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MARSOL WHITE BOOK ON THE STATE OF THE ART IN MANAGED AQUIFER RECHARGE MODELLING

A Literature Review

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Abstract

Of the several themes addressed in "MARSOL White Book on Managed Aquifer Recharge Modelling – Selected Results from the MARSOL Project", a synthesis of the work developed during MARSOL project, one should emphasize the literature review on MAR modelling. There was a collection of MAR models and applications both in terms of flow and transport and of hydrogeochemical modelling.

This paper aims to present a set of successful modelling applications on MAR methodologies as well as to briefly explain and summarize the capabilities of some of the software used. It can also serve as a reflection on MAR modelling throughout time as more complex models have been being developed.

Keywords: MAR, review, numerical modelling.

Theme: 9 - Investigação em hidráulica e recursos hídricos.

1. INTRODUCTION

In the context of Managed Aquifer Recharge (MAR) numerical modelling has been an important process in several applications, since the prediction of rise of groundwater mounds, to determine where groundwater can be most appropriately pumped, understand quality changes in infiltration water and aquifer water, predict the success of treatment induced by MAR methodologies or to calculate the necessary injected volumes to counter a saltwater intrusion problem. A proper estimation of AR, by means of arithmetic methods, depends firstly on the conceptual approach of the groundwater problem and secondly on the selection of the appropriate AR method (Pliakas et al. 2005), and its widely known that the Success of artificial recharge as a management technique depends highly on how well the system is understood (Sunada et al. 1983). Koukidou et al. (2010) referred numerical modeling as an invaluable tool that enables accurate and reliable assessment of alternative strategic management plans, with the results of well calibrated and verified models as a solid basis for justification of capital investment required for infrastructure that is necessary to support water resources management scenarios. It is then essential, as a state of the art overview, to compile several applications in different demo-areas and scales, where modelling was essential to refine artificial recharge strategies, to help to understand the main impacts of a MAR project or to what to expect in field experiments.

2. DEVELOPING THE LITERARURE REVIEW IN MAR MODELLING STATE OF THE ART

This brief literature review on MAR modelling aimed to understand the most commonly used software and modelling methods such as scale, boundary conditions and inputs and output representation. Data on the software used in MAR modeling exercises was collected, with the objective of create a first-approach library to these software capabilities. Later every case study found was briefly summarized as an example of the software use.

3. FLOW AND TRANSPORT MODELS USED IN MAR

The selection of these models resulted mainly from the literature review – the most used and referenced tools/software were chosen.

1. The CODE_BRIGHT program (originally developed by Olivella et al. 1995) is a tool designed to handle coupled problems in geological media (Restrepo, et al. 2016) was developed on the basis of a new general theory for saline media. Then the program has been generalized for modelling thermo-hydro-mechanical (THM) processes in a coupled way in geological media. Basically, the code couples mechanical, hydraulic and thermal problems in geological media. The theoretical approach consists in a set of governing equations, a set of constitutive laws and a special computational approach. The code is composed by several subroutines and uses GiD (Coll et al. 2016) system for preprocessing and post-processing.

2. Accordingly to Li et al. (2009) COMSOL (formerly known as FEMLAB) is a finite element analysis and solver software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. It includes a complete environment for modelling any physical phenomenon that can be described using ordinary or partial differential equations (PDEs). Coupled with Earth Science Module, the software code can handle time-dependent and stationary problems for one-dimensional (1D), 2D, and 3D systems with axisymmetric for 1D and 2D problems of fluid flow, heat transfer, and solute transport.

3. Trefry & Muffels (2007) described FEFLOW as a Finite-Element subsurface FLOW and transport modeling system with an extensive list of functionalities, including variably saturated flow, variable fluid density mass and heat transport, and multi-species reactive transport. It is a proprietary code and not freely available; it supports an array of features of interest in subsurface flow and transport. Theoretical and numerical methods and FEFLOW capabilities are well described in Diersch (2014). This software is applicable in groundwater, porous media and heat transport studies - from local to regional scale.

4. FEMWATER (Finite Element Model of Water Flow Through Saturated-Unsaturated Media) model developed initially by Athens Laboratory of the U.S. Environmental Protection Agency (AERL) and the U.S. Army Engineer Waterways Experiment Station (WES) from 3DFEMWATER (Yeh, 1987). The program structure was reformulated to allow its integration into the Department of Defense Groundwater Modeling System (GMS). FEMWATER capabilities are described by Lin et al. (1997).

5. Accordingly to Yu & Zeng (2010), HYDRUS is a software program for solving Richards equation for water flow and the advection-dispersion equation for heat and solute transport in variably saturated subsurface media. Variably saturated zones are fundamental to understanding many aspects of hydrology, including infiltration, soil moisture storage, evaporation, plant water uptake, groundwater recharge, runoff, and erosion. It uses the finite-element (FE) method to simulate one-, two- or three-dimensional movement of water, heat, and multiple solutes in unsaturated, partially saturated, or fully saturated porous media.

6. MOCDENSE is a two-constituent solute transport model for ground water having variable density developed by Sanford & Konikow (1985). The model couples the ground-water flow equation with the solute-transport equation. The digital computer program uses an iterative strongly-implicit procedure to solve a finite-difference approximation to the ground-water flow equation. The model uses the method of characteristics to solve the solute-transport equation. This incorporates a particle-tracking procedure to represent advective transport and a two-step explicit finite-difference procedure to solve equations that describe the effects of hydrodynamic dispersion and fluid sources. This explicit procedure has several stability criteria associated with it, but the consequent time-step limitations are automatically determined by the program. It is applicable to two-dimensional, cross-sectional problems involving ground water with constant or variable density. The model computes changes in concentration over time caused by the processes of advective transport, hydrodynamic dispersion, mixing or dilution from fluid sources. The concentrations of two independent solutes can be modeled simultaneously. Temperature is assumed to be constant, but fluid density and viscosity are assumed to be a

linear function of the first specified solute. If a second solute is specified, it is assumed to be of a trace amount such that it does not affect the fluid density or viscosity. The aquifer may be heterogeneous and anisotropic. The model has been used mostly in studies of either saltwater intrusion or dense contaminant plumes.

7. The acronym to Transport Of Unsaturated Groundwater and Heat (TOUGH), is a set of multidimensional numerical models for simulating the coupled transport of water, vapor, noncondensible gas, and heat in porous and fractured media (Pruess, 1987). Initially developed primarily for geothermal reservoir engineering, the suite of simulators is widely used for applications to nuclear waste disposal, environmental remediation problems, energy production from geothermal, oil and gas reservoirs as well as gas hydrate deposits, geological carbon sequestration, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, geochemical, and mechanical processes in permeable media.

8. MODFLOW and related programs – MODFLOW is a 3D finite-difference groundwater model that was first published in 1984 (McDonald & Harbaugh, 1984). It has a modular structure that allows it to be easily modified to adapt the code for a particular application. Many new capabilities have been added to the original model. MODFLOW-2005 (Harbaugh, 2005) is the most current release of MODFLOW. In this version groundwater flow is simulated using a block-centered finite-difference approach. Layers can be simulated as confined or unconfined. The modular structure consists of a main program and a series of highly independent subroutines. The subroutines are grouped into packages. Each package deals with a specific feature of the hydrologic system that is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving the set of simultaneous equations resulting from the finite-difference method.

MODPATH, originally published by Pollock (1989) is a particle-tracking post-processing program designed to work with MODFLOW, where the flow data produced in the budget is used by MODPATH to construct the groundwater velocity distribution that forms the basis for particle-tracking calculations. MODPATH Version 7 (Pollock, 2016) is the most recent version of the program.

MT3D-USGS (Bedekar et al. 2016) is a USGS updated release of the groundwater solute transport code MT3DMS (Zheng et al. 2001). MT3D-USGS includes new transport modeling capabilities to accommodate flow terms calculated by MODFLOW packages aiming to provide greater flexibility in the simulation of solute transport and reactive solute transport. Unsaturated-zone transport and transport within streams and lakes, including solute exchange with connected groundwater, are among the program capabilities. MT3DMS can be used to simulate changes in concentrations of miscible contaminants in groundwater considering advection, dispersion, diffusion and some basic chemical reactions, with various types of boundary conditions and external sources or sinks.

The SEAWAT program (Langevin et al. 2008) is a coupled version of MODFLOW and MT3DMS designed to simulate three-dimensional, variable-density, saturated groundwater flow. Accordingly to Guo & Langevin (2002) was developed to simulate three-dimensional, variable density, transient ground-water flow in porous media. The source code for SEAWAT was developed by combining MODFLOW and MT3DMS into a single program that solves the coupled flow and solute-transport equations. The SEAWAT code follows a modular structure, and thus, new capabilities can be added with only minor modifications to the main program. SEAWAT reads and writes standard MODFLOW and MT3DMS data sets.

9. MODRET (Computer MODEL to Design RETENTION Ponds) was originally developed in 1990 as a complement to a research and development project for Southwest Florida Water Management District (Jammal & Associates Division, 1993). The MODFLOW model was specifically modified for use with the MODRET model which incorporates modeling of weir and orifice overflow or overflow based on manually-specified elevation vs. flow relationship (rating curve). The scope of this project was to develop a practical design manual for site investigation criteria, laboratory and field testing requirements and guidelines to calculate infiltration losses from stormwater retention ponds in unconfined shallow aquifers.

4. FLOW AND TRANSPORT CASE STUDIES

A brief summary of MAR modelling applications and examples is chronologically presented.

Stefanescu & Dessargues (1998) studied the possibility of increasing the proportion of groundwater usage by increasing storage in shallow aquifer by artificial recharge methods due to scarcity problems encountered during summer and long periods of intense freezing in Bucharest water supply which was highly dependent on surface water. A regional scale 3D numerical model was assembled in MODFLOW, limited by the two main rivers in the region (Arges and Dambovita). MODPATH was used to calculate transport path and travel times.

Chatdarong (2001) aimed to study the recharge behavior in San Joaquin Valley agricultural area as well as the economic feasibility and practicality of artificial recharge facilities in the conjunctive use for irrigation purposes. HYDRUS-2D was used in the simulations if a two-dimensional model based on the study area infiltration ditch.

Woolfenden & Koczot (2001) conducted a study to evaluate the hydraulic effects of artificial recharge, started in 1994, of imported water from Sierra Nevada in Rialto-Colton Basin (San Bernardino County, California). The main objectives were to describe geohydrology and water chemistry, and determine the movement and ultimate disposition of artificial recharged water simulating long-term effects on water levels likely to occur in two different AR scenarios: (1) continued recharge in ponds, (2) discontinued recharge in ponds. MODFLOW finite-difference model was used to simulate flow and MODPATH through particle tracking allowed for the understanding of water movement.

Haimerl (2002) evaluated the effectiveness of groundwater recharge dams by assembling a 2D numerical model using HYDRUS. These structures, built in Wadi Ahin in the north of Oman, were used to store the water on the surface and enable a controlled release for artificial recharge in terms of managed recharge.

Numerical modelling was used to simulate and understand the role of the unsaturated zone directly beneath an unused artificial recharge site in the Cherry Valley alluvial fans, located in

San Gregorio Pass, California (USA) (Flint, 2003). The numerical model was developed in TOUGH2 finite-difference code.

De la Orden et al. (2003) used numerical modelling as a tool to evaluate the effects in groundwater of artificial recharge applied for a period of 10 years in Vergel, Alicante (Spain). The Plana de Gandía-Denia coastal aquifer model was developed using MODFLOW in PMWIN software (Chiang and Kinzelbach, 1998).

In the development and verification of a groundwater artificial recharge system in Xanthi plain, Thrace (Greece) where the main objective is the reactivation of an old stream bed of Kosynthos River, Pliakas et al. (2005) built a finite-difference MODFLOW numerical model as a tool to estimate impact of AR. It was considered by the authors as a significant tool for rational management of groundwater resources in the study area.

Santo Silva et al (2006) applied numerical modeling for studying the applicability of artificial recharge methods in Recife plain (Brazil) to decrease the drawdown observed in Cabo aquifer due to over-exploitation and increasing urban areas, using rainwater injection in wells. A 2D vertical grid aquifer scale model was developed using CODE-BRIGHT coupled with GiD software.

GABARDINE project, which aimed to demonstrate suitability of alternative sources of water in groundwater artificial recharge by developing advanced integrated technologies and management, showed some examples of numerical modelling applied do MAR. Lobo Ferreira et al (2006) compiles the description of numerical models for three different demo-areas in the project. One of the demo-areas was Campina de Faro aquifer system (Portugal), where a finite difference MODFLOW model was developed using Visual MODFLOW software to study the optimization of groundwater rehabilitation through artificial recharge aiming the minimization of diffuse pollution effects caused by typical Portuguese agricultural practices, by promoting artificial in a riverbed.

In Goyal et al. (2009) a finite-element groundwater flow model, using HYDRUS-2D, was used to simulate draw-up and drawdown of piezometric pressure heads in the aquifer storage recovery cycles of varying buffer storage volumes and residence times in a highly brackish, semi-confined aquifer under shallow water-table condition in Hisan region (India).

Lobo Ferreira et al. (2009) used numerical modelling to understand effect of artificial recharge methodologies concerning the use of infiltration basins located in Cap Bon (Tunisia) as a way to increase groundwater quality, the effect of saltwater intrusion and increase water availability for agriculture. The numerical model was assembled in Groundwater Modelling System (GMS) software using FEMWATER.

Koukidou et al. (2010) aimed to characterize the regional groundwater flow system in the Tirnavos alluvial basin and to develop and apply appropriate models for assessing artificial recharge as a way to restore and manage regional groundwater resources in eastern Thessaly (Greece). Simulation of the aquifer system was performed on FEFLOW software and was used for the feasibility assessment of alternative groundwater management strategies based on Aquifer Storage Recovery (ASR).

Carleton (2010) presented numerical modelling tools to provide quantitative methods for estimating the height of groundwater mounds beneath infiltration basins. MODFLOW-2000 was used to simulate the height and extent of groundwater mounds with various aquifer characteristics, recharge conditions, and basin areas, depths, and shapes.

Kareem (2012) used MODFLOW in Groundwater Modeling System (GMS) software to simulate the water conveyance from rainwater collecting ponds to underground reservoirs by well injection in Jolak basin, Karkuk (Iraq).

A three-dimensional MAR model of the Isfara Aquifer, Fergana Valley (Uzbequistan) was developed by Karimov et al. (2013) using Visual MODFLOW software.. The main objective was to evaluate the viability of MAR activities, initiated in Isfara River Basin located in the tail end of the Big Fergana Canal (BFC).

5. HYDROGEOCHEMICAL MODELS USED IN MAR

Accordingly to Barber (2002) field-scale reactions between mixing aqueous phases, minerals, organic carbon and ion exchange phases can be assessed relatively simply using equilibrium mixing-cells which can be used to provide a wide range of assessment of redox and pH-dependent reactions that could impact on the efficiency of an AR system. These assessments could also be used to provide quantitative evaluation of monitoring data of artificial recharge schemes. For the same author, in AR/ASR hydrogeochemical modelling is relevant concerning mineral dissolution that locally can increase hydraulic conductive but have an adverse impact in aquifer structural integrity or mineral precipitation that has the opposite effect contributing to clogging.

1. Accordingly to Dijkhuis & Stuyfzand (1996) and Stuyfzand (1998) INFOMI is the acronym for 'INFiltration Of MIcropollutants'. It is a finite element 1D-model using the 'mixing cells in series' concept, incorporating a highly variable input for the pollutants in surface water; in the infiltration basin,in a specific river segment, at the water/sediment interface and in the saturated zone. Advection and dispersion (+diffusion) in the aquifer system are modelled using algorithms of Appelo & Postma (1993).

2. Accordingly to Jacques and Simunek (2005), HP1 was obtained by coupling the HYDRUS-1D one-dimensional variably-saturated water flow and solute transport model with the PHREEQC geochemical code. The HP1 code incorporates modules simulating (1) transient water flow in variably-saturated media, (2) transport of multiple components, and (3) mixed equilibrium/kinetic geochemical reactions.

3. Commercial software HYDROGEOCHEM is a coupled model of hydrologic transport and geochemical reaction in saturated-unsaturated media. It is designed to simulate transient and/or steady-state transport of aqueous components and transient and/or steady-state mass balance of adsorbent components and ion-exchange sites.

4. Parkhurst and Appelo (2013) describe PHREEQC is a computer program that is designed to perform a wide variety of aqueous geochemical calculations simulating chemical reactions

and transport processes in natural or polluted water, in laboratory experiments, or in industrial processes. The program is based on equilibrium chemistry of aqueous solutions interacting with minerals, gases, solid solutions, exchangers, and sorption surfaces, which accounts for the original acronym—pH-REdox-EQuilibrium, but the program has evolved to include the capability to model kinetic reactions and 1D (one-dimensional) transport. Rate equations are completely user-specifiable in the form of basic statements. Kinetic and equilibrium reactants can be interconnected, for example, by linking the number of surface sites to the amount of a kinetic reactant that is consumed (or produced) in a model period. A 1D transport algorithm simulates dispersion and diffusion; solute movement in dual porosity media; and multicomponent diffusion, where species have individual, temperature-dependent diffusion coefficients, but ion fluxes are modified to maintain charge balance during transport. An inverse modeling capability allows identification of reactions that account for observed water compositions along a flowline or in the time course of an experiment.

6. HYDROGEOCHEMICAL CASE STUDIES

A brief summary of hydrogeochemical applications in MAR is chronologically presented.

Whitworth (1995) modelled recharge via subsurface injection in El Paso, New Mexico (USA) with PHREEQE (Parkhurst et al. 1980), by first simulating the mixing of the injected water and the ground water to see if mineral precipitation might occur. Parkhurst & Petkewich (2002) used PHREEQC for geochemical modelling of an ASR experiment in Charleston, South Carolina (USA). The purpose of the aquifer storage operation is to store potable drinking water in a sand and limestone aquifer underlying the city of Charleston. Barber (2002) presented a case study where a Soil Aquifer Treatment experiment in China was modelled using PHREEQC to assess possible chemical reactions on mixing of groundwater and injectant (potable water from a reservoir) and to understand reaction exchange with possible aquifer mineral matrices during a ASR experiment.

Prommer & Stuyfzand (2005) carried out a reactive transport modelling study to analyze the data collected during a deep well injection experiment in an anaerobic, pyritic aquifer near Someren (Netherlands). The MODFLOW/MT3DMS-based re-active multicomponent transport model PHT3D (Prommer et al., 2003) was used for the transport simulations of the injection site. PHT3D couples the three-dimensional transport simulator MT3DMS with the geochemical model PHREEQC (v2). Greskowiak et al. (2005) carried out a modelling study to provide a process-based quantitative interpretation of the biogeochemical changes that were observed during an ASR experiment in which reclaimed water was injected into a limestone aquifer at a field-site near Bolivar (Australia). For this a PHT3D model was developed from a calibrated three-dimensional flow and conservative transport. Eckert et al. (2005) applied hydrogeochemical modelling in 1D-reaction transport model PHREEQC (v2) (Parkhurst and Appelo, 1999) to assess the purification processes that occur during riverbank filtration, in order to understand the temporal changes of the river water quality and hydraulics influence of this methodologies. Schmidt et al. (2007) while studying the geochemical effects of induced stream-water and artificial recharge on the Equus Beds Aquifer, Kansas (USA) used PHAST to simulate flow and transport of chloride from the stream through the aquifer into a recovery well. PHREEQC (v2) was also used for major ion and trace metal chemistry modelling providing insight into environmental changes that may be occurring as a result of AR activities.

In a geochemical modelling exercise of an ASR project in Union County, Arkansas (USA), Zhu (2013) used PHREEQC to simulate the scenario of injecting partially treated surface water from Ouachita River into the Sparta aquifer at the city of El Dorado. Lu et al (2014) produced a hydrochemical assessment of the local harvested water and groundwater based on field data, lab experiments, and modelling carried out for artificial recharge proposal in the Pinggu Basin aquifer. PHREEQC coupled with the flow and transport models was used.

7. CONCLUSIONS

Following the literature review for MAR modelling, the main conclusion, considering that for every model there is a different set of input data required, so one of the most important factor in selecting the appropriate model to a specific area/study is to verify what data is available/obtainable in order to feed it as much as possible allowing it to produce reliable results.

Based on the decision making methodology for the application of pollutant transport models proposed by Diamantino et al. (2006) the final decision for the selection and eventually the purchasing of a new model will have to be based on local or regional available skills and knowhow on groundwater modelling at the governmental environmental institution. The authors do firmly support the idea of governmental environmental institution to establish research contracts with local Universities and/or State Research Labs, and, if available, eventually also with private firms with relevant expertise on groundwater assessment and modelling. Also, for the author, this will be a case by case political decision depending on the willingness of the governmental environmental institution to overcome existing or potential groundwater pollution problems that may affect the regional environment and the public health.

Used models vary, but finite difference MODFLOW base software seems to be by far more frequently used, both due to be easily available and well documented, there are several programs adapted to specific problems. Due to its complexity finite elements are not so abundantly used, although the FEM grid is far more adjustable to complex limits of study areas. On the other hand, FEM HYDRUS was commonly selected for simulations in vadose zone. In hydrogeochemical studies related to MAR, free PHREEQC software was the most used, mostly due to its very wide set of capabilities.

Aquifer and local (small area of the aquifer) seems to be the most common scales studied. Small scale models (infiltration basin or aquifer sandbox model recreation) are scarce. MAR modelling, at a large scale, has been used as a decision support tool as basis to decide the suitability of MAR methodologies, most effective measures of environmental problem containment and to explore scarcity scenarios.

MAR modelling is being used worldwide, in particular in semi-arid to arid regions where scarcity problem is common and MAR presents as reliable solution, and in areas the use of recycled water is increasingly used in SAT-MAR as a way to increase water quality and availability.

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