Chapter 19

Numerical and analytical models for natural water treatment systems in the Indian context

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19.1 WHY MODELLING INDIAN NATURAL TREATMENT SYSTEMS?

Modelling either by numerical or analytical approaches is a widespread approach in hydrogeology, but requires careful considerations of the model type and level of effort to be spent which in turn depends on the purpose of the study. Before starting to model, Anderson and Woessner (1992) proposed to answer the following generic questions:

- Is the model to be constructed intended for prediction, system interpretation, or a generic modelling exercise?
- What do you want to learn from the model? What questions do you want the model to answer?
- Is a modelling exercise the best way to answer those question(s)?
- Can an analytical model provide the answer or must a numerical model be constructed?

In this Chapter we will outline the use of groundwater models focusing on the strategic phases of Natural Treatment Systems (NTS) (feasibility in a given watershed, NTS design and implementation, NTS operation) as well as on the model selection (types of models). Generic numerical models are then developed for two NTS types, riverbank filtration (RBF) and Management of Aquifer Recharge (MAR) via infiltration ponds. The purpose of this modelling exercise is to determine important NTS performance parameters such as recovery rates, infiltration rates or travel times of the infiltrate in the subsurface. Investigation of modelling scenarios for each of the NTS types is another aim. Furthermore results of numerical modelling and selected analytical solutions are compared.

Real-world applications of different types of models within the case studies of the Saph Pani project as outlined in previous Chapter complete and illustrate this more generic approach (Chapter 14).

The specificity of NTSs is that they rely on natural processes. Those are complex interactions of surface water, wastewater and groundwater and the contaminants they may contain with the aquifer matrix, with microorganisms and plants. In contrast to completely engineered and controlled systems, the functioning of NTS needs to be understood first to be able to predict their performance. Once a conceptual model of the relevant processes has been established on the basis of a variety of measurements, analytical or numerical models can be set up to simulate the behaviour of the NTS. As for any numerical flow and transport model this is done through an iterative process of model setup and model calibration.

Both a completely natural and a partly engineered NTS can be, at the very beginning of their implementation, considered as a black box, contrary to engineered treatment systems. Their potential impact or performance will largely depend on the local climatic, hydrological, geological, and biological (including macrophytes, microphytes, microbia) conditions, on land use and, last but not least, on the quality and quantity of water to be treated. Measurements and monitoring are indispensable to get an insight into this black box system and are a prerequisite to any establishment of any model, even a conceptual one. The data situation will largely determine the complexity and the reliability of NTS models. Setting up a highly sophisticated model on a weak data basis will only create artificially precise simulations and predictions. In sum, modelling is inseparably linked to monitoring. A series of key questions need to be addressed before, during and after implementing of an NTS facility:

- What will be the impact of a NTS at local scale in terms of water availability and water quality improvement (or deterioration)?
- What will be the radius of influence on water quality and quantity of an individual NTS?
- Will its performance be durable over time?
- How will it behave in cases of changing boundary conditions (e.g. climatic, hydrologic, land use) or in the case of extreme events (droughts, floods)
- How can it be improved through adapted configuration (e.g. position of wells with respect to a river, pumping rates), or by adding engineered components to the system such as in-situ or pre- or post- treatment measures for water quality improvement?
- What will be the impact of NTS at the basin scale when a large number of individual systems are implemented and if different systems are combined within a watershed?

These questions will be asked from the very beginning of the planning phase and over the entire lifetime of the NTS project. Coupled surface-groundwater models, potentially with contaminant transport will provide the unique possibility to preview the feasibility of an NTS in the regional context, to optimize the choice of the site and the configuration and to optimize operating conditions in a way so as to meet fixed quantity and quality targets. Those targets are most frequently quantified through criteria like water quality acceptable for given uses such as drinking water, irrigation or industry, groundwater level evolution and salinity.

Especially in India, groundwater is an important resource, accounting for approximately 60% of irrigation water and 85% of drinking water and it is estimated that 60% of groundwater sources will be in a critical state of quantitative degradation within the next twenty years (Worldbank, 2010 and referenced therein). MAR is identified as a strategy to cope with dwindling water resources in India and "The National Groundwater Recharge Master Plan" is developed to assess the nationwide feasibility of MAR (CGWB, 2005). Modelling can accompany the implementation of NTS over different generic phases, common to all NTS types and regional contexts (Table 19.1).

Table 19.1 Planning phases of Natural Treatment Systems (NTSs) and case studies in India (Saph Pani project), see Chapter 14.

Phase	Examples from Saph Pani
Phase 1: Initial feasibility study in the regional context and choice of the NTSs	• Choice of NTSs (MAR) for saline intrusion management in the coastal Arani and Koratalaiyar watershed, Chennai, Tamil Nadu
Phase 2: Estimation of the radius of influence and positive/negative impact of an individual NTS	• Simulation of the behaviour of individual MAR-SAT* percolation tanks, Maheshwaram, Telangana
Phase 3: Planning of NTS implementation at watershed scale	• Implementation of MAR check dams in the coastal Arani and Koratalaiyar watershed, Chennai, Tamil Nadu
Phase 4: Estimation of the impacts on water quality and quantity at aquifer and watershed scale	• Scenarios of wetland impacts on water balance in the Musi watershed, Hyderabad, Telangana Simulation of contaminant transport/attenuation in an alluvial aquifer: RBF at Yamuna River, New Delhi
Phase 5: Optimisation of individual and watershed scale solutions	• Optimisation of well technology and exploitation schemes assisted by flow modelling for RBF in Haridwar, Uttarakhand

*Managed aquifer recharge (MAR) combined with soil-aquifer treatment (SAT).

19.2 WHAT MODELS FOR INDIAN NATURAL TREATMENT SYSTEMS?

The variety and degree of sophistication of models is large and, as stated above, has to be adapted to the problem to be solved and to the available data situation. Geometry of groundwater models range from 1D to full 3D and the chosen spatial resolution will determine the calculation times. Processes used for natural water treatment mainly take place at the interfaces of different compartments of the local or regional water cycle (surface flow, unsaturated flow, groundwater flow, seawater intrusion) so that there is need for integration of different types of models (river models, unsaturated-saturated groundwater models, density driven flow models). These models have revealed a major challenge for the simulation of the behaviour e.g. constructed wetlands at basin scale (Musi river study site, Chapter 14).

A complete response to the questions listed above (Chapter 19.1.1), that also addresses contaminant transport and water quality in general, may require the use of reactive transport models or even of state of the art bio-geochemical reaction modelling. Even simple models (analytical models) can provide sufficient information at least for a preliminary design or evaluation of NTS's but, most frequently, numerical models will be used. Standard numerical models are nowadays able to simulate up to full 3D advective and dispersive flow and transport of water and solutes. Supplementary features may be needed in a given context. Such features could involve, in the order of increasing complexity, the following processes:

- Density driven flow (in the context coastal aquifers salinisation), e.g. the Chennai case study (Chapter 14).
- Sorption and (bio-) degradation of solutes (e.g. through sorption isotherms, degradation factors) e.g. the New-Delhi RBF case study investigating ammonium transport (Chapter 14).
- Variable saturation flow (in the case of a significant thickness of the unsaturated zone, in particular if the latter plays an important role for water quality improvements in SAT systems) e.g. the Maheshwaram case study, which looked into infiltration processes when using infiltration ponds/tanks for MAR-SAT (Managed aquifer recharge combined with soil-aquifer treatment) (Chapter 14).
- Geochemical reactions through the combined use of flow-transport models and thermodynamic equilibrium models or thermo-kinetic models taking into account the reaction kinetics e.g. the Maheshwaram case study dealing with Fluoride mobilisation upon MAR (Chapter 14).
- Biologically mediated geochemical reactions (specific models available).

In this Chapter we will outline, through simulation of generic benchmark tests, the use of different types of groundwater models available for NTSs, in particular MAR and RBF. These generic model runs will allow selecting modelling approaches adapted to the problem to be treated and to the available calculation capacity and modelling tools. Applications of different types of models within the case studies of Saph Pani will illustrate this synthesis in Chapter 14.

19.3 SOME ANALYTICAL SOLUTIONS FOR NT SYSTEMS

Analytical solutions are simplifications and generally assume hydraulic properties to be homogenous and isotropic. Boundary conditions are often simplified and assumed to be constant. Nevertheless, analytical solutions for NT systems often provide a straight-forward approximation of important performance parameters such as recovery rates, infiltration rates or travel times of the infiltrate in the subsurface.

19.3.1 Bank filtration

Bank filtration (BF) systems in India are often utilized as the sole purification treatment along with limited post-treatment such as chlorination (Sandhu *et al.*, 2010). The purification capacity of the BF systems depends to a large extend on hydraulic parameters such as mixing ratio between native groundwater with induced surface water (bank filtrate) and the travel time of the bank filtrate to the abstraction well.

Simple analytical solutions for BF systems were developed by Rhebergen and Dillon (1999) and Dillon *et al.* (2002) to approximate travel time of bank filtrate from the surface water to the abstraction well. The authors assume an initially horizontal water table and do not consider riverbed clogging. Both river and well are fully penetrating the aquifer. All the water which is pumped is assumed to come from the surface water body in the final steady state condition. The minimum travel time ($t_{\min}$) of bank filtrate to the abstraction well is calculated according to:

$$t_{\min} = \frac{2\pi D n_e a^2}{3Q} \quad \left(\text{Dillon } et\ al., 2002\right) \tag{19.1}$$

where:
$t_{\min}$ = minimum travel time [d]
D = average saturated thickness [m]
n_e = effective porosity of the aquifer [–]
a = distance of the well from the bank [m]
Q = abstraction rate [m^3/d]

The minimum travel time ($t_{\min}$) is calculated under steady-state conditions and underestimates travel time for intermittent pumping conditions (Dillon *et al.* 2002). The analytical approach overestimates the proportion of bank filtrate in the abstraction well because rivers in nature are usually only partially penetrating the aquifer and analytical solution which assume full penetration will overestimate the infiltration from the river (Chen, 2001).

The share of bank filtrate in the abstraction well (q/Q) of the above example changes in time and can be calculated according to a generalized solution developed by Glover and Balmer (1954) based on the equations developed by Theis (1941):

$$\frac{q}{Q} = erfc\left(\frac{a}{\sqrt{4\alpha t}}\right) \quad \text{(Glover and Balmer, 1954)} \tag{19.2}$$

where:

q = rate of induced infiltration from the river (bank filtrate) [m^3/d]

α = aquifer diffusivity = transmissivity/storage coefficient, for unconfined conditions it can be calculated with K = hydraulic conductivity [m/d] according to KD/n_e [m^2/d]

t = time of pumping [d]

$erfc$ = complementary error function

q/Q = the proportion of water derived from the stream for transient pumping conditions.

As t increases to values where steady-state conditions can be assumed (approx. one year in the test cases), the solution approaches one (equal to 100% bank filtrate). Therefore, eq. 19.2 overestimates the share of bank filtrate because the influence of the stream (fully penetrating) is overestimated. As discussed above the critical parameters travel times and share of bank filtrate were worst case estimations, travel time is underestimated and the share of bank filtrate is overestimated. This makes it a conservative approach since both parameters, essential for the NTS purification capacity, are assumed to be better in reality: Longer travel times will lead to longer contact time with the aquifer material and a lower share of bank filtrate in the recovery well(s) results in stronger dilution so that the overall system performance will be higher than estimated by the analytical model.

In addition to the above example, Hunt (1999) derived a solution which takes into account a situation in which a river only penetrates partially into the aquifer system, the river has a semi pervious sediment layer and the river is not necessary located at the boundary of the model. The system Hunt describes gives a non-stationary solution for a phreatic aquifer system in which a well extracts groundwater and this extraction causes inflow from the river into the groundwater (Figure 19.1). Hunt presents a solution for the drawdown of the groundwater, both in space and in time, as well as a solution for the discharges from the river into the groundwater. The equations he provides for these two solutions are given in eq. 19.3 (drawdown $\omega\,(x,y,t)$ [m]) and eq. 19.4 (ratio between the infiltration and the extraction rate $\Delta Q/Q_w$):

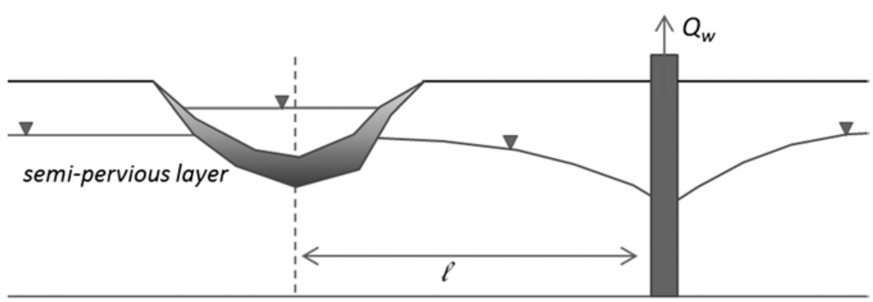


Figure 19.1 The problem considered by Hunt (1999).

$$\omega(x,y,t) = \frac{Q_w}{4\pi T}\left\{W\left[\frac{(\ell - x)^2 + y^2}{4Tt/S}\right] - \int_0^\infty e^{-\theta} W\left[\frac{(\ell + |x| + 2T\theta/\lambda)^2 + y^2}{4Tt/S}\right] d\theta\right\} \tag{19.3}$$

where:

λ = constant of proportionality between the seepage flow rate per unit distance (in the y direction) through the streambed and the difference between river and groundwater levels at $x = 0$ (location of the river) [m/d]

W = Theis well function (for example in Barry, 2000)

S = porosity [–]

T = transmissivity of the aquifer [m^2/d]

$$\frac{\Delta Q}{Q_w} = erfc\left(\sqrt{\frac{S\ell^2}{4Tt}}\right) - \exp\left(\frac{\lambda^2 t}{4ST} + \frac{\lambda\ell}{2T}\right) erfc\left(\sqrt{\frac{\lambda^2 t}{4ST}} + \sqrt{\frac{S\ell^2}{4Tt}}\right) \tag{19.4}$$

As a simplification, Hunt (1999) also assumes that the water level in the river does neither change with time as a result of runoff variations or of the infiltration into the groundwater.

19.3.2 Surface spreading methods

Surface spreading methods comprise NTSs such as infiltration ponds, soil-aquifer treatment or surface flooding. During surface spreading, the source water such as river water or surface runoff is collected and diverted to the area of recharge. Recharge takes place by percolation through the unsaturated zone to the groundwater table. In India, surface spreading is often operated without managed abstraction and the artificially recharged groundwater is consumed by the local community mostly for agricultural purposes (Gale *et al.* 2006). Important hydraulic parameters during surface spreading are the infiltration rate or the development of the groundwater mound beneath the recharge area, reducing the thickness of the unsaturated zone. Infiltration rates during surface spreading are subject to large temporal and spatial variations. This is caused by geological heterogeneities, by varying filling and extension of ponds but also by operational needs such as dry/wet cycles. The hydraulic performance of an infiltration system is therefore best expressed in long-term infiltration rates or hydraulic loading rates (Bouwer, 2002).

The Green-Ampt equation was developed to calculate the infiltration rate (V_i) from a ponded surface (e.g. infiltration basin) into a deep homogeneous porous media with uniform initial water content. The Green-Ampt model has been found to apply best to infiltration into initially dry, coarse textured media which exhibit a sharp wetting front.

The Green-Ampt solution was developed in 1911 and is based on Darcy's law:

$$V_i = K\left(\frac{H_W + L_f - h_{we}}{L_f}\right) \qquad \left(\text{Green and Ampt, 1911}\right) \tag{19.5}$$

where:

V_i = infiltration rate or hydraulic loading rate [m/s],
K = hydraulic conductivity [m/s],
H_w = depth of water in the pond or infiltration facility [m]
L_f = depth of the wetting front below the bottom of the pond [m]
h_{we} = suction or negative pressure head at the wetting front [m]. Approximately equal to the air entry pressure or bubbling pressure

Unsaturated K values are lower than saturated K (K_{sat}) values, because of the entrapped air. Bouwer (1978) refers to K/K_{sat} ratios of 0.5 for sandy soils and 0.25 for clays. Values of h_{we} describe the suction at the wetting front (negative pressure head). Typical values of h_{we} along with other important hydraulic properties for various soils can be found in Table 19.2.

Table 19.2 Hydraulic properties for various soils (modified after Rawls *et al.,* 1983).

Texture	Effective Porosity n_e [–]	Suction Head h_{we} [cm]	Hydraulic Conductivity K [cm/hr]
Sand	0.417	–4.95	11.78
Loamy Sand	0.401	–6.13	2.99
Sandy Loam	0.412	–11.01	1.09
Loam	0.434	–8.89	0.34
Silt Loam	0.486	–16.68	0.65
Sandy Clay Loam	0.330	–21.85	0.15
Clay Loam	0.309	–20.88	0.10
Silty Clay Loam	0.432	–27.30	0.10
Sandy Clay	0.321	–23.90	0.06
Silty Clay	0.423	–29.22	0.05
Clay	0.385	–31.63	0.03

Operators of infiltration ponds may also be interested in the height of groundwater mound which is created by a MAR facility. A minimum thickness of the unsaturated zone may be important to ensure a sufficient degree of natural treatment with respect to required water quality standards (Figure 19.2).

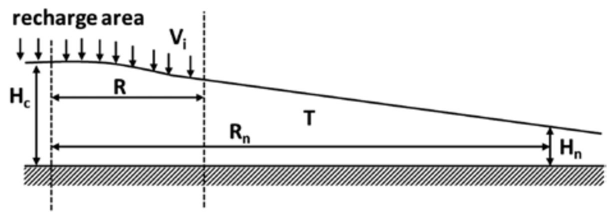


Figure 19.2 Cross sectional view illustrating geometry and parameters used for calculation of groundwater mound (Bouwer, 2002).

Bouwer *et al.* (1999) developed an analytical solution for round or square recharge ponds, where the groundwater flows radially away from the point of recharge. The ultimate or steady-state height of the groundwater mound right below of the centre of the recharge pond is calculated according to:

$$H_c - H_n = \frac{V_i R^2}{4T}\left(1 + 2\ln\frac{R_n}{R}\right) \quad \left(\text{Bouwer } et\ al.,\ 1999\right) \tag{19.6}$$

where:
R = radius or equivalent radius of the recharge area [m]
R_n = distance from the centre of the infiltration pond to the control area [m]
H_c = height of groundwater mound in the centre of recharge area [m]
H_n = height of water table in control area [m]
V_i = average infiltration rate (total recharge divided by total area) [m/s]
T = transmissivity of the aquifer [m²/s]

Control area is here defined as the area where the groundwater table is stable. The value of transmissivity in eq. 19.6 must reflect the average transmissivity of the aquifer at the steady-state stage of the mound.

In numerical groundwater models, infiltration rates or exchange fluxes (q) between the ground- and surface water are usually calculated by introducing a transfer or leakage coefficient ϕ_h [1/d]:

$$q = \phi_h (h_{\text{ref}} - h_{gw}) \tag{19.7}$$

in which:
q = Darcy flux [md^{-1}] of fluid (positive from river to groundwater) and
h_{ref}, h_{gw} = heads [m] in the river and groundwater respectively.

Assuming a simple surface spreading infiltration system represented by an initially fully rectangular canal with no other in- or outflow than the fluxes to or from the connected groundwater, the conservation of mass equation for such a unit can be written as follows:

$$\frac{\delta h_{\text{ref}}}{\delta t} = -\frac{Q_o}{A_r} \tag{19.8}$$

In which t [d] represents time and A_r represents the cross section area of the canal [m²].

It is assumed that the groundwater is initially way below the bottom of the canal and even after the canal has been drained completely, the groundwater still has no direct contact to the surface water. Substituting eq. 19.7 in eq. 19.8, taking into account that the width of the canal (B_r [m]) is water level independent, infiltration takes place along the complete wetted perimeter of the canal (bottom and lateral infiltration) and the lowest value of h_{gw} is limited to the bottom of the canal (constraining the infiltration), the time T_e [d] which is needed to empty the canal from a water depth wd_r1 to a depth wd_r2 can be calculated by:

$$T_e = -\left[\frac{B_r(\ln(wd_r) - \ln(B_r\phi_h + 2\phi_h wd_r))}{B_r\phi_h}\right]_{wd_{r1}}^{wd_{r2}} \tag{19.9}$$

For a canal with a triangular shape and a constant slope of the banks $1/\eta$ [–], the solution of T_e can be expressed in a slightly more convenient way:

$$T_e = -\left[\frac{\eta}{\phi_h \sqrt{\left(1+\eta^2\right)}} \ln(wd_r) \right]_{wd_{r1}}^{wd_{r2}} \tag{19.10}$$

As these equations also describe non stationary infiltration processes with varying water levels in the infiltration unit, they can be used to verify the results of numerical groundwater models simulating infiltration processes related to surface-spreading MAR structures.

19.4 USE OF NUMERICAL MODELS FOR NATURAL TREATMENT SYSTEMS

In contrast to analytical solutions, numerical models can be adapted to a wide range of site-specific conditions and problem statements. A large number of numerical models have been used to analyse various MAR systems ranging from basic hydraulic problems (Neumann *et al.* 2004) to complex temperature-dependant redox zonation and associated contaminant removal (Henzler *et al.* 2014; Greskowiak *et al.* 2006). Most numerical models, no matter if based on finite elements or finite differences, are generally capable to simulate three-dimensional advective, diffusive and dispersive flow and solute transport. In the following, we provide a brief description of commonly used codes:

MODFLOW (Harbaugh, 2005) is a modular, finite-difference flow model developed since the 1980's. The code is public domain free software, but there are several commercial and non-commercial graphical user interfaces available. MODFLOW can be combined with several packages to simulate fate and transport (MT3DMS, Zheng & Wang, 1999 and PHT3D, Prommer, 2006), density driven flow (SEAWAT, Langevin *et al.* 2007). It also provides modules for parameter estimation and uncertainty analysis (e.g. PEST, Welter *et al.* 2012). With this set of packages MODFLOW is a very powerful, robust and flexible modelling tool.

FEFLOW (Diersch, 2014) provides an advanced 3D graphically based modelling environment for performing complex groundwater flow, contaminant transport, and heat transport modelling. Regarding contaminant transport, multiple species as well as kinetic reactions between the species can be modelled. Both saturated and unsaturated flow regimes can be described. It uses a Galerkin-based finite element numerical analysis approach with a selection of different numerical solvers and tools for controlling and optimizing the solution process. FEFLOW is a completely integrated system from simulation engine to graphical user interface including a public programming interface for user code. By this interface, also integrated surface water–groundwater interactions can be modelled, for example using the plug-in IfmMIKE11. This module couples FEFLOW to the surface water modelling engine MIKE11 (DHI, 2014a). Its scope of application ranges from simple local-scale to complex large-scale simulations. Special features like biodegradation, density dependent flow and random walk analyses enable the use of FEFLOW also in very specific cases. With FEPEST FEFLOW offers a powerful tool for auto calibration and parameter uncertainty analyses.

MARTHE v7.0 is a complete numerical hydrosystem code designed for hydrodynamic and hydrodispersive modelling of groundwater flow and mass and energy transfer in porous media (Thiéry, 1990, 1993, 1995, 2010a). This code allows the three-dimensional simulation of flow and transport under saturated conditions and in the vadose zone (Herbst *et al.* 2005) using a finite volume method for hydraulic calculations (Thiéry, 2010b) and integrates a hydroclimatic balance (precipitation, evapotranspiration, runoff, infiltration, recharge) using the GARDENIA scheme (Thiéry, 2010c) as well as density driven flow. Full interaction between a surface water network and groundwater is implemented in MARTHE v7.0 and has been applied to river basins to predict the influence of climatological changes on river flows and to predict floods (Thiéry and Amraoui, 2001; Habets *et al.* 2010; Thiéry, 2010d). Reactive transport (flow and solute transport coupled to geochemistry) uses the REACT solver from Berkeley LBNL TOUGHREACT code (Xu *et al.* 2011). Coupling with the thermokinetic PHREEQC code for reactive transport modelling is currently being implemented. Furthermore, MARTHE was applied in the context of MAR systems (Gaus *et al.* 2007; Kloppmann *et al.* 2012). However in the release of MARTHE used for earlier studies, all surface water bodies are connected to the river network allowed to flow out of the system, but surface water cannot be stored in topographic depressions and re-infiltrate to the aquifer. For this reason, a specific module (LAC), allowing for a complete water balance (rainfall, evapotranspiration, infiltration, storage, water level changes and lateral extension) of MAR structures has been implemented and tested on the Saph Pani project study site of Maheshwaram watershed (Picot-Colbeaux *et al.* 2013).

MIKE SHE (DHI, 2014b) is a fully distributed, process-based hydrological model and includes process models for evapotranspiration, overland flow, unsaturated flow, groundwater flow, and channel flow and their interactions including solute transport. Each of this process is described by its governing equation or by a simpler conceptual representation and a user can tailor the model structure by choosing processes to be included and the solving methods. MIKE SHE is a comprehensive catchment modelling framework with applications ranging from aquifer management and remediation to wetland management, flooding and flood forecasting. MIKE SHE is dynamically coupled to MIKE11, which is a one-dimensional surface water model that simulates fully dynamic channel flows and is therefore able to represent river processes and river management. The process-based approach allows different model structures to be applied within the same modelling framework. In MIKE SHE, governing partial differential equations are solved by discrete numerical approximations in space and time using finite differences.

19.4.1 Calculating mixing proportions by water balance modelling

Water balance modelling or water budget calculation is the easiest procedure to analyse e.g. shares between the different recharge components. Typical problem statements in MAR systems comprise characterisation of sources of water which is abstracted in a well. By specifying sub-regions in the model domain (i.e. boundary conditions), the flow between each of the adjacent zones is calculated. This method may be applied in two- or three-dimensions using any groundwater flow model that includes water balance calculations (for example MODFLOW, MARTHE or FEFLOW). In case of more complex flow patterns, e.g. multiple wells and transient boundary conditions, it may be necessary to assess the water budget by more demanding particle tracking or solute transport approaches.

19.4.2 Calculating mixing proportions and travel times by particle tracking

Particle tracking is used to trace flow lines by simulating the movement of imaginary particles in a given flow field. When advective transport is the dominant process controlling solute mobility, particle tracking in groundwater flow models can be an alternative to more demanding solute transport models. Particle-tracking using model packages such as MODPATH (Pollock, 1994) or FEFLOW (DHI-WASY, 2013) provide a tool to calculate e.g. travel time of water between two points. In MAR and RBF systems, particle tracking was used e.g. by Abdel-Fattah *et al.* (2008) to investigate travel time of bank filtrate, riverbed infiltration zone length and well capture zone. During particle tracking, it is assumed that solute movement is controlled entirely by advection and that density-dependent flow, dispersion and diffusion are negligible. Random-Walk Particle Tracks, however, incorporate diffusion and dispersion, bringing field-line analysis a large step closer to the capabilities of a full advection-dispersion solution. As this option does not require the setup of a complete transport problem, pre- processing effort and computational cost remain comparably low. Random-Walk particle tracking is available in FEFLOW (DHI-WASY, 2013) and MARTHE (Thiéry, 2010a). Flow models can be transient or steady state and particle tracking can be calculated forward or backward in time.

Important performance parameters of MAR systems such as the share of bank filtrate in the abstraction well can be approximated by backward modelling of particles released around a well screen. The angle between the uppermost and lowermost streamline gives an approximation of the share of bank filtrate in the abstraction well (Chen, 2001). River water between these two lines flows to the abstraction well, while the water outside of these two lines does not flow to the well. The angle is then measured by visual inspection close to the well screen and compared to a complete full circle. This method will give only a rough approximation for simple models (e.g. single layer models). It has to be taken into account that in heterogeneous, multi-layer models, particles for each layer must be weighted according to the layer specific flow. This leads to laborious calculations and other methods may apply better. Travel times of bank filtrate to the abstraction well can be approximated by e.g. end point calculations in MODPATH. Travel time of particles from the abstraction well to their point of termination is calculated backward in time. Termination points are model boundaries e.g. the river.

19.4.3 Calculating mixing proportions and travel times by solute transport

In transient models, conservative solute transport can be used to approximate travel times and mixing proportions in MAR systems. Among other transport options, conservative transport can be simulated with MT3DMS (Zheng & Wang, 1999) and MARTHE (Thiéry, 1990, 1993, 1995, 2010a). In FEFLOW, a new feature called "Groundwater Age" offers a method to calculate groundwater ages, mean lifetime expectancies and mean exit probabilities also for non-conservative transient transport processes involving 1st order decay and linear retardation processes (DHI-WASY, 2013). By this, valuable information to estimate risk vulnerabilities or evaluate outlet capture zones and the origin of water, also under density dependent dominated conditions, can be provided. In MARTHE, transport in the aquifer considers advective, diffusive and dispersive components as well as exponential decrease for a given compound, chain degradation, a retardation factor or partition coefficient (Kd for adsorption-desorption), double porosity (equilibrium or with kinetics), Freundlich and Langmuir isotherms.

In MAR systems the point of recharge (e.g. the river or lake during bank filtration, infiltration pond or injection well) is assigned to species concentration C_0 of 1, while the rest of the model domain is assigned to species concentration of 0. The resulting breakthrough curve for continuous injection is shown schematically in Figure 19.3.

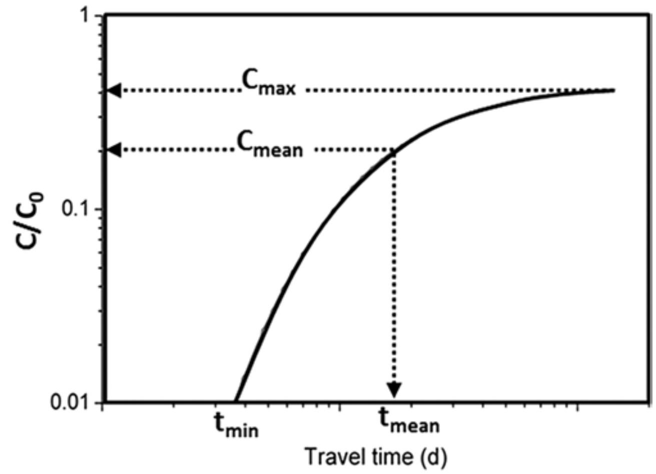


Figure 19.3 Log-log scale of an exemplary breakthrough curve of an ideal tracer and calculation of mean, minimum travel time and bank filtrate share in the abstraction well.

The proportion or share of bank filtrate in the abstraction well water is defined as the maximum concentration (C_{max}) during late, quasi steady-state conditions. The mean travel time (or dominant travel time) of e.g. bank filtrate to the abstraction well can be calculated by differentiating the cumulative breakthrough curve and retrieving the time at which its mean value is reached. Minimum travel time can, for example, be defined when one percent ($C/C_0 = 0.01$) of the maximum concentration is reached.

19.5 COMPARISON OF ANALYTICAL AND NUMERICAL SOLUTIONS

19.5.1 Bank filtration

Model descriptions

The BF model domain and associated boundary conditions are illustrated in Figure 19.4.

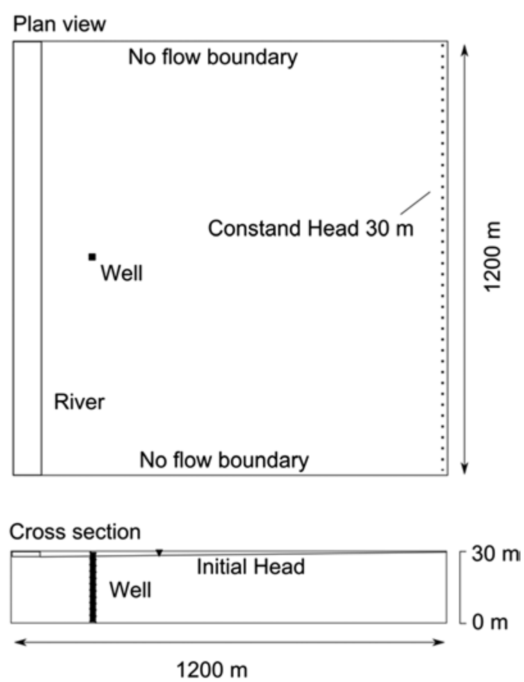


Figure 19.4 Model domain and boundary conditions for the bank filtration scenarios.

The cell size in the model domain is 20×20 m without any grid refinement. The abstraction well is fully penetrating. River stage is kept constant 1 m below the constant head boundary and vertical hydraulic conductivity is 1/10 of horizontal hydraulic conductivity. Two exemplary model scenarios have been used to compare analytical and numerical solutions for BF systems. Differences in the two BF scenarios are shown in Table 19.3. These scenarios represent two arbitrary, basic and simple capture zone characteristics, which can be approximated by using the presented analytical solutions. It was not intended to analyse the differences between the two scenarios in this study.

Table 19.3 Differences in model parameter between scenarios.

Parameter	Scenario 1	Scenario 2
Hydraulic conductivity [m/s]	1×10^{-4}	1×10^{-3}
Effective porosity [−]	0.15	0.25
Pumping rate [m^3/d]	1000	2000
Riverbed conductance [m^2/s]	0.04	0.4
Distance of pumping well from riverbank [m]	60, 80, 100	60, 80, 100

In FEFLOW, the riverbed conductance is applied as transfer rates T_{in} and T_{out}, which are calculated as follows:

$T_{in} = T_{out}$ = Riverbed conductance [m^2/s]/Element area [m^2] = 0.04/20 = 2×10^{-4} [1/s]

In each of the scenarios, the riverbed conductance was adjusted to the hydraulic conductivity of the aquifer in order to ignore any riverbed clogging effects. The river is represented in MODFLOW as well as in FEFLOW by a head-dependent flux boundary. This head is kept constant during all model scenarios. Water is flowing from the river to the groundwater when the head in the nearby cell is lower than the river stage. The flux between river and aquifer (q_{riv}) is calculated with riverbed conductance (C_{riv}) and the head difference between the river stage and the adjacent groundwater head (Δh):

$$q_{riv} = C_{riv} \times \Delta h \tag{19.11}$$

Clogging of the riverbed is expressed by riverbed conductance (C_{riv}) according to:

$$C_{riv} = \frac{K \times L \times W}{M} \tag{19.12}$$

where:
C_{riv} = riverbed conductance [m^2/s]
K = hydraulic conductivity of riverbed [m/s]
L = river length [m] in cell
W = river width [m] in cell
M = thickness of clogging layer [m]

Both equations are solved individually for each model time step at each model grid cell, which is identified as a river cell. This approach enables consideration of the temporally and spatially variable extent of the interactions between the groundwater and the surface water.

The BF model scenarios were first run in steady-state mode to calculate the water budget and particle tracking. In a last step, the flow model was coupled to a MT3DMS solute transport model using a third-order total-variation-diminishing (TVD) scheme for solving the advection term in transient mode. The TVD scheme is mass conservative and does not produce excessive numerical dispersion or artificial oscillation (Zheng & Wang, 1999). In FEFLOW, the particle tracking analyses taking into account dispersion as well as diffusion was performed using classic mass transport simulations as well as the calculation of lifetime expectancies with the Groundwater Age feature.

In a second example, the shown benchmark of Hunt (1999) was simulated using a coupled FEFLOW and MIKE11 setup using the plug-in IfmMIKE11 (Monninkhoff *et al.*, 2009). The model setup is shown in Figure 19.5.

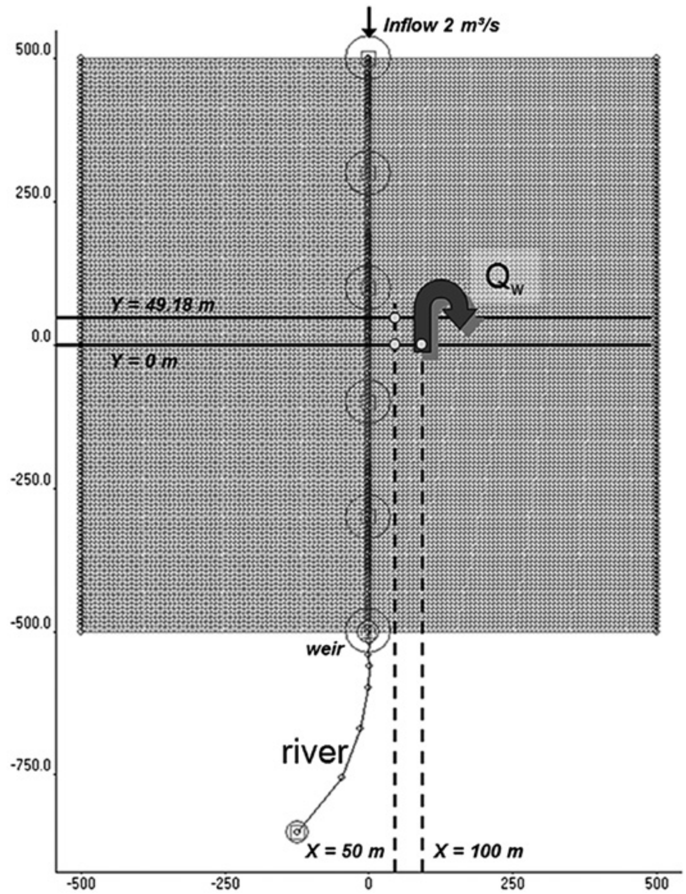


Figure 19.5 The problem considered by Hunt (1999) described by coupled groundwater and surface water system.

For this example, the MIKE11 model had to be built in a way that the river water level would not, or hardly, change as a result of the infiltration. For that purpose, a rather wide (200 m) and very smooth river bed (Manning–Strickler roughness coefficient Kst = 80 $m^{1/3}/s$) was defined. Furthermore, a constant upstream inflow rate of 2 m^3/s and a weir level of approximately 10 m at the downstream end of the coupled region ensured that the water level in the river along the FEFLOW model was infiltration rate-independent as well as constant along the river itself. MIKE SHE was verified using the Hunt benchmark as well (Illangasekare, 2001). For that verification λ in eq. 19.4 was set equal to $1*10^{-5}$ m/s. With a 200 m wide rectangular channel with a constant water depth of 2 m (the river bed was set at 8 m) an identical value for λ can be achieved using a global transfer coefficient equal ϕ_h of $42.4*10^{-4}$/d. By fixing a porosity of 0.2, a transmissivity of 0.001 m^2/s, a distance ℓ between river and well of 100 m and an extraction rate Q_w equal to 10’000 m^3/a, exactly the same conditions could be tested with IfmMIKE11.

Results

Differences of calculated minimum travel time by analytical and numerical approaches were found for the two BF scenarios (Table 19.4). These can be partly explained by the differences in the numerical approximation and discretization (MODFLOW and FEFLOW) and by the differences in conceptualization (in the numerical models the river was not fully penetrating the aquifer and a clogging effect has been taken into account by the FEFLOW model). Furthermore, it has to be noted that the calculation methods for deriving minimum travel times using particle tracking and solute transport are fundamentally different. In case of solute transport, a concentration threshold at the well determines the minimum travel time (which can be defined as $C/C_0 = 0.01$), taking into account dispersion, diffusion and mixing processes within the well capture zone. Using particle tracking, however, the minimum travel time from different starting points within the capture zone is derived. With the simple model setup at hand, the minimum travel time path always coincides with the shortest distance between the well and the river.

Table 19.4 Minimum travel time [d] calculated by different analytical and numerical approaches (longitudinal dispersivity = 5 m, transversal dispersivity = 0.5 m for solute transport).

	Well Distance from Riverbank [m]	Dillon *et al.* (2002)	Particle Tracking (Advection only)		Solute Transport (Advection + Dispersion)	
			MODFLOW	FEFLOW	MODFLOW (TDV)	FEFLOW[1]
Scenario 1	100	94	104	91	75	60
	80	60	67	57	39	43
	60	34	39	30	25	18
Scenario 2	100	79	132	109	101	91
	80	50	79	62	64	50
	60	28	43	31	29	24

[1]: Classic FEFLOW mass transport simulation; TDV = Total Variation Diminishing solution.

Despite these differences in model setup and calculation methods, the results clearly show that, compared to particle tracking results, on average the analytical solution from Dillon *et al.* (2002) produces lower travel times which confirms the conservative approach of the analytical solution, especially for scenario 2. If compared to the solute transport solutions, the analytical solution yields substantial higher travel times and underestimates dispersive effects during subsurface passage.

In Table 19.5, a comparison between FEFLOW simulations using particle tracking, the classic mass transport simulation and the Age Problem Class (Life Time Expectancy) is shown. The minimum travel time in the classic mass transport simulation is based on the explanation in Figure 19.3 and is therefore derived from the concentrations in the well. The evaluation of travel times using life time expectancies is based on mean travel times including dispersion and diffusion. From the resulting travel times, the minimum travel time between the river and the well is selected. Dispersion and diffusion in reality causes both longer and shorter travel times compared to mere advection based simulations. In this, the proportion of the longer travel times has the tendency to easily shift the mean towards older values, causing on average longer single travel times compared to pure advection based analyses (particle tracking). This also results in larger minimum travel times using the Age Problem Class. Like in the particle tracking, the minimum travel time is mostly located at the minimum distance between the riverbank and the well. The results show that according to the choice of definition of minimum travel time, significantly different results can be obtained. It is therefore important to determine which definition is most appropriate for the problem statement under consideration.

Table 19.5 Minimum travel time [d] calculated by different approaches in FEFLOW (longitudinal dispersivity = 5 m, transversal dispersivity = 0.5 m for solute transport simulations).

	Well Distance from Riverbank [m]	Minimum Travel Times [d]		
		Particle Tracking (Advection only)	Life Time Expectancy	Classic Mass Transport
Scenario 1	100	91	103	60
	80	57	68	43
	60	30	41	18
Scenario 2	100	109	120	91
	80	62	73	50
	60	31	41	24

In Figure 19.6 an exemplary result of Scenario 1 is shown with a well distance of 100 m from the riverbank, calculated with FEFLOW, taking into account advection and dispersion using the Age Problem Class (Life Time Expectancy).

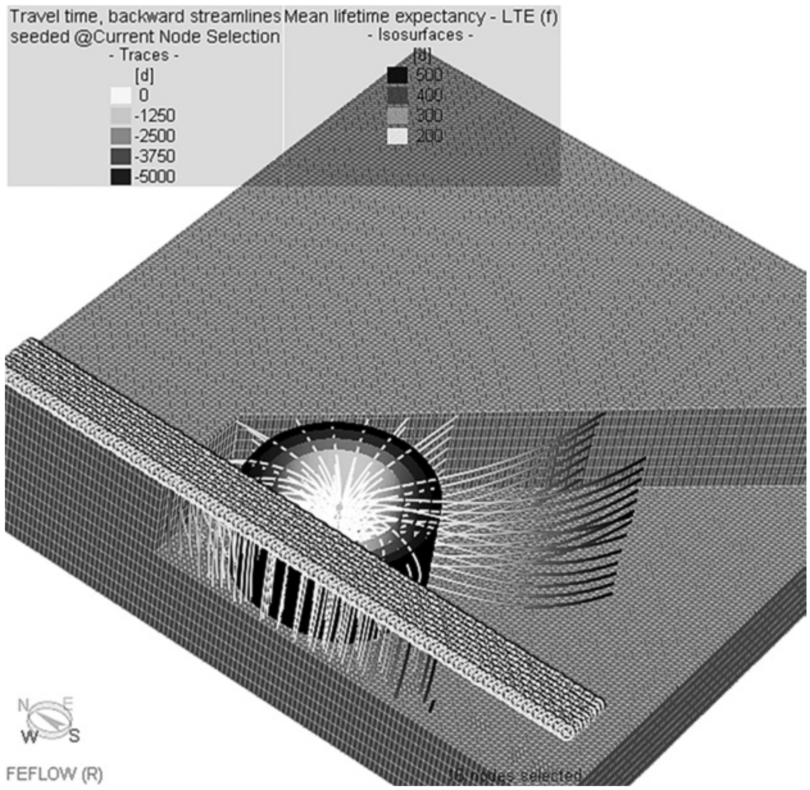


Figure 19.6 Result of a FEFLOW bank filtration simulation showing Lifetime Expectancies (advection and dispersion), Backward Streamlines (purely advection) and the river boundary nodes in slice 1. In FEFLOW, the Lifetime Expectancy (days) is defined as the time required for the water molecules to reach an outlet boundary of the aquifer.

Calculations of the share of bank filtrate in the abstraction well based on zone budget, particle tracking and solute transport come to almost identical results, whereas analytical solutions by Glover and Balmer (1954) largely overestimate the share of bank filtrate (%) compared to numerical solutions (Table 19.6).

Table 19.6 Percentage share of bank filtrate calculated by analytical and numerical (advection only) approaches.

	Well Distance from Riverbank [m]	Glover and Balmer (1954)*	Zone Budget (Water Balance)	Modflow	Feflow
Scenario 1	100	86	61	61	62
	80	86	63	63	64
	60	86	66	66	67
Scenario 2	100	94	17	17	17
	80	94	22	22	22
	60	94	27	27	28

*Calculated with t_{min} derived from eq. 19.1.

Minimum travel time and share of bank filtrate in the abstraction well can also be calculated based on breakthrough curves of conservative solute transport calculated for the abstraction well for different well distances (like shown in Figure 19.7 for the MODFLOW simulations).

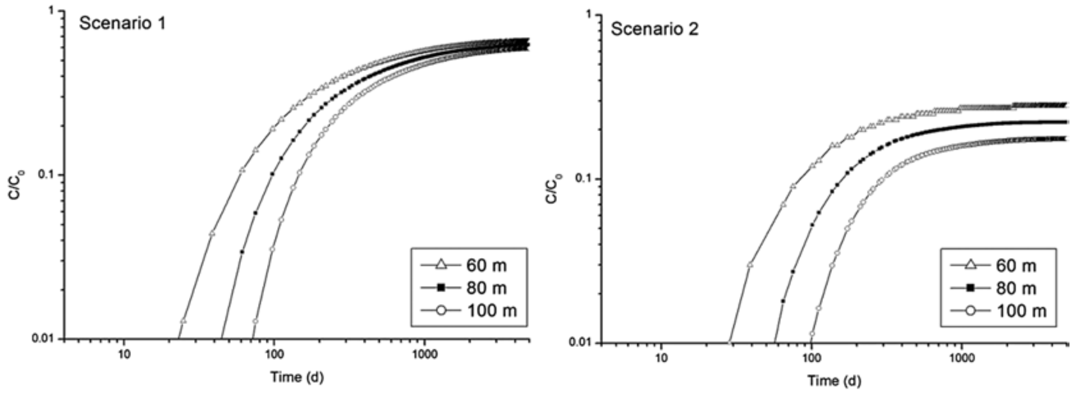


Figure 19.7 Log-log scale breakthrough curves of tracer indicating travel time (d) and share of bank filtrate (C/C_0) calculated by solute transport for 60 m, 80 m and 100 m distance of the abstraction well from the riverbank, MODFLOW simulations.

During these additional solute transport simulations, longitudinal dispersivity was kept constant with 10 m, which was approximated by one tenth of the maximum flow distance from the riverbank to the abstraction well according to (Adams & Gelhar, 1992) and transversal dispersivity was neglected.

In Figure 19.8 and Figure 19.9 the results for the benchmark of Hunt (1999) using IfmMIKE11 are shown. These figure show both the simulation results for the infiltration rate along the coupled river (Figure 19.8) as well as the drawdown along the line $y = 0$ and $y = 49.18$ m in Figure 19.5 at day 23 of the simulation (Figure 19.9). Within the figures, the analytical solutions presented by Hunt (1999) are also included. The analytical solutions and the IfmMIKE11 results are nearly identical. It is therefore concluded that these kind of MAR applications can be simulated using a coupled setup of MIKE11 and FEFLOW. The same setup has been successfully benchmarked by an OPENMI based coupling between FEFLOW and MIKE SHE (Yamagata *et al*., 2012).

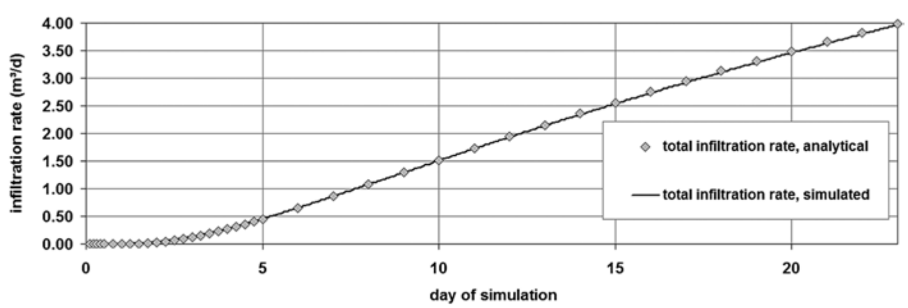


Figure 19.8 Comparison between the analytically solved and numerically simulated total infiltration rates over time along the coupled river branch using FEFLOW and MIKE11.

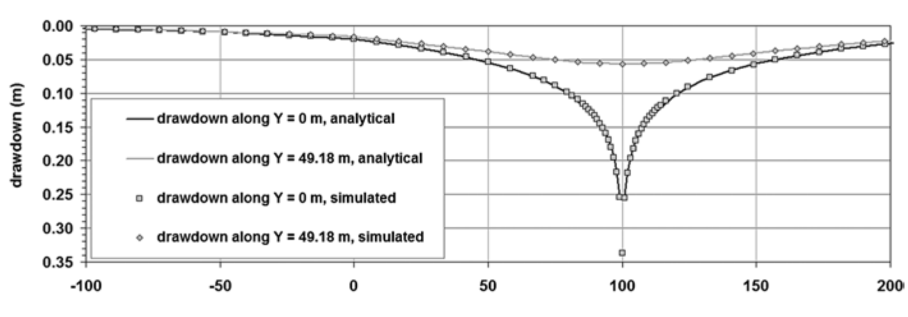


Figure 19.9 Comparison between the analytically solved and numerically simulated drawdown along $y = 0$ and $y = 49.18$ m at day 23 of the simulation using FEFLOW and MIKE11.

19.5.2 Infiltration pond

Model description

A simple model has been constructed to compare analytical and numerical solutions for infiltration ponds. The infiltration pond model domain and associated boundary conditions are illustrated in Figure 19.10.

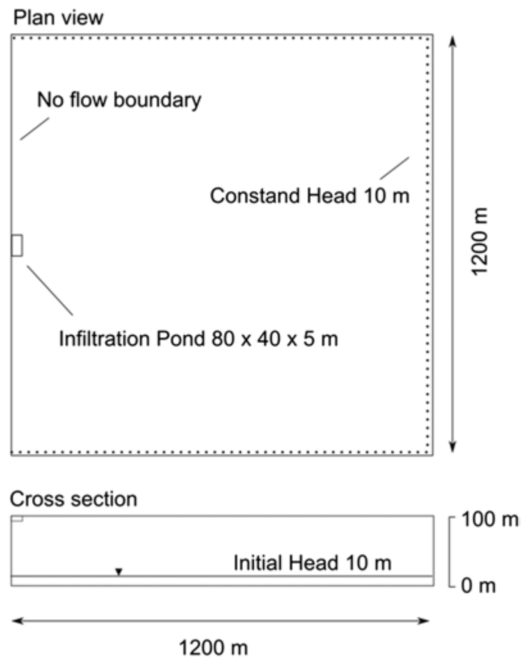


Figure 19.10 Model domain and boundary conditions for infiltration pond scenarios.

The infiltration pond is a square type with 80×80 m area, but, in order to save computational time, only half of the infiltration pond is represented by the model. The development of the groundwater mound beneath the infiltration pond was simulated using the unsaturated-zone flow package coupled to MODFLOW 2005 under steady-state conditions. Unsaturated flow is calculated based on a simplified Richard's equation (Niswonger *et al.*, 2006). In FEFLOW, the fully integrated 3D Richard's equation is used, applying a simplified Van Genuchten scheme. Model parameters used for the different pond scenarios are shown in Table 19.7.

Table 19.7 Differences in model parameter for infiltration pond scenarios.

Hydraulic Loading Rate [m/d]	Hydraulic Conductivity [m/s]	Effective Porosity [−]
1	1×10^{-4}	0.15
2	1×10^{-4}	0.15
3	1×10^{-4}	0.15
1	1×10^{-3}	0.25
2	1×10^{-3}	0.25
3	1×10^{-3}	0.25

Results

Analytical solutions from Bouwer *et al.* (1999) and numerical solutions for the development of a groundwater mound beneath a recharge pond for different hydraulic loading rates and hydraulic conductivities of the aquifer are shown in Figure 19.11.

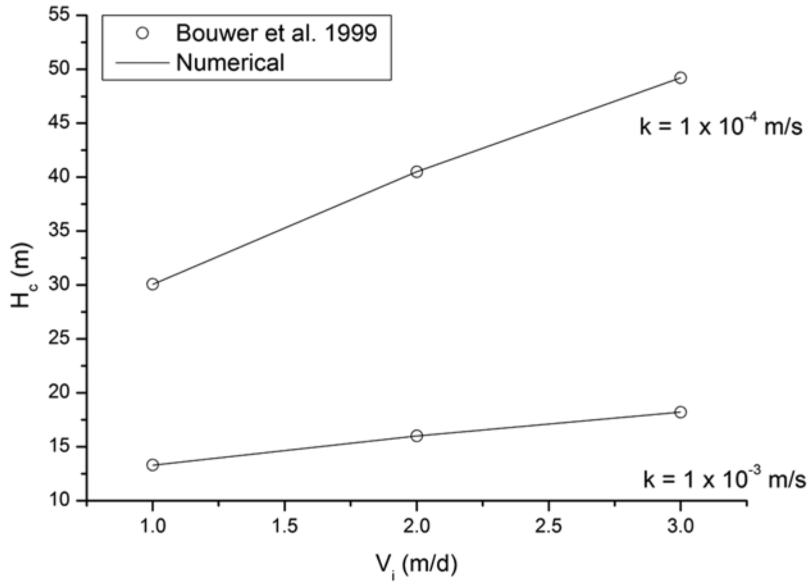
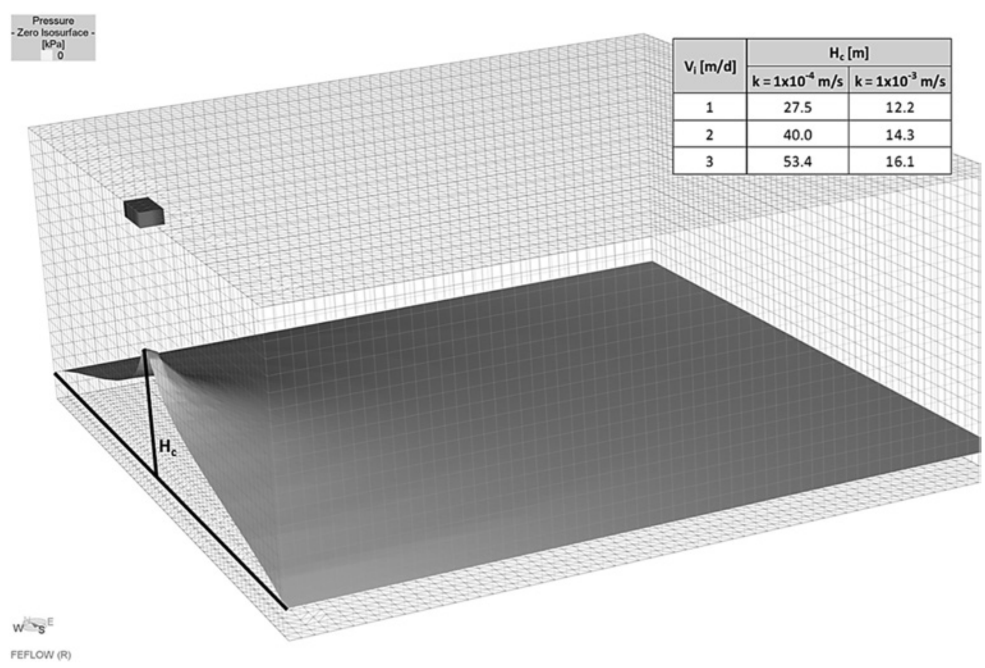


Figure 19.11 Comparison of numerical and analytical solutions of mounding height (H_c) below infiltration ponds using MODFLOW.

Calculations with MODFLOW and FEFLOW show that a sandy aquifer with $k = 1 \times 10^{-4}$ m/s and a 10 m groundwater thickness at the control area creates a mounding height of approx. 50 m ($V_i = 3$ m/d). Please note that these values are steady-state solutions and it may take years (up to 10 years) to develop equilibrium between percolation from the recharge structure and radial flow away from the recharge area. If the calculated groundwater mounding heights exceeds the thickness of the unsaturated zone (i.e. the zone below the recharge area is totally saturated), the groundwater mound must be controlled e.g. by pumping or by reducing the long-term infiltration rate. In Figure 19.12 an example of the FEFLOW setup and the simulated groundwater mounding beneath the infiltration pond is shown.



V_i [m/d]	H_c [m]	
	k = 1x10^{-4} m/s	k = 1x10^{-3} m/s
1	27.5	12.2
2	40.0	14.3
3	53.4	16.1

Figure 19.12 Results of FEFLOW simulations for different infiltration pond scenarios.

The value of transmissivity (T) in eq. 19.6 must reflect the average transmissivity of the aquifer during steady-state mound height. If T of the entire aquifer is used, eq. 19.6 underestimates the mounding height and if T only for the initially saturated thickness is used, eq. 19.6 overestimates the mound rise. Hence, the challenging part is to find a representative aquifer transmissivity. Bouwer *et al.* (1999) proposed to run pilot infiltration areas and to calculate T from that mound rise.

Eq. 19.9 and eq. 19.10, describing a transient infiltration process out of a rectangular and triangular shaped infiltration pond, have also been verified using a coupled numerical model under FEFLOW and MIKE11. The initial water depth of the river in both models is 10 m, the river width of the rectangular cross section is 25 m and the slope of the bank of the triangular cross section amounts 1:2. The transfer coefficient is equal to 0.1/d and the length of the river is 500 m. Using a maximum allowed time step of FEFLOW of 0.05 d, both the exchange discharges and the water depths of the latest version of IfmMIKE11 fit perfectly to the analytical solutions (Figure 19.13). As IfmMIKE11 is using an explicit coupling approach, also the influence of the maximum allowed time step of FEFLOW was tested. It was found that the lack of an iterative coupling causes discrepancies between the analytical and numerical solution if the FEFLOW time step exceeds a length of approximately 0.25 d.

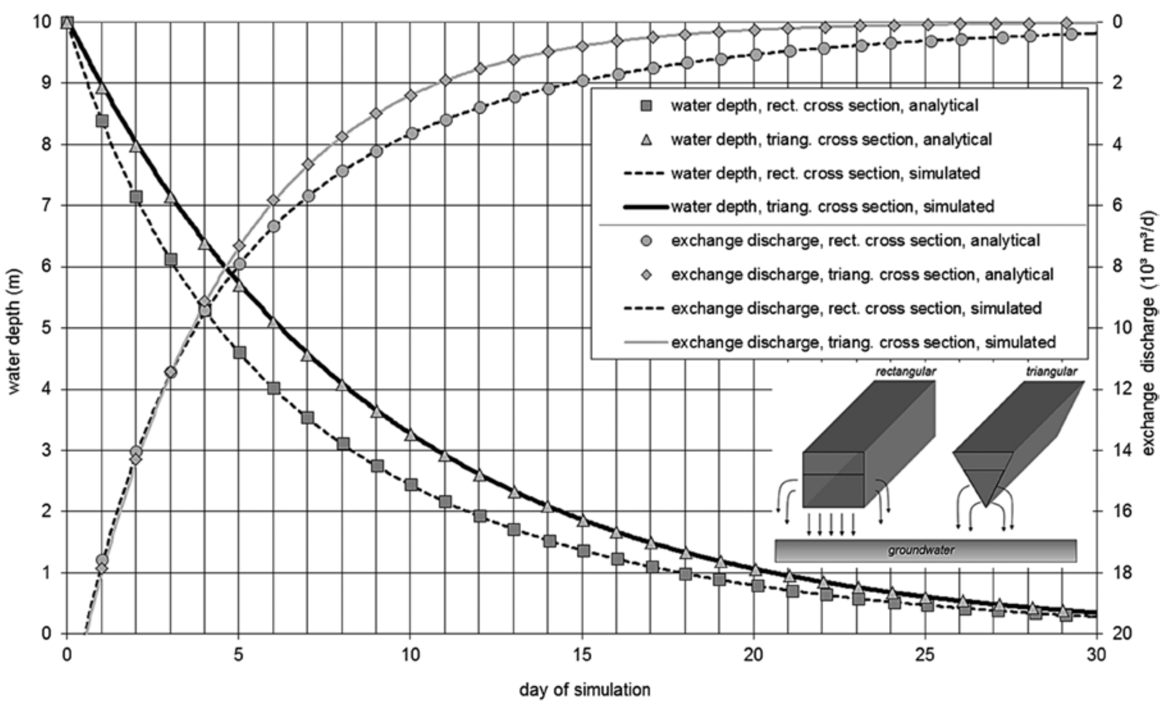


Figure 19.13 Comparison between the analytical solutions and simulated results for a rectangular as well as a triangular river cross section using a maximum FEFLOW time step of 0.05 d.

These simulations show that, besides bank filtration processes, also surface spreading MAR structures can be simulated using numerical coupled ground and surface water models. Furthermore, with the coupling of MIKE11 and FEFLOW also integrated multi-species and non-conservative mass transport processes can be described (Monninkhoff *et al.* 2011).

19.6 CONCLUSIONS

The examples presented in this Chapter show that by using numerical modelling a variety of different natural treatment techniques (MAR, RBF) can be accurately described. However, it has also been shown that particle-based, purely advective numerical calculations may yield substantial longer travel times of infiltrated source water to the abstraction well compared to solute transport. It is therefore recommended to use classical mass transport simulations to evaluate the minimum travel times, taking into account both dispersion- and diffusion-driven processes.

Besides the numerical tools presented in this Chapter, the included analytical solutions may provide a first approximation of important performance parameters of NTSs, but limitations and assumptions have to be taken into account. Integrated analyses of surface water and groundwater interactions, especially for geometrically complex MAR structures, in diverse geological environments or at a regional catchment levels, can only be performed using numerical modelling tools.

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Natural Water Treatment Systems for Safe and Sustainable Water Supply in the Indian Context

Saph Pani

Editors: Thomas Wintgens, Anders Nättorp, Lakshmanan Elango and Shyam R. Asolekar

Natural Water Treatment Systems for Safe and Sustainable Water Supply in the Indian Context is based on the work from the Saph Pani project (Hindi word meaning potable water).

The book aims to study and improve natural water treatment systems, such as River Bank Filtration (RBF), Managed Aquifer Recharge (MAR), and wetlands in India, building local and European expertise in this field. The project aims to enhance water resources and water supply, particularly in water stressed urban and peri urban areas in different parts of the Indian sub-continent. This project is co-funded by the European Union under the Seventh Framework (FP7) scheme of small or medium scale focused research projects for specific cooperation actions (SICA) dedicated to international cooperation partner countries.

Natural Water Treatment Systems for Safe and Sustainable Water Supply in the Indian Context provides:

- an introduction to the concepts of natural water treatment systems (MAR, RBF, wetlands) at national and international level
- knowledge of the basics of MAR, RBF and wetlands, methods and hydrogeological characterisation
- an insight into case studies in India and abroad.

This book is a useful resource for teaching at Post Graduate level, for research and professional reference.

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