

# Developments on Modeling of Groundwater Flow and Contaminant Transport

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Received: 29 December 2016 / Accepted: 23 May 2017 /

Published online: 9 June 2017

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**Abstract** Groundwater modelling is a useful tool to forecast hydraulic heads, changes in groundwater levels and changes in concentrations such as in cases of pollutant plume evolution and evaluating of aquifer protection strategies. Also, modeling can be used to hindcast changes in concentrations. Over the years, several numerical methods have been employed for the development of groundwater flow and transport models with the most popular being the finite difference and finite element approaches. In the present work, a review of the groundwater flow and transport models is presented based on their numerical method approaches in a chronological order. Also, all phases of building a groundwater model and all required information in each phase are included. Finally, the most well-known and used commercial groundwater simulators for flow and transport are presented.

**Keywords** Groundwater · Subsurface flow · Pollution · Simulation · Models

## 1 Introduction

In the last few decades, the use of numerical simulation models in science and engineering has become a powerful tool to describe and study physical systems and phenomena. In the area of groundwater hydrology and oil reservoir engineering, numerical simulation models are employed to describe hydrologic phenomena, movement of water and oil in the ground, and movement of contaminants. In addition, simulators are used to evaluate or predict long term impacts of water withdrawals and contaminant migration, and to examine groundwater management alternatives.

In general, a numerical simulator reduces one or more partial differential equations to a set of algebraic equations which can be solved for discrete values of the dependent variables. This reduction is accomplished using approximation techniques such as finite difference methods, finite element methods, and boundary element methods. The need of introducing the numerical

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simulation is due to the fact that analytical solutions were not adequate to describe a subsurface system accurately. The main reason of the inadequacy of the analytical solutions is the heterogeneity that characterizes the system.

In general, groundwater simulation models are used for: 1) forecasting groundwater level changes or changes in concentration, aiming to test aquifer protection strategies; 2) hindcasting concentration changes, aiming to determine a contaminant source or to design a field data collection network; and 3) evaluating the work of others, such as to assess conclusions of others through modelling.

In the past, several numerical models related to subsurface groundwater flow and mass transport have been presented with most of them involving saturated flow in porous media. Several models have also been developed involving flow in the unsaturated zone where the processes are more complicated and less well understood. We also have models that involve two or more liquids in the same porous medium such as in the petroleum industry and in cases of saltwater intrusion in coastal areas. The groundwater mass transport models describe the main processes of diffusion, advection and dispersion as well as some mass transfer processes such as decay and sorption. Although some mass transport models include reactions in the case of multiple reacting constituents, their performance is limited. One important issue for all models is the uncertainty of the model results which is due to several reasons such as limited number of field measurements, inaccurate geological or/and hydrological information, biases or measurement errors and weakness to measure certain parameters with accuracy.

All the groundwater numerical models solve a set of partial differential equations that describe the groundwater flow, the seepage velocity and the mass transport in case of groundwater contamination. Depending on the numerical methodology used for the solution of these equations, the models are divided in five (5) categories: 1) finite differences, 2) finite elements, 3) integrated finite differences, 4) boundary elements, and 5) analytical elements. The finite differences and finite elements are the most common methods for solving groundwater flow and mass transport problems. A computer program solves the set of algebraic equations arising from approximation of partial differential equations (equations of the system, boundary conditions and initial conditions) which comprise the mathematical model. The set of algebraic equations obtained in this way can be expressed in a matrix form. The choice between finite differences or finite elements depends on the problem to be solved and the user's preference. The finite differences are easy to be applied. Generally, they require fewer components for constructing the equation matrix. The finite element method is best to approach irregularly shaped boundaries compared to the finite differences method. Integrated finite differences can handle irregular domains in a similar way as finite elements. The selection of a method approach is usually based on the user's preference. Although occasionally there have been articles that support one or the other method, the seizures are not objective and fairer seems Gray's opinion (1984) that "*every method has special features that may be desirable for a specific application.*"

Regarding the unsaturated zone models, they are theoretically more complex and need more parameters than the saturated zone models, but they are particularly useful when the infiltration process and the recharge of the saturated zone are required. Their main characteristic is that they require the knowledge of the recharge rate to determine the upper boundary condition, since the infiltrated water introduced at the upper boundary of the unsaturated zone model will eventually reach the saturated zone.

In the following sections, a detailed review will be presented regarding groundwater flow and groundwater mass transport models.

## 2 Groundwater Flow Models

Groundwater flow models in the saturated zone are characterized by higher degree of simplicity compared to groundwater mass transport models. Actually, they solve the two partial differential equations related to groundwater flow and seepage velocity, which are Eqs. (1) and (2), respectively:

$$\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) - S \frac{\partial h}{\partial t} + \sum_{i=1}^r Q_i \delta(x-x_i) \delta(y-y_i) \delta(z-z_i) = 0 \quad (1)$$

where,

- $K_{xx}$  hydraulic conductivity in the x direction ( $LT^{-1}$ )
- $K_{yy}$  hydraulic conductivity in the y direction ( $LT^{-1}$ )
- $K_{zz}$  hydraulic conductivity in the z direction ( $LT^{-1}$ )
- $S$  specific storage coefficient ( $L^{-1}$ )
- $Q_i$  is the source/sink term at point  $i$  ( $L^3 T^{-1}$ )
- $\delta$  delta function
- $r$  number of sources / sinks

$$V_x = -K_{xx} \frac{\partial h}{\partial x}, \quad V_y = -K_{yy} \frac{\partial h}{\partial y}, \quad V_z = -K_{zz} \frac{\partial h}{\partial z}, \quad (2)$$

where,

$V_x, V_y, V_z$  are the  $x, y$  and  $z$  components of Darcy velocity, respectively [ $LT^{-1}$ ].

The first numerical models related to flow through porous media appeared in the early ‘50s in an attempt to obtain solutions for large problems of oil reservoirs. Pinder and Bredehoeft (1968) present a review of the pioneering work related to numerical methods in porous media. Thereafter, numerical simulation models received special attention and an extraordinary growth in their development followed.

Numerical groundwater flow models using a finite difference approach to approximate the derivatives of the algebraic equations were first presented by Remson et al. (1971), Mercer and Faust (1981) and Wang and Anderson (1982). The integrated finite difference (IFD) was reported by Narasimhan and Witherspoon (1978) and Fogg (1986).

Groundwater flow numerical models using the finite element approach were presented by Pinder and Gray (1977), Zienkiewicz (1977), Mercer and Faust (1981) and Huyakorn and Pinder (1983).

The method of boundary elements or the boundary integral method was employed by Liggett and Liu (1983), Liggett (1987) and De Marsily (1986).

In the recent past, artificial neural networks (ANN) have found application in groundwater management to predict the hydraulic head at a well location (Coppola et al. 2005; Feng et al. 2008; Lallahem et al. 2005; Nayak et al. 2006; Nikolos et al. 2008; Trichakis et al. 2009) as well as for the simulation of spatio-temporal groundwater levels (Tapoglou et al. 2014). A black box approach is used by ANNs to simulate the hydraulic head, taking as input hydrological parameters such as rainfall and temperature, as well as hydrogeological parameters such as pumping rates from nearby wells. Available field data are used to train the network and evaluate the training process.

### 3 Groundwater Mass Transport Models

Groundwater mass transport models solve a system of partial differential equations related to groundwater flow, groundwater velocity and mass transport. Specifically, first the flow equation is solved:

$$\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) - S \frac{\partial h}{\partial t} + \sum_{i=1}^r Q_i \delta(x-x_i) \delta(y-y_i) \delta(z-z_i) = 0 \quad (3)$$

with all terms as described in the previous section.

Knowing the hydraulic head  $h$ , the groundwater velocity equation is solved,

$$V_x = -K_{xx} \frac{\partial h}{\partial x} \quad V_y = -K_{yy} \frac{\partial h}{\partial y} \quad V_z = -K_{zz} \frac{\partial h}{\partial z}. \quad (4)$$

Finally, the mass transport equation is solved for the chemical concentration  $C$ ,

$$\begin{aligned} & \frac{\partial}{\partial x} \left[ D_{xx} \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y} + D_{xz} \frac{\partial C}{\partial z} \right] + \frac{\partial}{\partial y} \left[ D_{yx} \frac{\partial C}{\partial x} + D_{yy} \frac{\partial C}{\partial y} + D_{yz} \frac{\partial C}{\partial z} \right] \\ & + \frac{\partial}{\partial z} \left[ D_{zx} \frac{\partial C}{\partial x} + D_{zy} \frac{\partial C}{\partial y} + D_{zz} \frac{\partial C}{\partial z} \right] - \left[ V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} + V_z \frac{\partial C}{\partial z} \right] \\ & + Q(C^\omega - C) - \theta[1 + E(C)] \left( \frac{\partial C}{\partial t} \right) = 0 \end{aligned} \quad (5)$$

where  $C$  is the contaminant concentration [ $ML^{-3}$ ],  $\theta$  is the porosity of the aquifer,  $C^\omega$  is the concentration of the pumped fluid [ $ML^{-3}$ ],  $E(C)$  is a function representing chemical adsorption properties and  $D_{ij}$  [ $L^2 T^{-1}$ ] are the dispersion terms in the three main directions ( $x, y, z$ ).

The dispersion  $D_{ij}$  terms are defined as:

$$\begin{aligned} D_{xx} &= \left( a_L V_x^2 + a_T V_y^2 + a_V V_z^2 \right) / V + D_M \\ D_{yy} &= \left( a_T V_x^2 + a_L V_y^2 + a_V V_z^2 \right) / V + D_M \\ D_{zz} &= \left( a_V V_x^2 + a_V V_y^2 + a_L V_z^2 \right) / V + D_M \\ D_{yx} &= D_{xy} = (a_L - a_T) V_x V_y / V \\ D_{yz} &= D_{zy} = (a_L - a_V) V_y V_z / V \\ D_{zx} &= D_{xz} = (a_L - a_V) V_z V_x / V \end{aligned}$$

where,

- $D_M$  molecular diffusion coefficient ( $L^2 T^{-1}$ )
- $a_L$  longitudinal dispersivity (L)
- $a_T$  transverse dispersivity (L)
- $a_v$  vertical dispersivity (L)
- $V$  velocity of groundwater flow ( $LT^{-1}$ )

For the simulation of the groundwater flow and contaminant transport, field information is required related to the type of the aquifer (confined or unconfined), to the topography (ground elevation and aquifer's depth), to the geology (geological formation type, hydraulic conductivity, porosity, storativity), and to the hydrology (infiltration rates). It is also required that initial and boundary conditions for the flow and mass transport are determined.

The first attempts of groundwater numerical mass transport models using the finite difference method were presented by Welch et al. (1966) and Reeves et al. (1986). The finite element approach was used by Yeh and Ward (1981), Huyakorn and Pinder (1983), and Voss (1984).

As it was mentioned earlier, for the simulation of the mass transport equation, the solution of the groundwater flow equation is required first, therefore, most models presented in the past combine both the solution of groundwater flow and mass transport equations.

In Section 5, a summary of the most known groundwater flow and contaminant transport models is presented.

## 4 Building a Groundwater Flow and Mass Transport Model

In the present section the main phases of building a groundwater flow and transport model are presented.

### 1. *Starting phase*

The first step in building a model is to collect all information available for the area of interest which will be modeled. The information includes maps and reports as well as other references mentioned in the reports.

### 2. *Phase 1*

Based on the information collected in the previous phase, the following attributes must be determined for the area to be modeled:

#### *Geology*

In order to have a good representation of the geology, it is necessary to locate all well logs located in the area, to collect all geophysical information and soil map information. Based on these, a conceptual model of the stratigraphy can be made that also includes the lithology information. The main objective of this is to determine all geological formations and have a rough estimation of the hydraulic conductivity  $K$  and its distribution in the three main directions  $x$ ,  $y$ , and  $z$ , as well as of the porosity of each stratum.

#### *Aquifer parameters*

For the determination of the aquifer parameters one needs to collect and locate all pump and slug test data as well as all the hydraulic conductivity coefficients that have been determined using these data. Also, it is necessary to collect available grain size analyses, laboratory determinations of the hydraulic conductivity, porosity, absorption coefficient, carbon content and dispersivity. Values at known locations are normally interpolated to all other points. If little information is available, one must rely on lithological and stratigraphical interpretation in conjunction with soil map information (Pinder 1999).

### *Hydrological stresses*

In order to determine the hydrological stresses, all known pumping wells must be located and the pumping information must be obtained. Pumping must be specified in terms of discharge rates at each well location. If many wells are near one another, they must be combined. Also, meteorological data (especially rainfall) should be collected to compute the net infiltration value. In addition, leaking pipes, drains etc. must be identified and located on the map. Leakage must be specified wherever it exists, either as point value at a specific location or as a distributed leakage source.

### *Boundary conditions*

It is very important to locate all major water bodies that act as sources or sinks of groundwater, as well as ponds, water bodies that affect groundwater flow, and sources with known volumetric discharges such as leaking tanks. In case of mass transport modeling, it is required to locate sources of known concentrations or/and sources of known mass fluxes. First kind boundary (*Dirichlet*) conditions are constant head or constant concentration conditions, second kind (*Neumann*) boundary conditions are constant flow or constant mass flux conditions, and third kind (*Robin* or *Chauchy*) are leaky conditions.

### *Land uses*

The land use information is very important to determine sources of contaminants in cases of groundwater pollution. If there is deposition or movement of soil, it is necessary to know where and when that happened. After reviewing all available information, one should determine if there are in the area of interest leaking tanks, leaking drains, contaminated surface water bodies, surface spreading of solvents etc. An examination of the water quality will verify any of the aforementioned cases. Land uses are also particularly important in establishing the time of introduction of contaminants into the subsurface (Pinder 1999).

### *Water chemistry*

For the evaluation of the water quality, the following information must be collected: groundwater, surface water, soil and spring water quality analysis. Also, the possibility of existence of non-aqueous phase fluid in the subsurface should be investigated, as well as the possibility of organic daughter products. All this information can be used to determine the extent of the contaminant plume and the variability of the concentrations, and to locate contaminant sources (Pinder 1999).

## 3. Phase 2

This phase refers to the model input which includes the model geometry, the model grid and the time steps.

### *Geometry*

The area of the model should be larger than the area of interest and, if possible, it should coincide with hydrological boundaries. If no known boundaries exist in the area of interest, a constant head or constant flux boundary based upon observed water levels may be employed at a distance far enough from the area of interest, so as not to influence the simulation (Pinder 1999).

### *Model grid*

The most common approaches for the model grid are the finite difference and the finite element approaches.

1. Finite difference approach

A rectangular area slightly greater than the area defined by the boundary conditions is selected which is subdivided into smaller contiguous rectangles. If mass transport is involved, the rectangle width should be less than twice the dispersion coefficient divided by the Darcy velocity. The mesh can increase in size approaching the boundaries provided no contaminant transport occurs there. The hydrological boundaries must coincide with the edges of the rectangles. Special assemblages of rectangles are required for leakage areas (e.g., ponds), special infiltration areas (e.g., cups) and areas of different aquifer coefficients (Pinder 1999).

2. Finite element approach

In most cases triangular or quadrilateral elements are used to subdivide the area of the model. The same rule for selection of side lengths in the case of a contamination problem is used as in finite differences. Larger triangles can be used as the perimeter of the model is approached if no mass transport takes place. The perimeter of the model must correspond to the boundary conditions, but the model needs not to extend beyond the boundary conditions. All wells should be located at the vertices of the triangles and the corners of the quadrilaterals.

### *Temporal simulation*

A small (seconds to minutes) time step is needed when transient groundwater flow is simulated in the presence of pumping. It is prudent when simulating transport, to use a time step such that the time increment is less than the smallest space increment divided by the pore velocity. In the case of groundwater flow, the time step may be increased in size as the simulation advances, provided no new hydrological stresses are imposed on the system. In transport simulations, the time step should not be increased significantly. The time step multiplier should not exceed 1.5.

4. *Phase 3*

The last phase of groundwater modeling includes the calibration of the model. For the groundwater flow, the simulated water levels and the discharges/recharges should be compared to the measured ones. Also, seasonal changes in the water table should be compared to those observed in the field. For the contaminant transport, simulated concentrations and contamination patterns should be compared to field measurements.

## **5 Commonly Used Groundwater Flow and Contaminant Transport Models**

In this section, the most prominent and commonly used groundwater flow and mass transport models are presented in a chronological order.

**FEFLOW** It is a finite-element model for the simulation of 2D and 3D fluid density dependent flows, contaminant mass (salinity) and heat transports. It can simulate: phreatic

aquifers, perched water tables, moving meshes; saturated-unsaturated zones; salinity-dependent and temperature-dependent transport; and complex geometric and parametric situations. The model was firstly presented by Dr. Hans-Jörg G. Diersch in 1979. He developed the software in the Institute of Mechanics of the German Academy of Sciences at Berlin up to 1990. In 1990, he was one of the founders of WASY GmbH (German for Institute for Water Resources Planning and Systems Research Inc.) of Germany (Trefry and Muffels 2007). In 2007 the shares of WASY GmbH were purchased by the DHI Group. An analytical presentation of this code can be found in the book written by Diersch (2014).

**MODFLOW** It is the most prominent worldwide 3D finite-difference groundwater flow model developed by the U.S. Geological Survey in the early 1980s. The code was originally called USGS Modular Three-Dimensional Ground-Water Flow Model (McDonald and Harbaugh 2003). MODFLOW simulates the groundwater flow using a block-centered finite-difference approach and the layers can be confined, unconfined, or a combination of both. It also simulates flows from external stresses such as areal recharge, evapotranspiration, flow to wells, flow to drains, and flow through riverbeds. After the original release, several versions of MODFLOW have been presented, such as MODFLOW-88, MODFLOW-96, MODFLOW-2000, MODFLOW-2005, where additional features and abilities of the model were included. Later on some other models were linked to the MODFLOW model such as MT3D and SEAWAT. **MT3D** is a modular three-dimensional transport model developed by Zheng (1990) at S. S. Papadopoulos & Associates, Inc. MT3D simulates advection in complex steady-state and transient flow fields, anisotropic dispersion, multi-species reactions, and can simulate or assess natural attenuation within a contaminant plume. **SEAWAT** is a 3D variable density, transient groundwater flow in porous media. Actually it is a combination of MODFLOW and MT3DMS into a single program that solves the coupled flow and solute-transport equations (Kumar 2015). It has been used in many applications of saltwater intrusion problems.

**SUTRA** It is a 2D groundwater transport model for saturated and unsaturated flows, a complete saltwater intrusion and energy transport model. SUTRA employs a 2D hybrid finite-element and integrated finite-difference method to simulate: (1) fluid density dependent saturated or unsaturated groundwater flow and either (2a) transport of a solute in the groundwater or (2b) transport of thermal energy in the groundwater and solid matrix of the aquifer. The original version of SUTRA was released in 1984 (Voss 1984).

**PTC** It is a 3D mathematical model which calculates the groundwater flow and transport of contaminants in porous media by combining the finite element and finite difference methods. PTC uses partial differential equations to represent saturated groundwater flow described by hydraulic head, groundwater velocity components and contaminant transport. These equations are derived from conservation of mass principles and Darcy's Law. The algorithm involves discretizing the domain into approximately parallel horizontal layers. Within each layer a finite element discretization is used allowing for the accurate representation of irregular domains. The layers are connected vertically by a finite difference discretization. This hybrid coupling of the finite element and finite difference methods allows for the application of the splitting procedure. It was developed by Babu et al. (1987). Later on, it was developed as a Plug-In Extension (PIE) for the ArgusOne GIS program (Olivares 2001).



**FEMWATER** It is a fully 3D finite-element model that simulates density-dependent coupled flow and contaminant transport in saturated and unsaturated zones. It allows modeling of the saltwater intrusion as well as other density-dependent contaminants. It is the combination of two models 3DFEMWATER and 3DLEWASTE (Yeh and Ward 1981; Yeh 1987, 1990).

**3DFEMFAT** It is a 3D finite-element model of groundwater flow and transport through saturated- and unsaturated porous media. The first 2D version of the model was first presented by Yeh et al. (1994). It has been applied to model wellhead protection, infiltration, sanitary landfill, agriculture pesticides, hazardous waste disposal sites, density-induced flow and transport, saltwater intrusion.

**AQUA3D** It is a 3D model using the Galerkin finite-element method that solves the three-dimensional groundwater flow and transport problems for homogeneous and inhomogeneous as well as for anisotropic flow conditions. The model was developed by Vatnaskil (1998a, b).

## 6 Conclusions

Groundwater numerical models have been proved a useful tool to simulate groundwater flow and contaminant transport. Over the years, several commercial groundwater numerical simulators have been presented with the majority of them to be based on the finite difference and finite element numerical methods. When building a groundwater numerical simulator, it is very important to have accurate information on the aquifer parameters and to perform a detailed calibration in order to obtain correct simulated results. The selection of the appropriate code depends on the characteristics of the system to be modeled and on the modeling preferences: groundwater flow or mass transport, one, two or three-dimensional, transient or steady-state, density-dependent or not, unsaturated, saturated or combined flow, chemical reaction or not, etc. Based on all of the above, the right selection of the numerical groundwater model with the correct input can guarantee the accuracy of the simulated results.

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