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ORIGINAL ARTICLE

Utilizing unsaturated soil zone models for assessing managed aquifer recharge

Jana Sallwey[1] · **Jana Glass**[1] · **Catalin Stefan**[1]

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Abstract

Managed aquifer recharge (MAR) is increasingly used to balance out the divergence between natural groundwater recharge and overexploitation of groundwater resources. As testing and design of recharge facilities can be cost and time-intensive, modeling tools hold great potential to design field investigations as well as to augment and extrapolate from their results. Focusing on unsaturated soil zone models, this study first reviews 16 previous modeling studies showing their range of model types and applications. The review is accompanied by an example of the use of HYDRUS 2D/3D, an unsaturated zone model, to design a novel small-scale infiltration basin. The basin is going to be established as part of a field and laboratory research facility for MAR in Pirna, Germany. Modeling results assisted in determining the dimensions of the infiltration unit as well as the placement of measurement devices and experimental scenario planning. Finally, the strengths and constraints of this modeling approach for MAR assessment are discussed.

Keywords Managed aquifer recharge · Modeling · Unsaturated zone · Field experiments · Soil aquifer treatment

Abbreviations

MAR	Managed aquifer recharge
BC	Boundary condition
SAT	Soil aquifer treatment
ASR	Aquifer storage and recovery
ASTR	Aquifer storage, transfer and recovery

Introduction

Groundwater is crucial for the sustainable water supply of many regions as it is the principal drinking water source to more than 2.5 billion people worldwide (WWAP 2015). However, water scarcity is already a major threat to large parts of the world (Fedoroff et al. 2010). The increasing world population and its demand for fresh water as well as the effects of climate change could hasten the existing decline in water tables and groundwater storage in many aquifers already prone to stress and lacking effective management.

Managed aquifer recharge (MAR), which is the intended recharge of groundwater for later use or environmental benefits (Dillon 2005), is an emerging method to reverse these negative effects on groundwater resources. It is increasingly used to balance differences between temporal or local water demand and availability (Bouwer 2002; Dillon 2005). MAR is a means for sustainable groundwater management and often involves large-scale facilities. Technical facilities for groundwater enhancement include injection wells, infiltration ponds, and galleries or recharge dams (Hannappel et al. 2014). Building these recharge systems needs careful planning beforehand to achieve field conditions that can be controlled and managed, to reduce construction costs, and to understand the local hydrogeological conditions.

The planning of these MAR sites can be executed through field and laboratory investigations (Environmental and Water Resources Institute 2001; NRMMC-EPHC-NHMRC 2009). However, experimental set-up can be time- and cost-intensive. Therefore, it can be of advantage to accompany these practical investigations by modeling studies. Preliminary modeling can be undertaken to identify the parameters and processes which have the greatest influence on the local groundwater system and thus define the scope of future data collection. Pilot

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✉ Jana Sallwey
jana.sallwey@tu-dresden.de

[1] Technische Universität Dresden, Dresden, Germany

sites and preliminary studies are required by some MAR guidelines (Environmental and Water Resources Institute 2001; NRMMC-EPHC-NHMRC 2009). Such studies are aimed at defining the requirements and constraints of applying MAR as well as at optimizing the actual MAR site in terms of dimensions, monitoring, and operational parameters.

With respect to groundwater, modeling can be helpful in three different areas of application: (1) developing management strategies that optimize defined objectives; (2) understanding hypothetical hydrogeological questions, and (3) assessing predictive scenarios (Environmental and Water Resources Institute 2001). In addition to feasibility studies that evaluate possible locations for MAR sites, modeling objectives include the optimization and planning of design and operative parameters of an MAR site as well as the quantification of its impact on the groundwater (Kloppmann et al. 2012; Maliva et al. 2015; Ringleb et al. 2016). Past modeling studies have focused mostly on groundwater models and their potential for MAR assessment in the different phases of MAR site planning (Jha and Pfeiffer 2006; Valley et al. 2006; Kloppmann et al. 2012). Unsaturated soil zone models have been given only little attention in the context of MAR (Ringleb et al. 2016).

This paper focuses on the use of models of the unsaturated zone (also called vadose zone) for assessing MAR sites. Following a review of past unsaturated zone model applications, it showcases a practical study at a test site in Pirna, Germany. This test site is part of a research project that utilizes modeling, laboratory, and field experiments for understanding the processes that facilitate the planning of MAR sites under different boundary conditions. The experiments will be conducted to test the suitability of the different experiments for assessing MAR as well as to determine the constraints that arise with experimental set-ups at different scales and boundary conditions. Regarding boundary conditions, the focus will be on determining the optimal soil characteristics, loading rates, and wet/dry cycles for efficient MAR application. To achieve this, field and laboratory tests are run under very similar conditions to enable the comparison of the obtained results. The design of the field test site was supported by unsaturated soil zone modeling using HYDRUS 2D/3D (Šimůnek et al. 2016). Results show that the applicability of unsaturated zone models is highly restricted regarding model parametrization and the depiction of boundary conditions. They further showcase the strengths and constraints of this model type with regard to MAR analysis as well as adaption needs to enhance the potential for vadose zone model application.

Unsaturated soil zone modeling

The unsaturated soil zone

The unsaturated soil zone describes the subsurface region between the soil surface and the groundwater table. Pores may contain either water, gas, or both. Being a key element of the hydrologic cycle, the unsaturated zone connects the atmosphere, vegetation, and surface water bodies with the groundwater. Thus, it plays an important role in water resources planning as it defines the quantity and quality of natural and artificial groundwater recharge (Kim and Jackson 2012; Rossman et al. 2014; Turkeltaub et al. 2015). Especially in semi-arid and arid areas, groundwater recharge is the determining factor for the availability and sustainability of groundwater resources (Toews and Allen 2009; Szilagyi et al. 2011; Crosbie et al. 2013). Furthermore, the vadose zone plays an important role in the protection of groundwater resources as the passage through the unsaturated zone fosters filtering of organic matter (Vanderzalm et al. 2010), trace organic compounds (Montgomery-Brown et al. 2003), nitrogen (Zhang et al. 2005), and bacteria (Toze et al. 2004). This effect is used particularly for surface spreading methods to pre-treat infiltrated water before it reaches the groundwater especially when stormwater or treated wastewater are used for infiltration (Bekele et al. 2011; Nadav et al. 2012; El Arabi and Dawoud 2012; Azaroual et al. 2013).

To determine water movement in the unsaturated zone, many studies use numerical models based on the Richards' equation (Small 2005; Keese et al. 2005; Mathias et al. 2006; Wang et al. 2009), which is a nonlinear partial differential equation representing water movement in variably saturated soils (Eq. 1):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial \varphi}{\partial z} + 1\right)\right], \tag{1}$$

with K is the hydraulic conductivity, ψ is the pressure head, z is the elevation above a datum, θ is the water content, and t is time (Richards 1931). Due to its nonlinear behavior, the equation must be solved numerically. The relationship between water content and pressure head is described by the soil water retention curve. This function can be parameterized by the van Genuchten equation (Eq. 2):

$$\theta(\psi) = \theta_r + \frac{\theta_\mathrm{s} - \theta_\mathrm{r}}{\left[1 + (\alpha \times \psi)^n\right]^{1-\frac{1}{n}}}, \tag{2}$$

with θ_s is the saturated water content, θ_r is the residual water content, and ψ characterizes the pressure head. α and n are empirical van Genuchten parameters (van Genuchten 1980).

Richards' equation is valid for infiltration under isothermal and isotropic conditions. Its utilization may lead to only macroscopic representation of the actual natural soil status. For some MAR infrastructure, this generalization may cause high uncertainties, as microscopic processes affect the flow. It has been shown that wetting front instabilities often develop and govern the water flow under certain flow regimes (Glass et al. 1989), e.g., beneath clogged surfaces of infiltration units (NRMMC-EPHC-NHMRC 2009). As the Richards' equation fails to address this phenomenon, more elaborate models need to be considered (Assouline 2013). Preferential flow can be described using dual-porosity or dual-permeability models (Gerke and van Genuchten 1993; Šimůnek et al. 2003). In this experimental study, the development of a clogging layer was not regarded. Thus, water flow was modeled using the Richards' equation.

Most commonly used vadose zone models for MAR simulations include HYDRUS, MARTHE, FEFLOW, and TOUGH2 (Ringleb et al. 2016). HYDRUS is a computer software package available in 1D and 2D/3D used for the simulation of water, heat, and solute movement in variably saturated porous media (Šimůnek et al. 2016). It supports the representation of unsaturated soil hydraulic properties by van Genuchten (1980), Brooks and Corey (1964), Durner (1994), Kosugi (1996), as well as a modified van Genuchten function for soils near saturation. Hysteresis and dual-permeability are incorporated as well as a scaling procedure to approximate hydraulic variability in the subsurface. HYDRUS supports constant and time-varying head and flux boundary conditions that may change from one condition type to the other. Calculating ponded infiltration with adapting water tables is available for HYDRUS 1D and 2D.

MARTHE has been developed to simulate mass and energy flow in aquifers, rivers and unsaturated zones considering density effects due to changes in salinity or water temperature in 1D, 2D or 3D (Thiéry 1990). It supports the representation of unsaturated soil hydraulic properties by van Genuchten (1980), Brooks and Corey (1964), Brutsaert (1966) as well as logarithmic and pseudo-unsaturated functions. Boundary conditions implemented in MARTHE include open water bodies with free surface, constant, and time-varying fluxes as well as unitary gradients. Hysteresis is not included in the code, but dual-permeability modeling is possible.

FEFLOW has been designed to model flow, mass, and heat transport in porous and fractured media in 2D and 3D (Diersch 2014). Unsaturated soil hydraulic properties can be represented by van Genuchten (1980), Brooks and Corey (1964), Vachaud et al. (1973), and modified van Genuchten as well as exponential and linear functions. The retention parameters can be further defined by spline interpolation techniques. Boundary conditions can be specified as constant and time-varying head and flux boundaries with multilayer wells being a unique boundary condition to this code. Hysteresis can be regarded. FEFLOW can depict time-varying material properties which is of advantage to model clogging processes.

TOUGH2 enables the simulation of coupled transport of water, vapor, non-condensable gas, and heat in porous and fractured media (Pruess et al. 2012). The model can depict processes of hysteresis, macropores, and fractures. It provides extensive inverse modeling capabilities, with parameterization of boundary conditions and soil structure based on measured data. It allows for parameter determination of highly heterogeneous, anisotropic soil structures. Boundary conditions can be specified as constant and time-varying head and flux, as atmospheric and falling head boundaries (ponding).

Further information on vadose zone models has been compiled by Vachaud et al. (1990) and Šimůnek and Bradford (2008).

Reviewing unsaturated zone model application for MAR

The basis of this study was a literature review evaluating overall model utilization for MAR assessment (Ringleb et al. 2016), where case studies had been compiled from reviewed articles, scientific reports, and conference proceedings. Only publications written in English language had been considered. Data on vadose zone models were extracted from the compiled database of the study and evaluated regarding the applied MAR types and modeling objectives.

Since the beginning of the application of numerical models for MAR assessment, groundwater flow models have been the predominant model type (Fig. 1). Vadose zone models have rarely been utilized before 2006, and only in the past 10 years, their potential for MAR assessment has been studied (Ringleb et al. 2016).

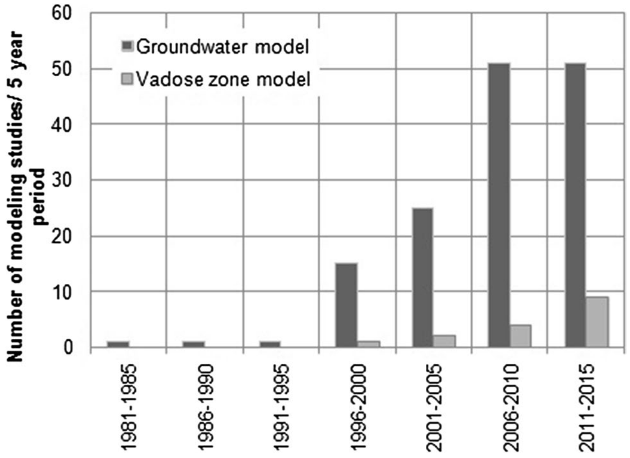


Fig. 1 Comparison of the historical application of vadose zone vs. groundwater flow models for MAR evaluation (after Ringleb et al. 2016)

Overall 16 publications were gathered that assessed MAR with the help of unsaturated soil zone models and 145 publications on saturated groundwater models (Table 1). Two-third of the studies were conducted for spreading methods and of those infiltration ponds and basins were the dominant MAR type (eight studies). Most of the 16 studies combined unsaturated zone modeling with further model types. Groundwater modeling was incorporated into nine of the analyzed studies. Transport modeling was of additional concern for nine studies.

To ensure the success of an MAR application, it is crucial to understand the impact of the system on the groundwater table. Determining the influencing zone of infiltration wells (Saharawat et al. 2006) as well as the infiltration behavior of recharge basins (Ting et al. 2006; Gvirtzman et al. 2008) has been studied with the help of vadose zone models.

Assessing the different sources of groundwater recharge and quantifying their volumes help to determine an appropriate recharge quantity. Differentiating natural and managed groundwater recharge has been undertaken by

Table 1 Vadose zone modeling studies with information on MAR types (SM-spreading methods, WSB-well, shaft and borehole recharge, IM-in-channel modification), additional modeling approaches (groundwater flow, solute transport), and modeling objectives (Ringleb et al. 2016)

	General MAR type	Vadose zone model	Groundwater flow modeling	Solute transport modeling	Groundwater management	Optimization, design	Geochemical processes	Saltwater intrusion	Soil aquifer treatment
Azaroual et al. (2012)	SM	MARTHE		×			×		×
Bhola et al. (2013)	IM	FEFLOW	×	×	×			×	
Browne et al. (2011)	SM	2D variable saturated flow	×	×			×		
Fernández-Escalante (2013)	SM, WSB	HELP			×				
Flint (2002)	SM	TOUGH2		×	×	×			
Gaus et al. (2007)	WSB	MARTHE	×	×			×		×
Gvirtzman et al. (2008)	SM	CPFLOW	×			×			
Händel et al. (2014)	WSB	HYDRUS, COMSOL				×			
Hasan et al. (2013)	SM	PCSiWaPro		×			×		×
Heilweil et al. (2015)	SM	VS2DI				×			
Kloppmann et al. (2012)	SM	MARTHE	×	×			×		×
McMahon et al. (2000)	SM	MODFLOW + SPLASH	×		×	×			
Monninkhoff and Kaden (2012)	WSB, IM	FEFLOW, MIKE-SHE	×	×	×	×		×	
Parkhurst and Petkewich (2002)	WSB	PHAST	×	×			×		
Saharawat et al. (2006)	WSB	HYDRUS			×				
Ting et al. (2006)	SM	TOUGH2	×		×				

Fernández-Escalante (2013) and McMahon et al. (2000) with the help of the models SPLASH (Arunakumaren 1997) and HELP (Schroeder et al. 1994). McMahon et al. (2000) further investigated how to differentiate MAR and excess irrigation. Determining different recharge sources not only helps with adapting a sufficient MAR infiltration volume but also demonstrates the potential of unmanaged recharge measures such as excess irrigation for sustainable groundwater.

Especially at sites where MAR methods such as in-channel modification are applied, modeling needs to cover the complex interactions between surface water and groundwater. Coupled surface water-groundwater modeling using FEFLOW and MIKE-11 (Monninkhoff 2014) helped to determine the impact of existing and future MAR facilities such as check dams, infiltration wells, and an underground dam on recharge and seawater intrusion in India and China (Monninkhoff and Kaden 2012; Bhola et al. 2013).

Unsaturated flow modeling has been applied to compare the feasibility of different MAR methods regarding their potential to maximize recharge volumes (Händel et al. 2014). Models can help in the MAR method selection process but even more so have been used in optimizing MAR schemes (Heilweil et al. 2015) and assessing site suitability for surface infiltration (Flint 2002). Understanding which parameters and technical design criteria have the highest influence on the infiltration process helps to design efficient and sustainable groundwater management solutions. An extensive modeling study with MARTHE has been applied at the Shafdan MAR site in Israel to plan and optimize the extension of the already existing MAR facilities (Kloppmann et al. 2012). The calibrated 2D flow and transport model was able to reproduce tracer breakthrough curves, the infiltrated tracer plume, and the water level increase during pilot experiments, and was taken as a basis for geochemical modeling using PHREEQC (Gaus et al. 2007; Kloppmann et al. 2012).

Vadose zone models can be useful to evaluate data from laboratory experiments. Soil column experiments are commonly undertaken to study transient flow and transport processes in the unsaturated zone. Numerical evaluation of such experiments was successfully used to assess how pollutants behave during the infiltration of treated wastewater (Kloppmann et al. 2012; Hasan et al. 2013) and to study the hydrodynamic changes in the soil during soil aquifer treatment (SAT, Azaroual et al. 2012). As field studies with emerging pollutants are often prone to legislative restrictions, modeling tracer behavior in the field can be a valuable addition to upscale results derived from column studies to obtain the necessary approvals for MAR (Kloppmann et al. 2012).

Assessing clogging development during MAR operation is an important aspect to consider for the maintenance of MAR schemes. In general, clogging is neglected during vadose zone simulations and hydraulic parameters are kept constant over time. Sensitivity analysis showed that the saturated hydraulic conductivity is a very sensitive parameter for unsaturated zone modeling. Thus, conductivity changes that may be attributed to clogging should ideally be included into modeling studies. The lack of inclusion inherits from the fact that clogging processes are rarely incorporated into vadose zone software making tedious manual adaption of the hydraulic conductivity over time necessary (Händel et al. 2014). A numerical clogging model has been specifically developed based on an unsaturated flow and reactive transport model to evaluate clogging during MAR operations (Pérez-Paricio and Carrera 1998; Pérez-Paricio 2001). It incorporates diverse clogging mechanisms including physical, chemical, and biological clogging, and can assist to improve the efficient operation of a MAR facility (Pérez-Paricio 2001). Furthermore, a 2D variable saturated flow model was used to model physical clogging by colloid transport during stormwater infiltration (Browne et al. 2011).

All regarded vadose zone models from the studies used the Richard’s equation (Eq. 1) or a derivative in combination with the Mualem/van Genuchten equation. To utilize these equations, a set of hydraulic parameters needs to be obtained for each soil type (saturated water content, residual water content, van Genuchten parameters α and n, and saturated hydraulic conductivity). These parameters have been determined through the literature values taken from studies (Carsel and Parrish 1988) or norms (DIN 2008) by Ting et al. (2006), Gaus et al. (2007), and Hasan et al. (2013). Determination through neural networks (Händel et al. 2014) or through calibration to measured field data (Gvirtzman et al. 2008; Browne et al. 2011; Kloppmann et al. 2012; Heilweil et al. 2015) is a more exact way to obtain sought parameters. They were further determined by characterizing the soil water retention curve through field data (Parkhurst and Petkewich 2002; Azaroual et al. 2012). As the information on soils often relies on point data, one parameter set is used for a soil layer and the layers are generally assumed as homogenous. This simplification is practical but does not represent the heterogonous nature of most soils, including preferential flow. Anisotropy is seldom regarded in the studies as the ratio between horizontal and vertical conductivity is not measured. A study from Händel et al. (2014) found that the horizontal component of K is very sensitive for modeling ASR wells, whereas the vertical component is highly sensitive for recharge basins. The effect of hysteresis is another aspect to regard for water retention curves. Hysteresis is included in most modeling software (e.g., HYDRUS, CPFLOW) but often neglected as parameterization of the different retention curves for infiltration and dewatering is tedious. Gvirtzman et al. (2008) assessed differences in the reproduction of the drying and wetting phase during modeling, but found that parameterizing hysteresis was impractical as many different retention curves were needed throughout the soil profile for the same time step. This high need for information requires so many assumptions that fitting these hysteresis parameters becomes meaningless. Overall, it can be stated that the determination of hydraulic parameters is accompanied with many uncertainties and assumptions. Thus, they are often fit to the specific case by calibration to measured field values (Flint 2002; Browne et al. 2011; Bhola et al. 2013; Heilweil et al. 2015).

The representation of boundary conditions for unsaturated soil zone models is underlain by some assumptions and simplifications. The hydraulic head of the groundwater boundary condition is often modeled as static (Ting et al. 2006; Azaroual et al. 2012; Händel et al. 2014) or variable (Gaus et al. 2007; Heilweil et al. 2015). Moving groundwater tables should be incorporated into studies, as the effect of groundwater depths on infiltration rates has been shown to be important by Händel et al. (2014) and Heilweil et al. (2015). However, changes of groundwater tables on the groundwater flow regime are assumed to be negligible (Gaus et al. 2007; Heilweil et al. 2015). The upper boundary condition is often simplified without regarding precipitation and evaporation as these flows are either of no relevance for the modeling objective or are significantly lower than the recharged infiltrate and thus negligible (Gvirtzman et al. 2008; Händel et al. 2014; Heilweil et al. 2015). The representation of infiltration basins is either by constant heads (Gvirtzman et al. 2008; Händel et al. 2014), changing heads or infiltration rates (Gaus et al. 2007; Hasan et al. 2013). It should be noted that some models do not account for ponding and changing water tables in the recharge basin cannot be represented, even though they have a large effect on infiltration rates. Boundary conditions at the side of the domain are usually no flow conditions as groundwater regimes are rarely regarded. A few studies showed that within a limited time frame, the no flow representation has no effect on the final results (Händel et al. 2014). The initial condition (moisture content) in the soil profile is a parameter that is given a little attention and that is usually represented as one homogenous value throughout the whole domain based on soil-specific natural moisture contents (Gaus et al. 2007) or point measurements (Gvirtzman et al. 2008).

Discretizing the model domain must be balanced out to allow for numerically stable models with acceptable computational time. In general, model elements should be relatively small at regions with steep hydraulic gradients (in this case MAR facilities) and can gradually decrease with depth as changes in pressure heads are much slower (Šimůnek n.d.). Information on discretization is rarely discussed in the studies regarded. Cell sizes generally range between 1 m (Heilweil et al. 2015) and 5 m (Händel et al. 2014) and domain boundaries have lengths of up to 100 m. The model built by Gaus et al. (2007) is the only exception with a particularly larger model area of 1800 hectares.

Browne et al. (2011) stated that due to the assumptions and simplifications, modeling should be approached as conservative scenarios only showcasing the worst case that can be improved with better support by field data. Uncertainties in the hydraulic parameters and their assumed homogeneity were one of the biggest problems encountered in the vadose zone modeling studies (Gvirtzman et al. 2008; Hasan et al. 2013; Heilweil et al. 2015). Using the constant head boundary condition for infiltration basins instead of simulating gradual increase or decrease was another model deficiency that affected the results (Gvirtzman et al. 2008; Händel et al. 2014).

Materials and methods

Numerical simulations with HYDRUS 2D/3D were undertaken to determine the size and geometry of the pilot scale facility and the number and location of measuring devices. Further simulations were conducted to design the experimental scenarios. The scope of the scenarios was to test the influence of infiltration duration, seepage volumes, and built-in materials on the quantity of groundwater recharge.

The sediments at the test field site are characterized by fluvial deposits and in the upper layers by anthropogenic deposits. The aquifer itself consists of layers ranging from fine sands to coarse gravel. Marine sedimentary rocks form the aquifer base (Dietze and Dietrich 2012). Groundwater depth ranges between 8 and 10 m below surface, and is highly dependent on the water level in the nearby river Elbe.

To minimize external influences and to control the climatic conditions, the infiltration unit will be covered with a climate tent. Knowledge and control of climatic conditions ensure the comparability to laboratory experiments which are run in parallel. Fixed technical conditions of the size of the climate tent were given (length: 4.3 m, width: 2.5 m, compare Fig. 2). Underneath the infiltration facilities, a basin will be excavated that enables the soil material within the basin to be replaced with different media. The size of this basin was varied in three dimensions in the simulations: length 1.5–3 m, width 1–1.5 m, and depth 1–2 m. The field experiments are planned with various soil types to assess their suitability for different infiltration scenarios. The original soil was removed for this purpose. Properties of the soils were defined by grain size analysis. The soil type in the surrounding area was defined as sand, the material in the excavated trench as loamy sand. The hydraulic parameters used for the solution of Eq. 2 were defined by neural network prediction using the ROSETTA software (Schaap et al. 2001) and the determined grain size distributions (Table 2).

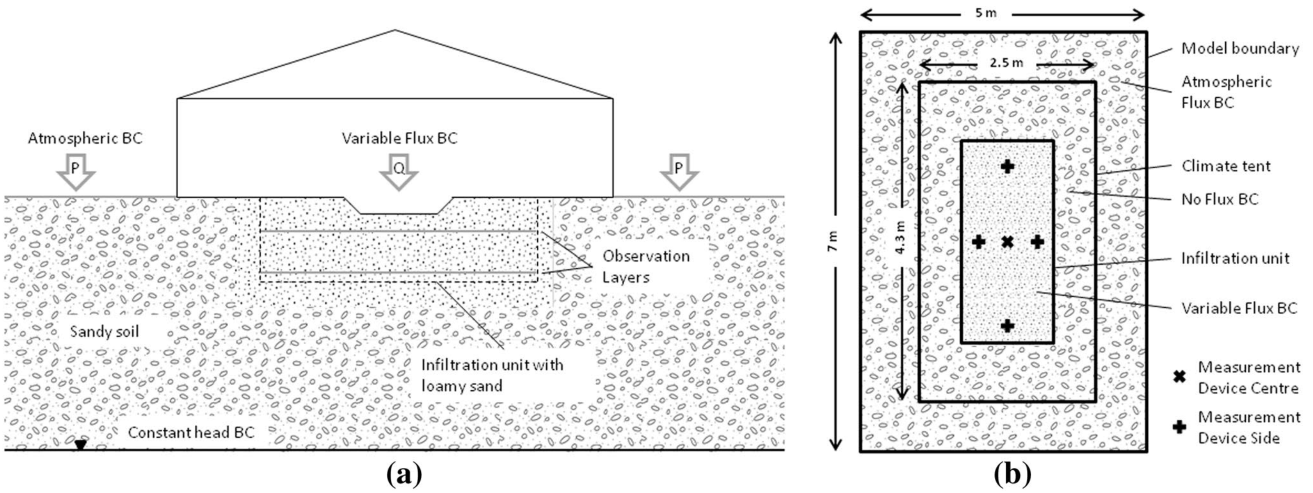


Fig. 2 **a** Experimental set-up and plan view of field scale infiltration test site and **b** top view of test site including corresponding boundary conditions (BC) applied in HYDRUS simulations

Table 2 Soil parameters used in HYDRUS simulations for materials inside and outside of the infiltration basin, with Ks is the saturated hydraulic conductivity

	θ_r (−)	θ_s (−)	α (1/m)	n (−)	K_s (m/s)
Soil in infiltration basin	0.05	0.378	3.51	4.239	0.00015
Soil outside of infiltration basin	0.045	0.431	14.5	2.68	0.00085

The overall depth of the model was set to 10 m. Width and length of the model were set to 5 and 7 m, respectively (Fig. 2). The depth, width, and length of the infiltration basin were varied throughout the simulations. The varying groundwater level was not considered in the model. The minimum groundwater level was assumed as static to simplify the lower boundary condition as fluxes cannot be determined over varying groundwater tables by HYDRUS. The lower boundary was set as a constant head boundary condition. The upper boundary condition (BC) for the area outside of the greenhouse was set as atmospheric with a 50-day precipitation time series for Pirna. Evapotranspiration was not considered in this study. On top of the infiltration trench, the upper boundary condition was also set as atmospheric boundary with the exception of continuous infiltration scenarios that were depicted as a constant head boundary. For the atmospheric boundary condition, the model applies the defined flux BC if the boundary is unsaturated and switches to a pressure head BC once the specified boundary becomes saturated (pressure head equal to zero). As no previous knowledge of the initial conditions was obtained, preceding simulations were undertaken to generate a natural distribution of soil water depending on the standard rain profile for Pirna.

Simulations for each infiltration scenario were undertaken for 50 days. Time step widths for the simulations were adjusted automatically by HYDRUS. The initial time step width was set to 1 s. The spatial discretization of the model domain was undertaken using triangular prism and dividing the domain into 150 vertical layers. Layer thickness at the top was 0.026 m and increased to 0.079 m at the bottom. 535,208 mesh elements were created with the largest mesh size of 0.35 m near the boundaries of the model. The mesh was refined for the area inside of the climate house with the largest mesh size being 0.15 m. For the infiltration area, the mesh was again refined and the smallest mesh size in this area was set to 0.07 m. Spatial refinements were undertaken until the model ran in a stable manner considering the recommendations made by Šimůnek (n.d.).

Results

Planning of infiltration unit size and geometry

One aspect of the infiltration basin that needed to be discussed before the construction was the possibility to exchange the built-in soils. With the intended extent of 1 m × 2 m and a depth of 2 m, every exchange of soil would request 4 m^3 of soil. This implies a high organizational effort as the exchange must be done by hand. Therefore, pressure head measurements in the depth of 0.7, 1, 1.5, and 2 m were compared. The pressure head changes in the four depth levels were evaluated at two different positions of the infiltration basin with the 50-day rain profile as the infiltration scenario (Fig. 3a in the middle of the basin, Fig. 3b at the side of the basin).

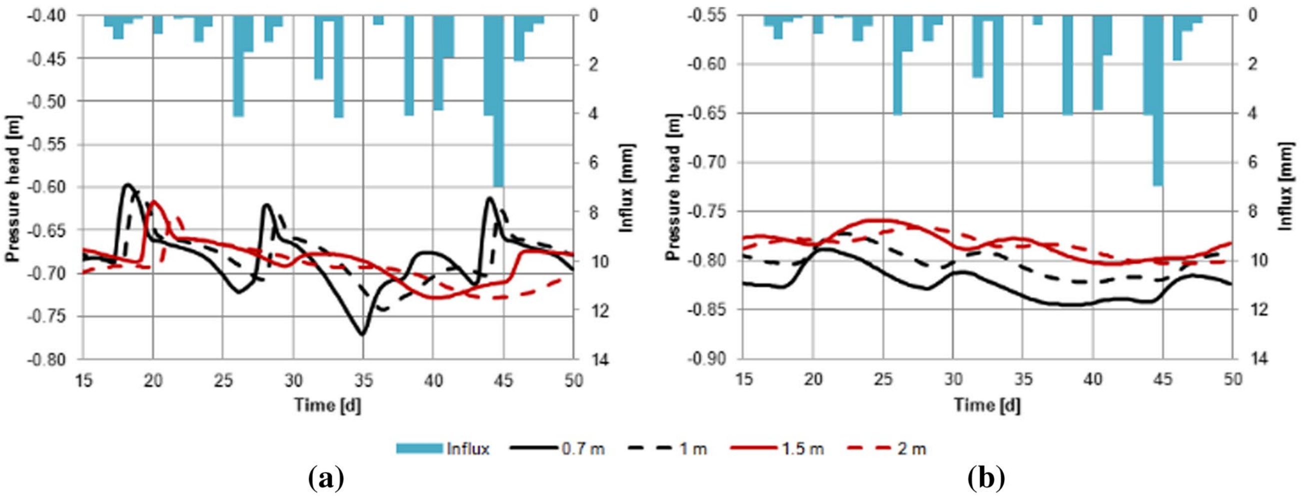
Results show that the profiles at 0.7 and 1 m depth as well as 1.5 and 2 m depth behave very similar. The average values of the pressure head as well as the reaction to infiltration peaks compare well. Hence, it was decided that a depth of 1.5 m for the infiltration basin is sufficient. Consequently, the soil volume that needs to be exchanged decreased from 4 to 3 m^3.

Assessing the placement of measuring devices

The observation network must be planned carefully to avoid unnecessary use of measurement tools. The type, location, and number of measurement devices need to be tested to define their optimal placement within the measurement area.

Simulations were undertaken that compared the pressure head evolution at 26 possible locations. The observation points were arranged in two planes below the surface (0.7, 1.5 m). For the standard distribution, measurement tools were placed at 0.25 m from the boundary of the infiltration unit (Fig. 4, red and green points). The influence of the boundary on the resulting pressure heads was tested by comparing measuring points with a smaller distance (0.07–0.10 m) with those placed at 0.25 m to the boundary (Fig. 4, black and red points). In addition, pressure heads at three different observation points in the center of the basin with a distance of 0.5 m to the infiltration unit boundary were compared (Fig. 4, blue points).

The results of the standard distribution show that only the observation points in the center (Device 12, 11) behave significantly different from the rest. Comparing the observation points in the edges of the basin, it can be seen that it makes a remarkable difference if the devices are situated 0.1 m from the border (Device 1–4) or if they are situated 0.25 m from the border (Device 8–10, 13). For the observation points in the center of the basin, no clear difference



(a) (b)

Fig. 3 Pressure head distribution **a** in the center and **b** at the side underneath the infiltration unit showcasing water movement in different depths below surface

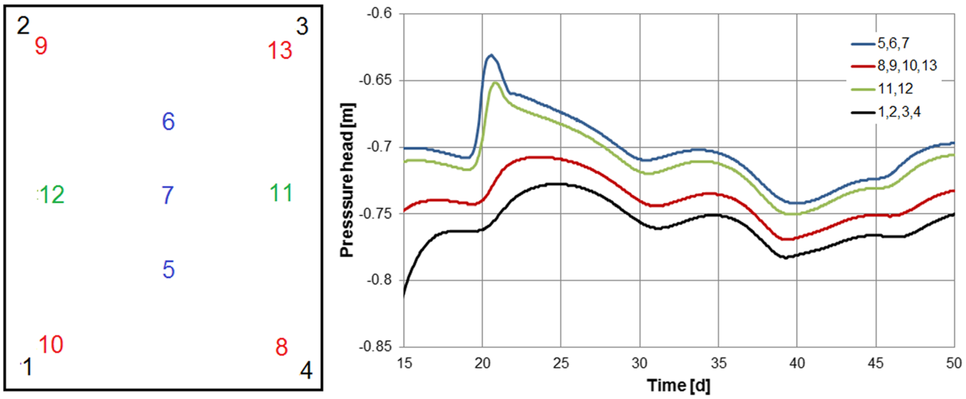


Fig. 4 Comparison of possible placement options for measurement devices in 1.5 m depth comparing the effect of centered devices vs. devices at the side, the effect of boundaries of the infiltration basin, and the influence of location in the center of the basin. Influx scenario is consistent with scenario shown in Fig. 3. For better visibility, only one graph is plotted per device cluster

can be noted. They also show very similar behavior to the central devices (11, 12) at the side of the basin.

In conclusion, it can be stated that the tools should not be situated too close to the infiltration unit border as they would be influenced by the boundary. In case of homogenous irrigation of the whole area of the basin, it is not necessary to install six devices in each depth as local diversion is very small. To save costs, a distribution with one device in the center and two measuring tools at the side of the basin should be favored, e.g., locations 7, 8, and 12. It should be kept in mind that irrigation schemes with different local influxes or the introduction of varying land use conditions (e.g., partly sealed surfaces) form other requirements on the measuring devices. Disturbance is another factor to consider as especially the devices placed in the center of the basin cause disruptions in the natural flow and should be placed thoughtfully.

Experimental scenario planning

Infiltration rates were varied between different steady-state and intermittent transient rates. Each of these simulations ran for 50 days with infiltration starting after 14 days to ensure no influence of the initial conditions in the soil which had only been estimated. In Table 3, an overview of the infiltrated water and the amount of water reaching the groundwater table after the depicted time frame is given. In no case, surface ponding occurred. The scenarios with the highest infiltration rates resulted in the highest groundwater recharge ratios (10 L/h 14 days and 10 L/h 21 days). At least 363 L of water must be infiltrated to result in groundwater recharge (0.1 L/h increase). In general, it can be stated that including drying periods has no advantage in terms of maximizing the volume of infiltrated water. In all cases, increasing the duration of infiltration breaks resulted in lower percentage of infiltrated water. However, in later experiments, not only the quantity of infiltrated water but also the quality will be considered. Therefore, the influence of the breaks on the quality of infiltrated water, e.g., increase in oxygen, must be assessed as well. Comparing scenarios with similar infiltration quantities (1 L/h for 21 days and 3 L/h for 7 days) shows that higher infiltration rates will lead to faster groundwater recharge.

Only experimental designs with duration of up to 50 days are practicable for the planned field experiments. Four different infiltration scenarios are going to be conducted in 1 year, but field experiments are restricted to seasons where the soil is not frozen. To achieve recharge at the groundwater level within the time frame of 50 days, recharge rates of at least 3 L/h must be considered.

Increasing the drying period of the hydraulic loading cycle prolongs the residence time in the unsaturated soil zone. Drying periods lead to a more natural water distribution in the soil zone as well as continuous saturation, whereas short and large infiltration scenarios lead to the best recharge ratio but also to rapidly decreasing water contents in the unsaturated soil zone. Both scenarios could

Table 3 Simulated scenarios for an infiltration unit of 2 m^2 with corresponding amounts of infiltrated water and groundwater recharge (in L)

Scenario	Infiltration (L)	Groundwater recharge (L)	Total recharge/ total inflow (%)
Standard rain scenario for Pirna	166	0	0
1 L/h for 1 day, then increase of 0.1 L each h for next 3 days	363	4	1
1 L/h for 1 day, 3 L/h for 1 day, 10 L/h for 1 day, 20 L/h for 1 day	845	353	42
1 L/h for 7 days	174	0	0
1 L/h for 1 day, 1-day break (×7)	174	0	0
1 L/h for 1 day, 3-day break (×7)	174	0	0
1 L/h for 14 days	348	0	0
1 L/h for 21 days	522	3	1
3 L/h for 7 days	525	73	14
3 L/h for 1 day, 1-day break (×7)	525	64	12
3 L/h for 1 day, 3-day break (×7)	525	0	0
3 L/h for 14 days	1040	501	48
3 L/h for 21 days	1570	971	62
10 L/h for 7 days	1740	1209	69
10 L/h for 1 day, 1-day break (×7)	1740	1141	66
10 L/h for 1 day, 3-day break (×7)	1740	923	53
10 L/h for 14 days	3480	2992	86
10 L/h for 21 days	5220	4672	90

be used for different infiltration approaches (quantity vs. quality and artificial vs. natural recharge).

Modeling these different scenarios and loading cycles may help in understanding the effects of incorporating drying cycles or increasing loading rates. Three scenarios were chosen to show the different water distribution in the deeper unsaturated zone (Fig. 5). Two similar scenarios where only the hydraulic loading rate was increased from 3 L/h [scenario (a), Fig. 5a] to 10 L/h [scenario (b), Fig. 5b] were compared to a scenario without drying times [scenario (c), Fig. 5c]. The biggest visible difference between the scenarios lies in the shape of saturation. While for the scenario without breaks a circular saturation starting beneath, the infiltration basin could be detected, the spreading in the scenarios with breaks is more homogenous in the center and decreases more rapidly to the sites. Overall, the horizontal moisture distribution patterns in scenario (b) and (c) show only little change in water content height throughout the plane. For scenario (a), the moisture content difference within the plane increases significantly. Figure 6 showcases these differences in a horizontal cross section. Moisture distribution for scenario (a) and (b) is very similar in height and homogeneity in the center of the basin. Towards the boundaries, there is a rapid decline for scenario (a).

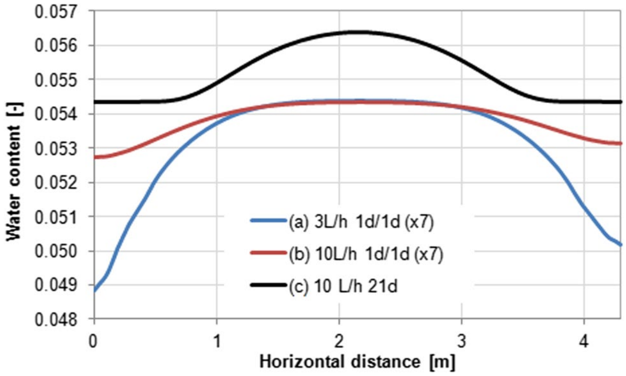
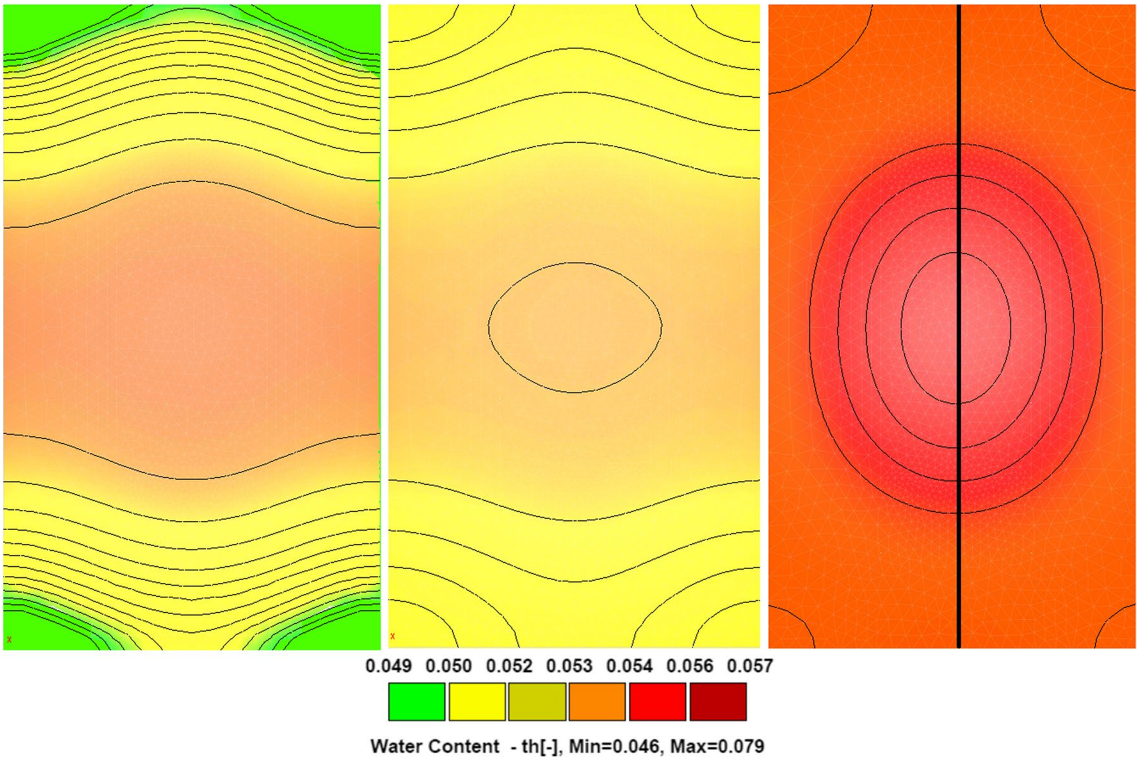


Fig. 6 Cross section of horizontal moisture distribution of three different infiltration scenarios simulated 5 m below surface after 50 days. Location of cross section is marked in Fig. 5c with a black line

Water content for scenario (c) is significantly higher throughout the whole cross section, but the overall behavior is similar to that of scenario (b). Even though the moisture difference between scenario (b) and (c) is much closer, the visual distribution patterns of (a) and (b) are more alike (Fig. 5). This suggests that for the distribution of water in the lower vadose zone, not only the amount of water but also the drying times are a defining factor. The



(a) 3 L/h 1d/1d (x7) **(b)** 10 L/h 1d/1d (x7) **(c)** 10 L/h 21d

Fig. 5 Horizontal water content distribution of three different infiltration scenarios simulated 5 m below surface after 50 days results further indicate that the vertical boundaries could have an influence on the results, so in subsequent studies, the model domain should be extended to ensure the reliability of the results.

The flux across the groundwater boundary has been plotted in Fig. 7 and shows the time distribution of groundwater recharge and further the height of recharge over the course of the three scenarios. Recharge for scenario (a) is negligible within the time frame of 50 days, whereas for scenario (c), almost all recharged water reaches the groundwater table before the 50 day mark. Recharge increase is relatively constant over time for scenario (c), whereas for scenario (b), the cyclic behavior of the recharge can still be detected at the groundwater level. During the recharge flux decrease, a characteristic pattern can be observed for scenario (b) and (c) which has also been cross-checked and validated with other scenarios from Table 2. The flux decrease starts with a rapid decline, it is followed by a slower phase of decreasing flux and it ends in an almost constant phase. This could be attributed to the combination of the soils in the basin and the surrounding area as they have different drainage characteristics which together form this pattern.

Further studies concerning the experimental design of the scenarios have been conducted regarding soil types (not included). The influence of soil types on the quantity of infiltrated water is straightforward: the sandier the soil, the higher the infiltration potential. Thus, modeling soil scenarios for quantitative assessment is dispensable. However, simulations showed that with certain soil combinations, capillary barriers can develop, e.g., when materials of lower permeability are built into highly permeable surroundings. Simulations could help to depict field scenarios where capillary barriers evolve and consequently could be avoided by choosing adequate built-in materials.

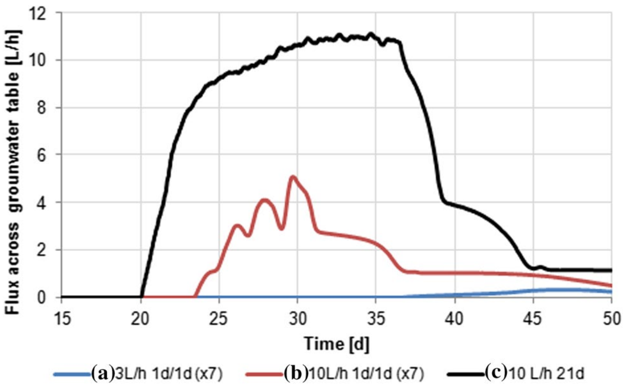


Fig. 7 Total value of the boundary flux across the lower boundary (ground water table) for three different scenarios

Discussion

For a literature review on the use of unsaturated soil zone models for MAR assessment, only 16 studies were found, most of which had been published in the past 10 years. The scope of these studies showed that there is a wide potential for the use of vadose zone models. They have been applied to plan and optimize MAR systems, assess the impact of MAR on the unsaturated zone and the groundwater, and to evaluate geochemical processes during MAR operation. In addition, it has been tested whether unsaturated zone models can substitute groundwater flow modeling for MAR assessment. Further objectives include the comparison of different MAR methods as well as the assessment of coupled surface and groundwater systems. Two-thirds of the evaluated studies concerned spreading methods. In general, water movement in the unsaturated zone is often not modeled by itself, but studies are rather combined with groundwater or transport modeling.

The potential of vadose zone models has not yet been fully utilized. Only very few studies concerned the design and optimization of pilot studies and real MAR sites. Modeling at different stages of the pilot experiments as well as the actual MAR site construction holds great potential for saving costs and time. Additional modeling can help to understand the hydraulic processes at the catchment area or the site itself. The aim of such modeling studies can be the identification of parameters which have greatest influence on the recharge processes and help define the scope of future data collection. Testing and monitoring programs for hydrologic parameters are required by some MAR guidelines (Environmental and Water Resources Institute 2001; NRMMC-EPHC-NHMRC 2009). Pilot or test sites are generally run to find a good compromise between what is theoretically desirable and practically achievable by applying MAR to a specific site (Environmental and Water Resources Institute 2001). As the results are scale-dependent, test sites should be constructed at the scale desired for the later MAR site. For shallow groundwater basins, monitoring of several wetting and drying cycles is advised. For deep groundwater basins, test operations of several months should be conducted. Thus, a careful design of these test sites is essential to manage temporal and spatial requirements. Location of observation points and frequency of data collection as well as the observed parameters need to be defined. This is a critical part of the test program as it is time-consuming and costly. Concerning the timeframe, it is essential to conduct test runs of adequate length to obtain the response of the groundwater basin to the infiltrated water, e.g., the time span, the infiltrated water needs to reach the groundwater table. Careful planning can confirm that the scope is correct and that the proposed budget is adequate.

As it has been shown, modeling can be helpful for the design of MAR sites and their experimental set-up. By modeling an MAR test site in Pirna, Germany, the dimensions of the infiltration unit were determined considering technical as well as economic criteria. Assessment of the number and location of measurement devices helped to identify the minimum number of devices needed and their optimal placement. Thus, unnecessary investment into observation units was prevented. Furthermore, possible hindrance of the water movement in the soil could be reduced by minimizing the number of measurement devices. Experimental scenario planning gave an idea which scenarios are feasible for the set conditions, e.g. limited time frames. It also provided a first indication on the amount of water that needs to be infiltrated to get a response from the aquifer. A theoretical study on soil material showed the potential for the development of a capillary barrier.

Using a model for predictive purposes requires a thorough calibration of the model. However, calibrating a test site model is problematic as there are little to no previous measurements to work with. Thus, first results of the model need to be evaluated carefully. During the operation of the test site, subsequent data collection and model calibration need to be undertaken to verify the simulation results and to adjust the experimental measures. Preliminary sensitivity analyses may help to identify parameters that need to be focused on during calibration. It further helps to understand the system dynamics and prioritize main focus of data collection (Anderson et al. 2015). As for surface infiltration systems, the unsaturated zone is the most sensitive region. Therefore, focus should lie on estimating the hydraulic parameters defining this model compartment. This is especially true when clogging occurs as this process may change the respective soil parameters.

For this study, the soil data are essential factor for uncertainty. Only within the infiltration unit, the soil can be described as homogenous. Information on the outside material is not sufficient. For the location of the infiltration unit, there are no soil data available beneath 4 m of the soil surface, and hence, only assumptions can be made from surrounding boreholes. During the construction of the test site, investigations on the underlying soil material will be undertaken and later be included into the study. There is an anthropogenic layer with debris that is not easy to parameterize as it includes larger pieces of metal and bricks. Thus, the parameterization of the outside material is uncertain and the uncertainty needs to be considered when evaluating the results.

High requirements regarding the soil parameterization are a restriction for the utilization of unsaturated soil zone models. Obtaining the van Genuchten parameters which are needed to solve the Richards' equation is laborious. Using predefined parameters from databases or pedotransfer functions that assist to derive these parameters from sieve analyses may be helpful but are also the cause for further uncertainty. Parametrization of the Richards' equation for soils coarser than sand is still a matter of research (Dann et al. 2009; Thoma et al. 2014). Furthermore, vadose zone models require a finer discretization than groundwater models. Hence, model extent is generally smaller as large areas with fine discretization result in extensive computation time. Unsaturated soil zone models are available in different complexities and dimensions. The possibility to choose between models in 1D, 2D, and 3D provides means for simplified simulations and less extensive data requirements as well as computational demands.

The complexity and incorporated processes of each model must be checked beforehand to justify their application for a specific MAR study. In the Pirna case study, ponded infiltration with adapting heads could not be modeled as it is not available for HYDRUS 3D. The simplification of using an atmospheric boundary condition was viable as the applied fluxes did not exceed the soil infiltration capacity and no surface runoff was detected. With higher fluxes applied or a longer duration, all water exceeding the infiltration capacity of the soil would be removed as surface runoff or increase the surface pressure head to unrealistic levels, thus leading to water balance errors. As ponded infiltration is part of many spreading methods and in-channel modifications, this a major disadvantage of HYDRUS 3D in terms of MAR assessment. In this case study, the inability of the software to calculate fluxes over a changing groundwater table is not significant as the groundwater table is much lower than the zero-flux plane, and thus, groundwater table changes would not result in differing recharge rates. However, for studies with shallow groundwater tables, this would be a serious drawback in terms of applicability.

In addition to the already mentioned possibilities for the utilization of vadose zone models, further potential lies within the qualitative assessment of the infiltration scenarios. Especially, for SAT, the purification capacity of the soil material underlying the infiltration basin needs to be tested. Integrating colloid transport into the modeling study could help to assess pathogen fate and potentially physical clogging. Next to column studies, long-term simulations can help to predict the evolving purification capacity and the clogging potential. Thus, infiltration set-up with sufficient breaks between infiltration events can be designed to guarantee proper aeration of the soil. The evaluation of clogging development could potentially depict the point of time when the soil material must be exchanged or restoration measures need to be applied to guarantee steady infiltration capacities.

Further potential for the application of vadose zone models include the differentiation between natural and managed groundwater recharge and the comparison of different MAR methods regarding their qualitative and quantitative effectiveness. As the vadose zone is the connecting compartment between surface processes and the groundwater, it should ideally be considered for its possible contribution to coupled groundwater–surface water studies. This is especially relevant for studies concerning large-scale MAR facilities such as check dams and underground dams.

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Compliance with ethical standards

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