated flow of wastewater through a soil. Transport parameters and degradation are studied in laboratory soil columns and numerical modeling. HYDRUS-1D model (Šimůnek *et al.*, 2009) is used to simulate wastewater transport in the soil-water environment. Synthetic wastewater and steady water flow are used so that our results can be reproduced. The water did not contain any solids, to exclude physical clogging. As the removal of solids is a first step in water treatment and drip irrigation requires the removal of small particles such as sand, silt, clay, or organic debris, the synthetic wastewater used in this

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Table 1: Composition of synthetic wastewater for a COD of 300 mgL^{-1} (Houtmeyers, 1978). All concentrations are in proportion. The pH is, however, adjusted by adding $NaHCO_3$ concentration as last constituent in order to obtain a pH in the range of 7 to 8

Constituent	Mg L^{-1}	Contribution	Source of
Glucose	225	500 C	Carbon
NH_4Cl	150	40 N and 100 Cl	N and Cl
KH_2PO_4	11	2.5 P	P
K_2HPO_4	14	2.5 P	P
$MgSO_4.7H_2O$	100	40 SO_4	S
$NaHCO_3$	450	pH 7.5	pH adjustment
$CaCl_2$	5	Some Ca	Ca
$FeCl_3$	0.1	Some Fe	Fe

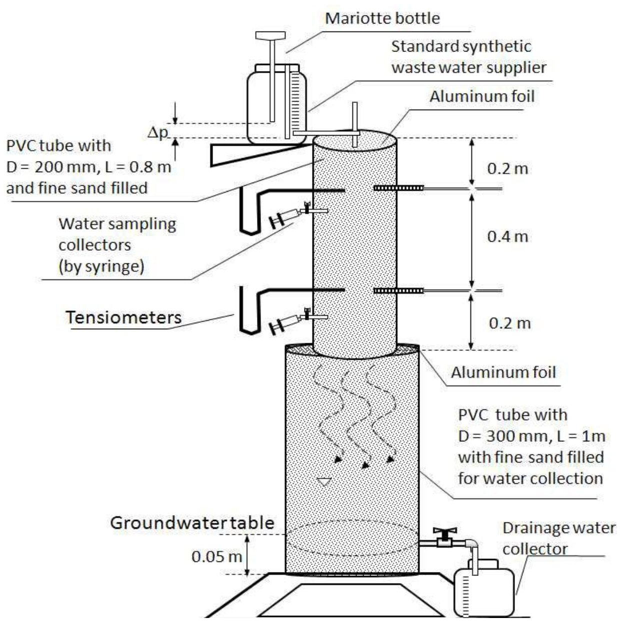

Fig. 1: Experimental setup for transport experiments in unsaturated porous media. All measurements are situated in the top column with 200 mm ID. The bottom column serves as a boundary condition

study is similar to wastewater after a primary treatment.

Materials and Methods

Experimental Setup

Twelve soil columns were constructed in order to characterize the water flow and transport parameters in one-dimensional vertically downward directed flow experiments. As shown in Fig. 1 a PVC tube with a 200-mm inside diameter (ID) and a length (Les) of 800 mm was placed on a larger PVC tube with ID = 300 mm and Leb =1000 mm.

At the top boundary of the upper soil column steady state water flux consisting of either demineralized water or synthetic wastewater was established with a Mariotte bottle. Water samples were taken using Rhizon extractors placed at 25 cm and 65 cm from the top. In the top columns water potential was monitored by tensiometers. Soil water content and electrical conductivity were measured simultaneously by Time Domain Reflectometry (TDR) according to Wyseure *et al.* (1997). TDR measurements were logged by a Tektronix 1502B cable tester with RS232 interface connected to a computer and to a SDMX50 multiplexer (Campbell Scientific Ltd., Shepshed, UK) and controlled by WinTDR software (Jones *et al*., 2002; Or *et al*., 2004). In addition, tensiometers for measuring hydraulic potentials were inserted horizontally along the column, on two different longitudinal transects at soil depths of 20 and 60 cm.

Synthetic Wastewater Irrigation

Synthetic wastewater was used in order to obtain reproducible results. The chemical composition (major ions and pH) of synthetic wastewater is presented in Table 1.

Glucose, NH_4Cl and phosphate were provided as the carbon, nitrogen and phosphorus source, respectively. This mixture has a C/N/P ratio of 100/8/1. $NaHCO_3$ was added as an alkalinity source and adjusted pH in the range of 7.0–8.0.

Treatments were expressed in Chemical Oxygen Demand (COD) concentrations. COD is determined by the amount of dissolved oxygen that a sample will absorb from a hot acidic solution containing potassium dichromate and mercuric ions. Four treatments with different concentrations were applied in randomized complete block design with 3 replications. Identical unsaturated, steady-state water flux conditions (1 cm h^{-1}) were applied by Mariotte bottles. The treatments consisted of T1 (COD 300 mgL^{-1}), T2 (COD 200 mgL^{-1}), T3 (COD 100 mgL^{-1}) and T4 (COD 0 mgL^{-1}as a control). Demineralized water was used for mixing the synthetic wastewater. Table 1 gives the concentration of major components: glucose, NH_4Cl, KH_2PO_4, K_2HPO_4, $MgSO_4$ -$7H_2O$, $NaHCO_3$ and concentrations of trace salt minerals, $CaCl_2$ (5 mgL^{-1}), $FeCl_3{\cdot}6H_20$ (0.1 mgL^{-1}).

Model Selection and Parameter Optimization

In this paper, we used a one-dimensional numerical model, HYDRUS-1D (Šimůnek *et al.,* 2009), which solves the Richard's equation for water flow and solves the CDE for solute and heat transport. The HYDRUS-1D program uses the Levenberg- (Marquardt, 1963) parameter optimization method for the inverse estimation of soil hydraulic and solute transport parameters by minimizing the following objective function OF (b) defined as (Simunek *et al*., 1998):

$$OF(b,\theta)=W_h\sum_{j=1}^{N1}\ \sum_{i==1}^{N2}\left|\theta_m-\theta_o(b)\right|^2 \qquad (11)$$

Where W_h is the normalization factor for water content, which is inversely proportional to the measurement of variance; N_1 represents different locations of water content measurements, N_2 is the number of observations for water content, b is the vector of optimized parameters and θ_o *(b)* is the corresponding model predictions for the vector of optimized parameters b (e.g., θ_r, θ_s, α, n and K). The subscripts m and o refer to the measured and optimized values, respectively.

The objective function for the transport parameters of dune sand is given by:

$$OF(b) = W_{EC} \sum_{j=1}^{N1} \sum_{i=1}^{N3} \left| EC_{w,m} - EC_{w,o}(b) \right|^2 \qquad (12)$$

Where EC_w is the bulk electrical conductivity, W_{EC} it's a normalization factor, and N_3 is the number of electrical conductivity measurements. For the simultaneous optimization of both soil hydraulic and solute transport parameters, the objective function is the sum of the objective functions given in Eqs. (11) and (12).

Main parameters affected solute transport in the model: (i) excluded volumetric water content; θ_v, (ii) dispersivity; λ and (iii) degradation constant; µ. The simulations were performed to: (1) determine the λ, V and D before, during and after the application of wastewater (2) estimate the degradation kinetics of synthetic wastewater under different concentrations by inverse modeling. We did inverse modeling with the Break through Curve; *BTC* to determine the transportation (pore water velocity and dispersivity) parameters; which were then used in inverse modeling with the *COD*-data to find the degradation. Having determined *D* and *V* we can than determine the degradation constant.

Results and Discussion

Hydraulic Properties

Soil water contents at soil depths of 20 and 60 cm of the columns were numerically simulated using the water content and electrical conductivity features implemented in Hydrus-1D. The results of modelling were compared to the soil water content and soil electrical conductivity from laboratory data collected from each column (by TDR) and simulated data for every treatment on longitudinal dispersivity at soil depths of 20 and 60 cm. The results in this section are presented to have an idea about the water regime in the soil columns. The pressure head and water content measurements in two depths varied between -25 and -35 cm and 0.112 and 0.192 (cm^3/cm^{-3}) during the experiments, respectively.

The model results agree well with the measured water contents during experiments. Average error values were at 0.0216, 0.0083, 0.0122 and -0.0060 (cm^3/ cm^{-3}), and root mean square error values of 0.0893, 0.0345, 0.0505 and 0.0248 (cm^3/ cm^{-3}), for T1, T2, T3 and T4, respectively. For all the treatments (T1, T2, T3 and T4), the model systematically overestimates the soil water content by 0.01 to 0.04 (cm^3/cm^{-3}).

Simulation soil water content distribution in the soil columns was first performed by using HYDRUS -1D, and then the graphs remade with other software. Fig. 2 depicts variation of water content and time during experiments. Overall, the values calculated demonstrate a good agreement between the model and TDR data.

Simultaneous Optimization

Numerical model HYDRUS -1D was first calibrated to inverse estimate the soil hydraulic properties and soil longitudinal dispersivity by using the measured soil water content and relative EC data from the Breakthrough experiment.

From the steady-state flow experiment, we only estimate porosity (the saturated water content) and longitudinal dispersivity. The final optimized parameter values of van. Genuchten model, longitudinal dispersivity and convection-dispersion equation (*CDE*) and solute transport parameters for the different pulse-response

Table 2: Summary of the simultaneously optimized van Genuchten soil water retention and solute-transport parameters for all columns *before the experiment* with waste water. Parameters estimated by Hydrus-1D for coarse dune sand, with a steady state flux applying demineralizd water (1 cm h^{-1}) with $\theta(v)$, average soil water content (cm^3 cm^{-3}); θ_s, saturated water content (cm^3 cm^{-3}); λ, dispersivity (cm); *V*, pore water velocity (cm h^{-1}) and *D*, dispersion coefficient (cm^2 h^{-1}). Also included are values of the minimized objective function (*SSQ*) and the R^2 values of the optimizations

Column	Before treatment	θ(v) ($cm^3 cm^{-3}$)	θ_s ($cm^3 cm^{-3}$)	λ (cm)	V (cm h^{-1})	D ($cm^2 h^{-1}$)	SSQ (-)	R^2 (-)
1	T3	0.141	0.358	0.12	2.42	0.29	0.266	0.957
2	T2	0.142	0.329	0.31	3.42	1.06	0.372	0.564
3	T4	0.111	0. 313	1.40	3.76	5.26	0.111	0.973
4	T1	0.084	0.340	0.68	4.30	2.92	0.121	0.768
5	T1	0.100	0.324	0.74	4.14	3.06	0.216	0.923
6	T2	0.113	0.349	0.64	3.49	2.23	0.376	0.915
7	T3	0.090	0.360	1.08	4.05	4.37	0.222	0.936
8	T4	0.081	0.344	0.88	4.66	4.10	0.126	0.792
9	T4	0.110	0.352	0.34	4.02	1.37	0.363	0.762
10	T1	0.082	0.333	1.50	6.42	9.63	0.182	0.934
11	T2	0.087	0.351	0.65	4.42	2.87	0.138	0.673
12	T3	0.083	0.353	0.12	4.72	0.57	0.126	0.972

Table 3: Summary of the simultaneously optimized van Genuchten soil water retention and solute-transport parameters for all columns *during the experiment* with waste water. Parameters estimated by Hydrus-1D for coarse dune sand, with a steady state flux applying waste water (1 cm h^{-1}) with $\theta(v)$, average soil water content (cm^3 cm^{-3}); θ_s, saturated water content (cm^3 cm^{-3}); λ, dispersivity (cm); V, pore water velocity (cm h^{-1}) and D, dispersion coefficient (cm^2 h^{-1}). Also included are values of the minimized objective function (*SSQ*) and the R^2values of the optimizations

Treatment	Week	θ(v)	θ_s	λ	V	D	SSQ	R^2
		(cm^3 cm^{-3})	(cm^3 cm^{-3})	(cm)	(cm h^{-1})	(cm^2 h^{-1})	(-)	(-)
	1	0.094	0.341	0.22	2.16	0.48	0.112	0.924
	2	0.085	0.334	0.41	2.34	0.96	0.152	0.913
	3	0.082	0.337	0.01	1.83	0.02	0.594	0.812
T1	4	0.141	0.343	0.32	2.28	0.73	0.468	0.756
	5	0.083	0.341	0.11	1.42	0.16	0.852	0.867
	6	0.095	0.341	1.00	0.84	0.84	0.901	0.546
	7	0.125	0.343	0.01	2.18	0.02	0.390	0.369
	8	0.088	0.345	0.34	2.22	0.75	0.776	0.698
	1	0.085	0.339	0.33	2.23	0.74	0.135	0.945
	2	0. 111	0.344	0.01	3.19	0.03	0.237	0.764
	3	0.092	0.347	0.07	2.02	0.14	0.358	0.873
T2	4	0.097	0.341	0. 96	1.04	0.99	0.126	0.769
	5	0.105	0.331	0. 15	2.11	0.32	0.453	0.874
	6	0.111	0.344	1.00	1.14	1.14	0.134	0.567
	7	0.123	0.340	1.35	2.08	2.81	0.112	0.678
	8	0.088	0.341	0. 01	0.92	0.09	0.142	0.932
	1	0.091	0.344	0.45	2.14	0.96	0.267	0.351
	2	0.124	0.337	1.00	3.02	3.02	0.342	0.456
	3	0.111	0.341	0.23	3.01	0.69	0.256	0.678
T3	4	0.113	0.334	1.30	0.93	1.21	0.234	0.789
	5	0.127	0.336	1. 01	1.02	1.03	0.217	0.875
	6	0.111	0.334	0.30	2.20	0.66	0.132	0.946
	7	0. 093	0.337	0. 38	1.73	0.00	0.112	0.957
	8	0.087	0.342	0.43	1.31	0.56	0.123	0.869
	1	0.087	0.341	1.35	2.07	2.79	0.234	0.934
	2	0.100	0.341	0.75	2.42	1.82	0.312	0.926
	3	0.103	0.344	0.24	2.05	0.49	0.123	0.946
T4	4	0.093	0.344	0.14	1.89	0.26	0.145	0.932
	5	0.088	0.335	0.15	2.03	0.30	0.124	0.957
	6	0.111	0.341	1.00	1.62	1.62	0.214	0.856
	7	0.082	0.342	1.00	0.88	0.88	0.435	0.678
	8	0.088	0.344	1.00	1.03	1.03	0.567	0.579

Table 4: Summary of the simultaneously optimized van Genuchten soil water retention and solute-transport parameters for all columns after the experiment with waste water. Parameters estimated by Hydrus-1D for coarse dune sand, with a steady state flux applying demineralizd water (1 cm h^{-1}) with $\theta(v)$, average soil water content (cm^3 cm^{-3}); θ_s, saturated water content (cm^3 cm^{-3}); λ, dispersivity (cm); V, pore water velocity (cm h^{-1}) and D, dispersion coefficient (cm^2 h^{-1}). Also included are values of the minimized objective function (*SSQ*) and the R^2 values of the optimizations

Treatment	Week	θ(v)	θ_s	λ	V	D	SSQ	R^2
		(cm^3 cm^{-3})	(cm^3 cm^{-3})	(cm)	(cm h^{-1})	(cm^2 h^{-1})	(-)	(-)
	1	0.111	0.341	0.155	4.57	0.71	0.103	0.556
T1	2	0.112	0.336	3.13	5.22	16.34	0.112	0.778
	3	0.111	0.338	1.432	4.77	6.83	0.222	0.889
	4	0.091	0.348	3.030	5.11	15.48	0.202	0.975
	1	0.112	0.338	0.030	4.82	0.14	0.113	0.946
T2	2	0.107	0.341	0.13	3.96	0.51	0.135	0.657
	3	0.096	0.342	0.230	3.91	0.90	0.114	0.969
	4	0.091	0.345	0.330	5.11	1.69	0.204	0.634
	1	0.112	0.343	1.130	4.75	5.37	0.125	0.982
T3	2	0.078	0.345	1.535	5.13	7.87	0.257	0.866
	3	0.091	0.335	0.675	4.92	3.32	0.122	0.872
	4	0.078	0.344	0.031	3.91	0.12	0.314	0.767
	1	0.105	0.335	0.075	5.11	0.38	0.233	0.946
T4	2	0.111	0.342	0.350	4.56	1.60	0.221	0.878
	3	0. 102	0.343	1.352	3.72	5.03	0.206	0.779
	4	0.097	0.336	0.08	4.75	0.38	0.327	0.863

Table 5: Optimal parameters of degradation constant by inverse modelling with HYDRUS- 1D with μ, degradation kinetic constant (1/day). Also included are values of the minimized objective function (*SSQ*) and the R^2 values of the optimizations

Treatment	μ (1/day)		SSQ (-)	R^2 (-)	Mass balance error (%)
	cod25	cod60			
T1	2.212	2.315	0.433	0.974	0.090
T2	2.351	2.421	0.321	0.981	0.112
T3	2.216	2.332	0.216	0.968	0.152
T1-T2-T3	2.523	2.433	0.427	0.964	0.091

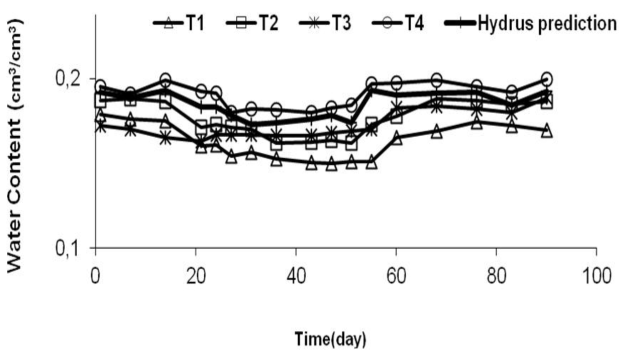

Fig. 2: Variation of volumetric water content with time by TDR and Hydrus-1D for a constant water-flux (1cm h^{-1}). Treatments T1, T2, T3 and T4 are 300, 200, 100 and 0 COD (mg L^{-1}), respectively, and started from day 0. For time more than 80 days demineralized water was used. The lower water content in the middle of the experiment is likely due to higher temperature

experiments before, during and after the experiment with waste water are summarized in Tables 3, 4 and 5. The value of optimized parameters, residual sum of squares (SSQ), and regression between the observed and predicted values (R^2) are listed in these Tables.

The simulated and observed values of optimized parameters and residual sum of squares (SSQ) for the convection-dispersion equation (*CDE*) and solute transport models are very similar for the different treatments. The predicted values for (θs) were more or less the same for all Breakthrough experiment. Much of the differences in the λ values for the all columns during experiments were due to differences in the van Genuchten parameters ($\theta_{s)}$ caused by non-homogeneous bulk density of the soils.

Finally, optimized values of the longitudinal dispersivity (λ) showed no significant change in all treatments. However, these small variations in longitudinal dispersivity between the columns might be due to small change in the soil water content during experiments.

Solute transport parameters *D* and *V* were estimated by the Hydrus-1D model. The values found for the dispersion coefficient and pore water velocities before, during and after the experiment with wastewater are also summarized in Table 3, 4 and 5. The pore water velocities predicted by Hydrus-1D software were in good agreement with the pore water velocities estimated by combining the column cross-sectional area, water flux rates, and the soil water contents.

The observed variances were all attributed to the experimental error. No treatment effect was significant. The variation between the columns was much larger than between the treatments, so effect could be detected. As for the water content and conductivity no change in properties was observed during the experiment with wastewater. The Hydrus predicted the observed BTC very well with R^2 values ranging from 0.901 to 0.986.

COD Degradation

Having determined longitudinal dispersivity, pore water velocities and dispersion coefficient from the first step we performed inverse modeling with the *COD*-data to find the degradation of synthetic wastewater. The degradation kinetics of synthetic wastewater under different concentration was assumed to follow first-order kinetics. Optimal parameters of degradation constant by inverse modelling with HYDRUS-1D are summarized in Table 6. The CDE model described well the BTCs of degradation constants of the synthetic wastewater, as is reflected by high values of the determination coefficient R^2 (0.96–0.98). Overall first-order degradation constants, μ were 2.315, 2.421 and 2.332 (1/day) for COD 300, 200, 100, respectively. The final degradation constant appeared to be the same for all treatments. The degradation constant for all treatments was 2.443(1/day) during experiments.

The COD degradation rates were calculated from the slope of the synthetic wastewater depletion curves. With the time the efficiency of the degradation of synthetic wastewater dropped, shown as decreasing degradation kinetic constant μ. The inverse estimation of μ by Hydrus on the measured COD at 25 and 65 cm depth were possible for all measurements.

The sensitivity of the parameters λ and μ in optimization was explored and showed that λ and μ are not very sensitive resulting in different profiles. On the other hand changes in *D* do not have much impact on the degradation. As there was no reason to believe that the adsorbed waste water would not degrade at the same rate as the waste water in the solution, we assume that all the wastewater removed from solution is also degraded. Although first-order degradation kinetics describes the overall degradation measured in the laboratory, it is very likely that the degradation taking place is variable in time and column replication. This is it not necessarily contradictory to growth of bacteria. In the dune sand soil, the natural supply of carbon is small. It therefore seems plausible that the microbial population in the soil columns will grow when supplied with synthetic waste water.

These results of model provide useful estimates for the rates of synthetic wastewater in irrigated soils. However, the rate-estimates obtained might not be the true values for the real field conditions due to the complexity of microbial degradation and the lack of detailed information of e.g. types and distribution of microorganisms.

Our findings can be implemented and tested in real field conditions. A recommendation is to take soil water samples within the first 50 cm of the soil. In addition the roots will also extract water and nutrients. A field experiment could compare the fate of wastewater with and without crops in order to differentiate between degradation and crop uptake.

Conclusion

Municipal wastewater reuse is believed to be a potential intervention strategy for developing nonconventional water resources. In this study the effect of wastewater on the soil hydraulic properties, the solute transport and transformation behaviour was studied by conducting steady state waste water application treatments on undisturbed one-dimensional sand columns. Information on the fate of water and synthetic wastewater was obtained using tonsiometers, time domain reflectometry and soil water sampling. The Levenberg-Marquardt algorithm in combination with the HYDRUS-1D code was used to inversely estimate the soil hydraulic and solute transport parameters.

Our simulations show that under unsaturated flow conditions and at three different concentrations of synthetic wastewater no significant differences in solute transport parameters are noticeable. Optimized parameters and sum of squared residuals (SSQ) for the CDE and transport models are very similar for the different treatments. The estimated values for θ_s were more or less the same for all experiments. Much of the differences in the optimized λ values for all columns during experiments were due to differences in the VG parameters (θ_s) caused by non-homogeneous bulk density of the soils. First-order degradation was observed. However, the degradation constant decreased with time and this decrease was independent of the concentration of the wastewater. We estimated that the degradation constant after a long time is 2.52/day. Our steady state flux of 10 mmh^{-1} maintained during 80 days was well above intensities experience under irrigation. Therefore, for synthetic wastewater similar to domestic waste water, we can conclude that the average residence time in the soil along with the degradation is sufficient so that groundwater will not be contaminated. Like in water treatment residence time and degradation rate are the crucial characteristics.

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