Predicting the Impact of Treated Wastewater Infiltration on Groundwater Recharge by Simulating Reactive Transport in the Unsaturated Zone

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Abstract

Due to demographic increase and climate change, it is necessary to look at alternative ways to replenish groundwater resources. One possibility is to infiltrate treated wastewater directly into the ground and use the filtering capacity of the soil. To prevent the pollution of groundwater, one must ensure that not only the quality of treated wastewater is suitable for infiltration, but also that the soil has good filtration capacities. This is a sustainable alternative to groundwater recharge if natural precipitation is insufficient, especially in semi-arid and arid areas. This paper presents the results of a project investigating the infiltration of treated wastewater from small-scale wastewater treatment plants (WTPs) into the unsaturated soil zone. These small-scale WTPs use a preliminary sedimentation, followed by a biofilm reactor and secondary treatment. Consequently, the treated wastewater has a high quality and is therefore suitable for direct infiltration into the unsaturated soil zone. To forecast the transport and the transformation processes and the concentration of infiltrated treated wastewater into the unsaturated zone, different scenarios were modeled with the help of the software, PCSiWaPro®. For this purpose, the software tool PCSiWaPro® was further enhanced to include wastewater transport and transformation as well as the small-scale sewage treatment plants classes. To account for the relevant biogeochemical reactions, PCSiWaPro® was coupled to the geochemical software PHREEQC. To validate the enhanced simulation software, column experiments were conducted. The results from column experiments and from modeling have improved the understanding of the complex processes in the unsaturated zone and its relationship with the saturated zone. It is now possible to efficiently design and operate small-scale wastewater treatment plants and to predict groundwater recharge.

1. Introduction

According to the European Water Frame Directive (EU-WFD, 2000), all the member states must achieve a good chemical and ecological status for all water bodies until 2015. The EU-WFD establishes quality criteria that takes into account the local characteristics of the groundwater body and its chemical status and introduces measures to prevent or limit its pollution. As a large proportion of the groundwater recharge comes from the treated wastewater, important steps in collecting and disposing it have been taken. But there is still significant groundwater recharge originating from small-scale wastewater treatment plants (WTPs). Until now, the treated wastewater has been directly discharged via drainage pipes. Since both discharge methods are expensive, the concept of infiltrating the treated wastewater directly into the ground for small-scale individual systems is being investigated.

The main objective of this work is to develop a software tool for simulating the transport and transformation of contaminants in variable saturated porous media coming from WTPs, based on laboratory and field experiments. Thus, the results of the modeling and the experiments can further improve the designs of small-scale WTPs, increase their operational efficiency, and recharge groundwater.

2. Modeling Unsaturated Zone Processes

2.1. Theoretical Background

The water flow process in variably-saturated porous media can be described using the Richards equation (Richards, 1931), which considers both unsaturated and saturated regions simultaneously:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left[K\left(K_{ij}^A \frac{\partial h}{\partial x_j} + K_{iz}^A\right)\right] - S \tag{1}$$

where θ is the volumetric water content [L^3L^{-3}], h is the capillary pressure head [L], x_i (i=1, 2) are the spatial coordinates [L], t is the time [T], K_{ij}^A are components of a dimensionless anisotropy tensor K^A, K is the unsaturated hydraulic conductivity function [LT^{-1}], and S is a sink/source term [T^{-1}], which is considered here as the amount of water removed by roots of plants. Since the capillary pressure head is a dependent variable and both the hydraulic conductivity K and the volumetric water content θ are dependent on the pressure head, the Richards equation is highly non-linear. Therefore, the solution process has to be conducted in an iterative manner. The unsaturated soil hydraulic properties are described by using the equations developed by van Genuchten (1980) and Mualem (1976). The water content in an unsaturated porous medium depends on the capillary pressure head in the pores, given by:

$$\theta(h_c) = \theta_s + \frac{\theta_s - \theta_r}{\left[1 + (\alpha \cdot h_c)^n\right]^{1-\frac{1}{n}}} \tag{2}$$

in which θ_r and θ_s denote the residual and saturated water contents, and the exponent n is the van Genuchten parameter.

The partial differential equation governing two-dimensional chemical transport during transient water flow in a variably-saturated porous media is given by:

$$\frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial c}{\partial x_j}\right) - \frac{\partial q_i c}{\partial x_i} + \mu_w \theta c + \mu_s \rho s + \gamma_w \theta + \gamma_s \rho - S c_s \tag{3}$$

where c is the solute concentration [ML^{-3}], s is the sorbed concentration [ML^{-3}], q_i is the i^{th} component of the volumetric flux [LT^{-1}], and μ_w and μ_s are the first-order rate constants for solutes in the liquid and solid phases [T^{-1}], respectively; γ_w and γ_s are zero-rate constants for the liquid [$ML^{-3}T^{-1}$] and the solid phases [T^{-1}]; ρ is the bulk density [ML^{-3}], S is the sink/source term in the water flow equation (1), c_s is the concentration of the sink/source term [ML^{-3}], and D_{ij} is the dispersion coefficient tensor [L^2T^{-1}]. The four zero-and first-order rate constants may be used to represent biodegradation, volatilization, precipitation and radioactive decay.

2.2. Software Tool PCSiWaPro®

The PCSiWaPro® is a software tool developed at the TU Dresden. It is based on a soil physical model implemented in the numerical code SWMS_2D, developed by Šimůnek et al., (1994). The PCSiWaPro® can simulate 1D and 2D vertical plane or axially symmetrical flow and transport processes in the unsaturated zone under steady-state and transient conditions. It numerically solves the Richards equation (1) and the convection-dispersion equation, using the finite elements method. Moreover, it has a flexible choice of boundary conditions, the consideration of hysteresis-like processes in the unsaturated zone, and a parameter identification algorithm. It considers sorption and zero- and first-order degradation. To account for hydrological conditions (e.g., precipitation, evapotranspiration, surface runoff, root water uptake), PCSiWaPro® is coupled with a Weather Generator module (WettGen) (Nitsch et al., 2007, Blankenburg, 2008).

As this numerical tool is intended for application by enterprises that investigate contaminant transport in groundwater and the degree of pollution of different contaminated sites, there is substantial demand to develop a complex software tool that covers all areas of interest (i.e., surface, unsaturated and saturated zone). Therefore, PCSiWaPro® is also coupled to the geochemical software PHREEQC (Appelo et al., 2005) to consider the relevant bio-geochemical reactions in the unsaturated zone (inter-dependent complexation reactions, cation exchange, precipitation-dissolution, volatilization, redox-reactions), and to the groundwater flow and contaminant transport simulation tool model PCGEOFIM (Boy et al., 2005) shown in Figure 1.

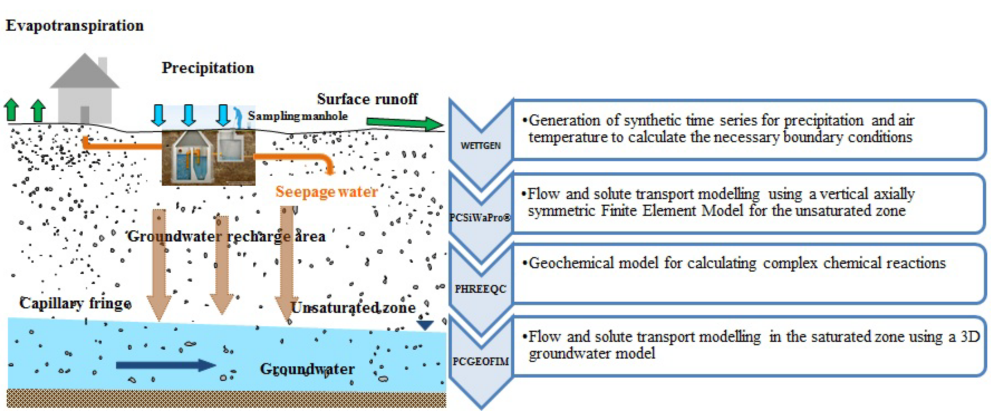

Figure 1. Conceptualization of coupled numerical codes for simulating surface, unsaturated and saturated zone processes.

2.3. Software Tool PHREEQC

The well known bio-geochemical program, PHREEQC (Parkhurst, 1995), is based on an ion-association aqueous model and is capable of a variety of chemical equilibrium reactions, kinetically determined reactions, solution and precipitation processes, and ion exchange processes. In several databases, the chemical properties of the individual substances and the possible reaction equations are stored. In a control file, the definition of the solution and the resultant chemistry of the solution are calculated.

2.4. Coupling PCSiWaPro® and PHREEQC

PCSiWaPro® accounts for sorption, retardation, and zero- and first-order degree degradation, and in the case of wastewater, it is also necessary to consider biogeochemical reactions. The well known geochemical model PHREEQC was chosen to be coupled with PCSiWaPro® due to its modular structure and extensive geochemical databases.

While PCSiWaPro® simulates the transport of water and wastewater in the unsaturated soil zone, PHREEQC focuses on the bio-geochemical reactions. The simulation tool has to consider different soil types, small-scale sewage treatment plant classes, as well as a mixture of contaminants and their inter-relations. Therefore, a set of databases for soil types, typical organic and inorganic wastewater contaminants, sewage treatment plant classes, and boundary conditions have all been further implemented to make the tool more user-friendly (Figure 2).

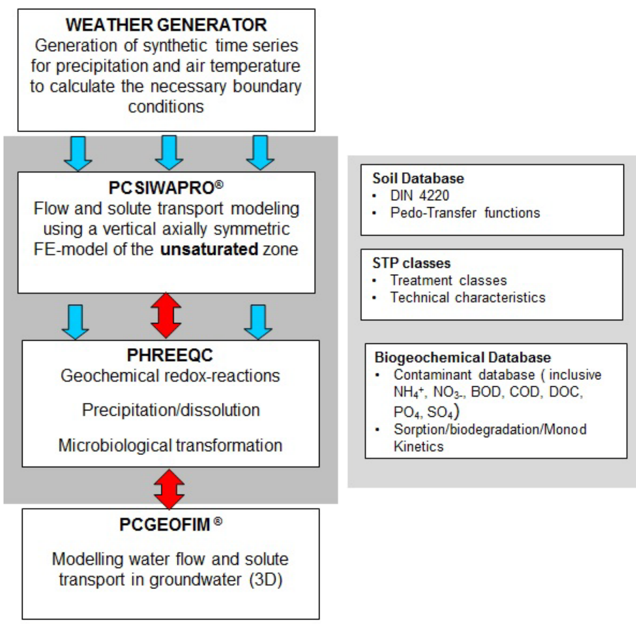

Figure 2. Coupling of numerical simulation codes and databases.

Figure 3 illustrates the program structure of the coupling between the two numerical models. In the discretized time domain of the numerical model, the three simultaneous and dependent processes of flow, transport and reaction are separated using a non-iterative splitting approach where Δt is the length of the coupling step. The coupling time step is further reduced in the case of geochemical reactions if necessary. As a result of decoupling, concentrations are assumed independent of reactions in the solute transport calculations. Likewise, the liquid phase saturation is considered independent of concentrations and reactions during flow calculation. During the geochemical step, performed by PHREEQC, the solution composition is considered independent of both flow and transport.

The coupling scheme between the PCSiWaPro® and PHREEQC takes places online, which means that for each time step, the codes exchange the following data:

1. Simulation of the water flow for the calculation of the convective transport performed by PCSiWaPro® (independent of concentrations and reactions)
2. Simulation of solute transport for each individual substance performed by PCSiWaPro® (independent of reactions)
3. Calculation of the bio-geochemical equilibrium and kinetics reactions for each node performed by PHREEQC (independent of flow and transport). The changes in the concentrations after the reactive step are the new initial concentrations for the next transport time step calculation. The concentrations in the immobile phase remain in the corresponding node and play no role for the mass transfer. A maximum one-day time step for the reaction is necessary to depict a realistic illustration of interactions between water and nutrient budgets.

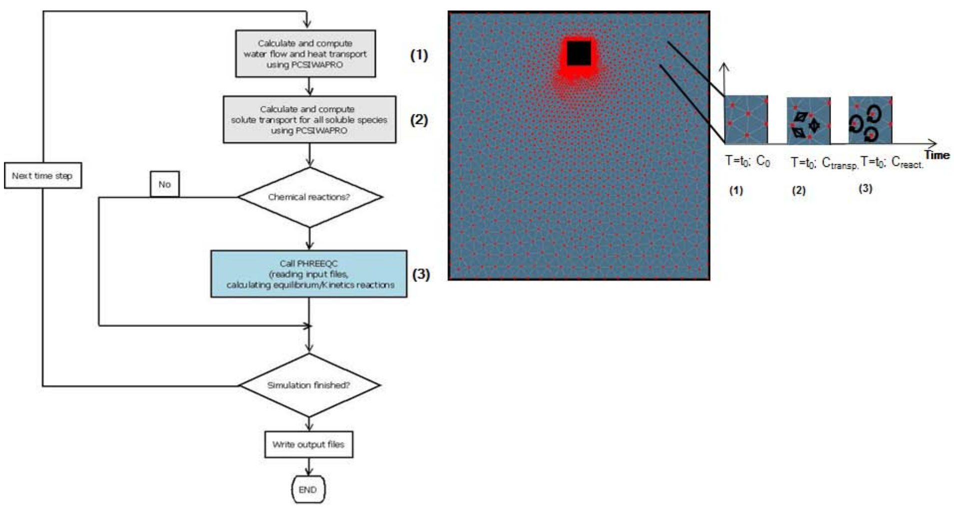

Figure 3. Coupling between the PCSiWaPro® and PHREEQC in a 2D cross-section.

3. Validation Through Column Experiments

As the software PCSiWaPro® is further developed to include small–scale WTPs, it is necessary to validate the results of the numerical simulations. Accordingly, a series of column experiments were performed in the laboratory to answer following:

- Which soil has the best natural attenuation capacity in order to ensure a good seepage water quality?
- How does the treated wastewater quality influence the infiltration capacity of soils (clogging aspect)?
- How do the infiltration rate characteristics (continuous/pulse, amount) influence the infiltration and natural attenuation capacity?
- Does the thickness of the unsaturated zone have a significant impact on the residence time of the seepage water and the natural attenuation capacity?

The experiments consisted of three columns, each with a different soil type described in Table 1. The in situ soil from the case study sites of Kleinopitz and Biehain in Saxony (Germany) was used for the column experiments. The 150 cm long columns were made of Plexiglas having an internal diameter of 15 cm. The treated effluent was infiltrated in the upper part of the column with the help of a peristaltic pump. Infiltration occurred eleven times daily, according to human diurnal water consumption. To determine the soil water potential in the column, two tensiometers were installed at different heights. Moreover, to have on overview of the temperature, a soil temperature sensor was attached. The measured data was directly recorded on a data logger.

Table 1. Soil parameters and initial conditions.

Soil type	van Genuchten parameters				Infiltration rate $[m^3 d^{-1}]$	Precipitation $[mm\ y^{-1}]$	Duration of experiments [d]
	θ_s $[cm^3cm^{-3}]$	θ_r $[cm^3cm^{-3}]$	α $[cm^{-1}]$	n [-]			
Coarse sand with gravel (KRB23)	0.38	0	0.15	1.34	0.1	676	365
Medium silty sand (KRB10)	0.38	0	0.2	1.23	0.1	676	365
Medium sandy silt (B5)	0.38	0	0.262	1.35	0.1	676	185

The quality of the inflow wastewater into the column and outflow was determined and compared to the legal limit for drinking water according to the German Drinking Water Directive (TWO: Die Trinkwasserverordnung, 2012) as listed in Table 2.

Table 2. Quality of some investigated parameters/contaminants and their legal limit.

	pH	COD	DOC	NO_2^-- N	NO_3^--N	NH_4^+-N	TKN	P_{ges}	E.coli
Unit	[-]	$[mg\ L^{-1}]$	$[mg\ L^{-1}]$	$[mg\ L^{-1}]$	$[mg\ L^{-1}]$	$[mg\ L^{-1}]$	$[mg\ L^{-1}]$	$[mg\ L^{-1}]$	/100 ml
Concentration in inflow	65	90	18.5	102	57.6	15.2	16.5	19.2	269
Legal limit TWO, 2012)	6.5-9.5	-	-	0.15	11.3	0.39	-		0

In the column with medium sandy silt (red line in Figure 4–left), a complete reduction of ammonium could be observed during the experimental duration of 185 days. However, an increase in the nitrate concentration was observed due to nitrification (Figure 4–right). The nitrate concentrations in the effluent were about 20 mg L^{-1} higher than the concentrations in the infiltrated wastewater. In the medium silty sand, a complete reduction of ammonium could be observed after 250 days. This result was achieved by decreasing the amount of infiltrated treated wastewater. An increase of nitrate could also be registered for this time. The reduction of the ammonium in the coarse sand with gravel was only between 25% and 50% and subject to major fluctuations. Due to the sufficient oxygen present in the soil column, denitrification was not observed.

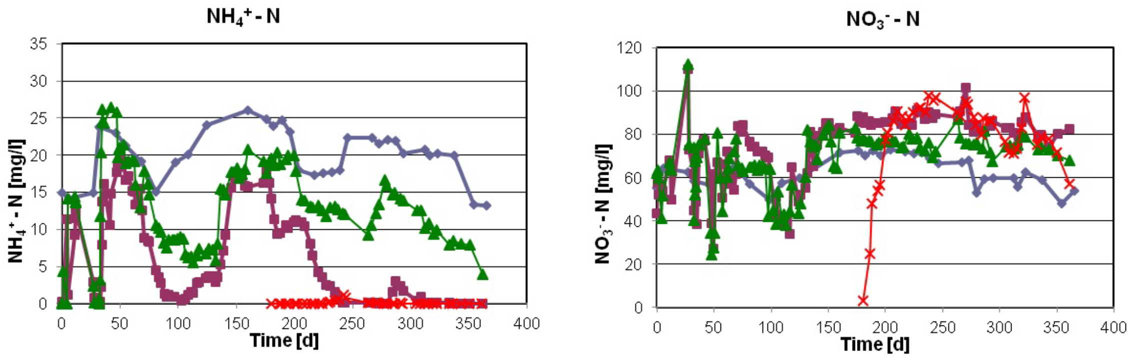

Figure 4. Ammonium Nitrogen (left) and Nitrate-Nitrogen (right) behavior in different soils (Blue- inflow; Green–coarse sand with gravel; Purple–medium silty sand; Red–medium sandy silt)

The reduction of COD and removal of DOC, TKN, and Total Phosphorous is presented in Table 3. It is observed that the highest removal of all parameters occurs in medium sandy silt. A higher removal was observed for COD and DOC in coarse sand with gravel, compared to medium silty sand. On the other hand a higher removal was observed for TKN and Total Phosphorous for medium silty sand, compared to coarse sand with gravel.

Table 3. Removal of COD, DOC, TKN, and Total Phosphorous observed during column experiments.

Soil class	COD	DOC	TKN	P_{Total}
	[%]	[%]	[%]	[%]
Coarse sand with gravel (KRB23)	70	40	30	0
Medium silty sand (KRB10)	50	20	70	75
Medium sandy silt (B5)	90	75	80	100

The reason for the low removal efficiency in the coarse sand with gravel and medium silty sand was the prevalent, non–optimal environmental conditions for the occurrence of biological degradation in the columns (low pH–value due to lower buffering capacity of soil). Another reason for low removal efficiency in the coarse sand with gravel and medium silty sand was the short residence time of the treated wastewater in the soil caused by the higher hydraulic conductivity. However, in the medium sandy silt, ideal conditions are present, as can be demonstrated by the highest removal of the concentrations of the infiltrated wastewater. Although the medium silty sand and the medium sandy silt have similar soil physical properties as shown in Table 1, the natural attenuation is more efficient in medium sandy silt due to the higher portion of fine grained silt compared to medium silty sand. Consequently, the finer grained soil type provides a larger specific surface area for the geochemical processes to occur.

4. Example Application

The PCSiWaPro® software was applied to the Kleinopitz case study site to predict the on-site transport of treated wastewater. A 2D numerical model was prepared (Figure 5) using input parameters and data (Table 1) obtained from the field and laboratory experiments to simulate the seepage of the treated effluent from small–scale WTPs (Tomoda, 2012). The upper boundary condition was the atmosphere, while the lower boundary represents the groundwater table.

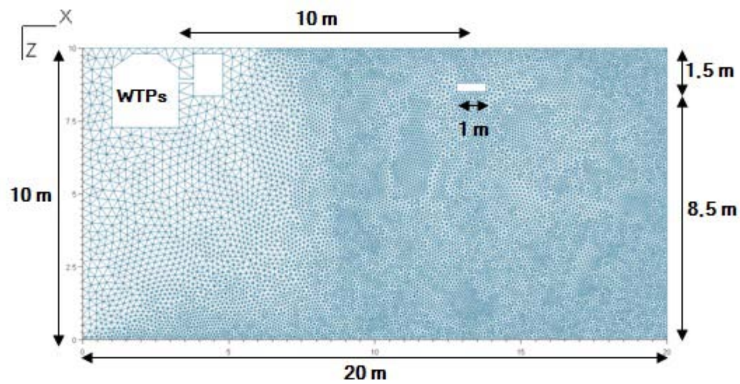

Figure 5. Graphical representation of the numerical model.

Several questions needed to be answered before performing a solute transport and reactions simulations, the most important being:

- Does the thickness of the unsaturated zone significantly impact the residence time of the wastewater and natural attenuation capacity?
- Where should the infiltration area be located to prevent contamination of any possible drinking water well?
- Which soil hydraulic parameters influence the seepage of the treated effluent?

The results in Figure 6 show the groundwater recharge from different scenarios, where the groundwater table depths of 10 m, 6.5 m, and 3.5 m have been used. Two different infiltration rates of 0.1 and 0.3 m^3d^{-1} for three different soil types were applied. When an infiltration rate of Q_{in} =0.1 m^3d^{-1} is applied (Figure 6–left) to all three different groundwater table depths, the travel time is always fastest for medium sand (compared to medium silty sand and medium sandy silt). As expected, the minimum travel time of 25 days to a GW table depth of 10 m is shortest for medium sand, compared to 27 and 33 days for medium silty sand and medium sandy silt, respectively. Irrespective of the depth of the GW table, a maximum groundwater recharge of 0.1 m^3d^{-1} is eventually attained for an equal infiltration rate of 0.1 m^3d^{-1}.

In case of medium sand and medium silty sand, when an infiltration rate of 0.3 m^3d^{-1} is applied, the minimum travel times are similar for both soil types. Thus the minimum travel time is 2, 6, and 10 days for a GW table depth of 3.5, 6.5 and 10 m, respectively. An eventual equivalent groundwater recharge rate (compared to the infiltration rate) of 0.3 m^3d^{-1} is also attained for these soil types but at a relatively faster rate compared to an infiltration rate of 0.1 m^3d^{-1} over a 60 day simulation period. The short travel time of water through the unsaturated zone to the groundwater table implies insufficient time for geochemical reactions to optimally occur. Only the medium sandy silt, with longer travel times, lower groundwater recharge rates, and greater depths to the groundwater table, could be a good candidate for infiltrating treated effluent from small scale WTPs, as also demonstrated by the column experiments.

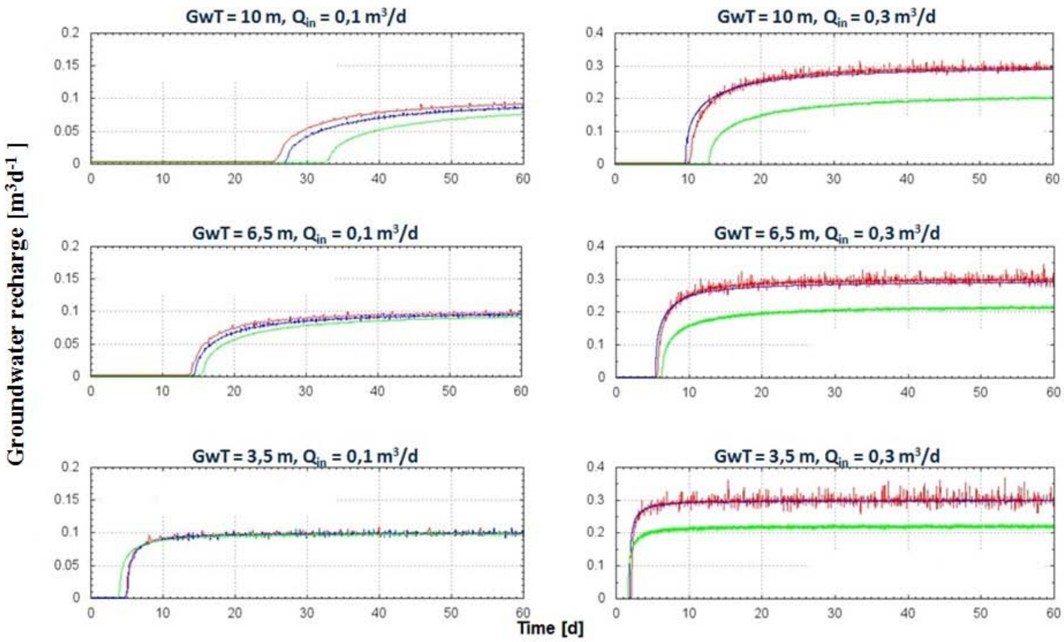

Figure 6. Groundwater recharge for different groundwater tables (GwT) and infiltration rates (Q_{in}) (blue–medium silty sand green–medium sandy silt, red–medium sand.

5. Conclusions

This paper presented a coupled finite element model that uses PCSiWaPro® for simulating water and solute transport in an unsaturated zone and the geochemical model PHREEQC for its capability of simulating chemical equilibrium and non–equilibrium reactions. The numerical model was validated by column experiments, where different soil types, infiltration rates and effluent qualities were considered. From the column experiments and the numerical simulation, one can conclude that medium sandy silt is the best suited soil type for infiltrating the treated effluent from small–scale WTPs because it has the longest travel time, and therefore sufficient time for bio–chemical reactions to take place. However due to the shallow depth to the GW table (up to 10 m), it is important to limit the infiltration rates to 0.1 m^3 d^{-1} or less.

The most difficult task in simulating the solute transport in unsaturated soils is the effective characterization and quantification of the effects of the chemical reactions on transport processes. In this context, one of the advantages of coupling is that PCSiWaPro® completely integrates the PHREEQC geochemical model, and thereby allows the user access to a large range of chemical reactions. It provides the ability to include the effects of a large number of different types of chemical processes on solution compositions on a per time–step basis. Another advantage is the extensive databases, which make the numerical PCSiWaPro® code a user-friendly software tool, especially when the necessary data collection cannot be performed through laboratory and field investigations. To demonstrate the robustness of the coupling scheme between the codes, the numerical software still needs to be extensively verified for more complex systems.

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