FEM MODELING VS. RANDOM WALK MODELING FOR POLLUTION SPREAD IN GROUNDWATER FLOW

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Abstract

Reasonably pure water is one of the most important resources of the 21st century, and the increasing demand as well as the climate change make it increasingly difficult to satisfy the demand with surface water. Groundwater is a suitable alternative, but anthropogenic changes have much more impact, so modeling and simulation is used to a great extend to forecast the possible results of such human interferences. As the basics physical laws governing the flow and transport of groundwater lead to PDE's, in geohydrology simulation almost always leads to the numerical solution of PDE's. The well known Finite Element Method and the less known Random Walk Method are the two far ends in the possible numeric techniques available for the mixed hyperbolic-parabolic PDE resulting from the attempt to model the transport of substances, and sometimes lead to fundamentally different results on the same problem, especially when used in conjunction with other stochastic and statistic modeling techniques usually applied in modeling the groundwater bearing geological strata, which basically provide the data for the flow model the transport is based on. In this paper the merits and shortcomings of these techniques in their application in groundwater modeling and simulation are discussed, compared and illustrated in a few examples.

Keywords: FEM, FD, Groundwater modeling

Presenting Author's Biography

Florian Judex studied applied mathematics at the Vienna University of Technology, an wrote his master thesis on system identification. At the moment he is working on his PhD thesis on groundwater modeling for the ARC Seibersdorf Research Center, as well as for the research unit "Numerics and Simulation of Differential Equations" at the Institute for Analysis and Scientific computing at the Vienna University of Technology.

1 The Basics of Groundwater

1.1 The Motivation for Groundwater modeling

Reasonably pure water is one of the most important resources of the 21st century, and the increasing demand as well as the climate change make it increasingly difficult to satisfy the demand with surface water.

Groundwater is often an alternative, but it's exploration and exploitation are much more difficult and expensive. Furthermore, groundwater has much higher response times to changes, and damage done to groundwater bodies is much more difficult to remediate then in case of surface water. Therefore modeling and simulation is one of the most important tools in groundwater engineering, as predictions of the anthropogenic changes are a vital part of every project in this field.

The increasing use of groundwater is also leading to the discovery of many polluted groundwater bodies which where unknown up to date, and transport modeling is used when track down the source of the pollution to make a remediation possible.

1.2 Groundwater Bodies

Groundwater resides in the pores of a groundwater bearing geological strata, the so called aquifer. The dimensions of aquifers can vary greatly, from small local aquifers with a few square kilometers to huge systems like the Nubian Sandstone Aquifer System beneath the Sahara spanning over 2 million square kilometers and containing approximately $3.7 \cdot 10^{14} m^3$ of water. Depths vary from just aquifers just below the ground surface recharged by rainfall to aquifers in a depth of several hundred meters which were filled over a million years ago and are non-renewable resources.

The main types of groundwater bodies are the unconfined groundwater bodies, where the aquifer is situated above an geological strata with a very low hydraulic conductivity (also called aquitard), and the confined groundwater bodies where the aquifer is between two aquitards, leading to a pressurized aquifer.

1.3 Basic Equations for Groundwater Flow

In order to simulate the transport of soluble substances in groundwater bodies, first the flow field of the aquifer has to be established. To be able to treat confined aquifers, the equations are not formulated for the groundwater table, but the piezometric head $h[m]$

$$h = z_0 + \frac{p}{\rho g} \qquad (1)$$

where $z_0[m]$ denotes the bottom elevation of the aquifer, $\rho[kg/m^3]$ the density of water, which depends mainly on the pressure $p[kg/ms^2]$ and roughly equals the level of the watertable if the aquifer would be unconfined. The change in groundwater storage, which is given by the specific storability $S[1/m]$, the thickness of the aquifer $m[m]$ and $h(\vec{x}, t)$ depends on the gradient of groundwater flow $\vec{v}(x, t)$

$$Sm\frac{\partial h}{\partial t} = -\nabla v. \qquad (2)$$

In turn the flow $\vec{v}$ can be derived via Darcy's law

$$j = m\mathbf{K}\nabla h \qquad (3)$$

from the gradient of the head, with $\mathbf{K}[m/s]$ denoting the tensor of the hydraulic conductivity Combining these two equations and adding a generalised term Q for sources and sinks leads to the flow equation for groundwater

$$S\frac{\partial h}{\partial t} = \nabla(\mathbf{K}\nabla h) + Q. \qquad (4)$$

All three types of boundary conditions appear in groundwater modeling. Average groundwater flow fields will have velocities between$10^{-7} m/s$ and $10^{-4} m/s$, and it is common in groundwater engineering to use m/d as a unit when characterising groundwater bodies. In practice, the tensor $\mathbf{K}$ is replaced by a constant k_f, leading to the standardised form of the flow equation

$$S_0\frac{\partial h}{\partial t} = k_f \Delta h + Q. \qquad (5)$$

In case of an unconfined aquifer m has to be replaced by $h - z_0$, while the storage term changes from Sm to $Sm + n_d$ to take in account that the water can expand into the drainable porous volume n_d above the piezometric head. The source term will include the recharge by precipitation, which is a source distribute over whole domain.

1.4 Basic Equation for the Transport

Once the flow $h(\vec{x}, t)$ field is established, transport can be modelled. The porous velocity $\vec{u}(\vec{x}, t)[m/s]$ used for the convective propagation of the transported substance is much higher then the darcy velocity used for the groundwater flow. They are connected via the effective porous volume n_e which is a dimensionless variable and denotes the percentage of the soil which is really used for the groundwater flow.

$$u = \frac{v}{n_e} \qquad (6)$$

In conjunction with Fick's law for dispersion the PDE for the concentration $c(\vec{x}, t)[kg/m^3]$ can be formulated

$$R\frac{\partial c}{\partial t} + \nabla(uc) = \nabla(D\nabla c) - R\lambda c + \tilde{Q} \qquad (7)$$

Here $D[m^2/s]$ denotes a tensor resulting in the combination of molecular diffusion and the mechanical dispersion in the pores of the aquifer. The dispersion is again linked to the porous velocity a fourth order tensor $\alpha[m]$ which is in practice replaced by two scalar values for transversal (α_T) and lateral (α_L) dispersion with respect to flow direction. $\tilde{Q}$ is a generalised source/sink term for the transported substance, λ a possible degradation and R a retardation caused by a possible interaction between the substance and the aquifer soil.

1.5 Modeling and Simulation of the Groundwater Flow

Although the laws and equations governing the flow of groundwater are well studied and sound, modeling and simulation is still difficult process, mainly because the low availability of data. All geophysical methods which can be used from the surface require the solution of an ill posed inverse problem, and are therefore limited in their usability and the quality of their output. Data gathering usually has therefore be done by using boreholes, which are expensive and take a lot of time to construct. Once a borehole is established, there are two types of experiments:

- Local experiments, in which the borehole itself is investigated. These include the experimental determination of the hydraulic conductivity from the drill core, the flow density via flowmeters or the flow direction using colloidal borescopes.
- Global experiments, in which a large surrounding of the borehole is investigated. These include among others pumping tests to determine an regional average of the hydraulic conductivity and tracer tests to determine the direction and speed of groundwater flow.

Furthermore location, type and exact values for the boundary conditions also depend on the amount of information available. For example a river can be modelled by a boundary condition of the first type if it has a good connection to the aquifer and it's rate of flow is high enough, or of the third type if the connection is limited. Table 2 shows the parameters which have to be either

1. determined by experiments,
2. estimated on the basis of geological maps and tables or
3. determined by identification.

Given the cost of boreholes and experiments, the second option is the one most often chosen. After the parameters are determined flowfield is computed or computation and identification is done. The methods used range from FEM or FD down to linear interpolation between measurement or even statistical linear models.

In most cases, the variation in time of many of the parameters, especially the recharge, is also unknown. Instead of the transient problem only the steady state problem is solve, leading to further averaging.

As the identification of the flow model already is an ill posed problem, quite often several realisations of the same flow field are used as possible starting points for transport modeling. Figures 1 and 2 show an example where for the same boundary conditions - 10 meters piezometric head at the left side, 0 meters on the right side, impervious at the bottom and the top - a flow field was computed from conductivity matrix with finite differences . The height of 12 meters, the size of 3 by 3 kilometer aquifer and an average hydraulic conductivity of 10^{-3} are all quite realistic values. FD instead of FEM was chosen because it is the method implemented in MODFLOW[1], a public domain software provided by the United States Geological Service (USGS). When used in conjunction with the Processing MODFLOW front end provided by the ETHZ [2], the model for the figures 1,2,3,4 and 5 can be set up in under 10 minutes if the user has a bit of proficiency.

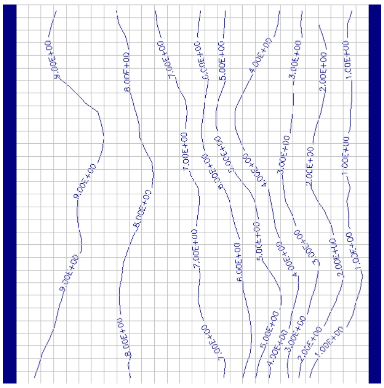

Fig. 1 random realisation of a flow field

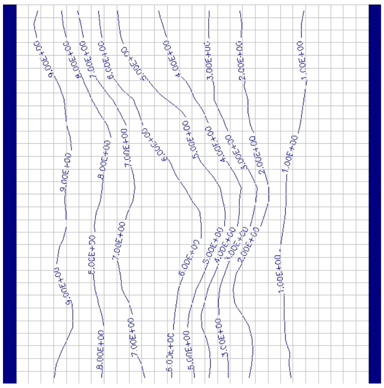

Fig. 2 random realisation of a flow field

The realization of the conductivity matrix was done with MODFLOWS field generator with parameters shown in table 1.

1.6 Finite Element modeling

As the finite element method is one of the most used methods in modeling and simulation of PDE's, it basics will not be discussed here.

Tab. 1 Parameters for the conductivity field calculation

Parameter	Value
Mean Value (log10):	-3
Standard deviation (log10):	0.434
Correlation length/field width (x-direction):	0.1
Correlation length/field width (y direction):	0.1

Tab. 2 Scale of Parameters in Groundwater modeling

Parameter	Scale / Range
S_0	$< 10^{-4}$
k_f	$10^{-9} - 10^{-2}$
n_e	$0 - 1$
R	$0 - 1$
λ	≤ 1
α_L	$10^{-1} - 10^{1}$
α_T	$\alpha_L \cdot 10^{-1} - \alpha_L$

The only thing one has to keep in mind for when using the finite element method for transport and flow modeling in aquifers, is that the transport modeling often has to use a different grid than the flow modeling. Details can be found for example in [3]

2 Random Walk modeling and Simulations

The Random Walk Method is a Monte Carlo Method which theoretical basis and application in theoretical physics date back to [4]. The mass of the transported substance is split into a number of particles which are placed at the source. In each timestep the particles are individually moved. The movement consist of a deterministic part corresponding to the convective movement in the flow field, and an stochastic part corresponding to the dispersion. For 1-D on step can be written as

$$x(t+\Delta t) = x(t)+u'(x(t),t)\Delta t+Z\sqrt{2D_L(x(t),t)\Delta t} \tag{8}$$

where u' denotes

$$u'(t) = u(\mathbf{x}(t),t) + \frac{\partial D_L}{\partial x}. \tag{9}$$

Z is the random element, a (0,1) normal distributed random variable. As D_L as directly proportional to u this term only is only important near to sources and sinks, where the small dispersion coefficient is enhanced by the high gradient of the head.

It is easily extended to three dimensions, and it's computational computation complexity increases linear. It's precision of course increases with the number of particles used. In case of a non-instantaneous source, the independence of the particles can be used for a superposition in time.

Compared to numerical solutions based on grids like FEM or FD, and even partial based algorithms like MOC or MMOC, where grids are only used for the dispersive step, there is no numerical dispersion during the computation. Only once the simulation is complete an a result has to be extracted from the data generated, a grid is used to compute sum of the masses of the particles in each cell, and deriving the concentration from this mass.

Figures 3 and 4 show two results of a random walk simulation of a transport problem in a constant flowfield in y direction, computed with custom MATLAB code.

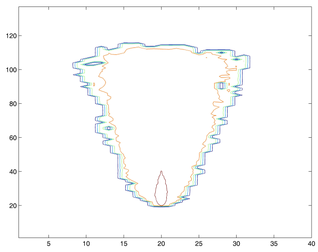

Fig. 3 random-walk simulation of transport

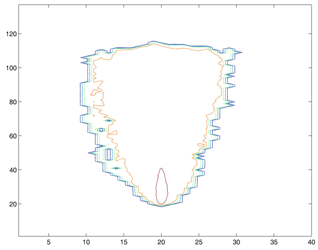

Fig. 4 random-walk simulation of transport

3 Finite Elements vs. Random Walk

Most natural aquifers are very heterogeneous. All of the parameters governing flow and transport will vary in space, especially including the geometry. Most of the changes are unknown, and even extreme changes on small spaces can occur. For example an old riverbed will result in a band of gravel with a high hydraulic conductivity, resulting in the hydraulic equivalent of a short circuit.

Figures 6 and 7 show the results of transport model based on the flowfields in figures 1 and 2, while figure 5 is the transport computed with the simple linear flowfield based on the average k_f value of 10^{-3} The effective porous volume of 0.25 used is a reasonable value for sandy gravel, a common type of aquifer. If the question to be answered is whether the border is reached or not, the deterministic solution would have been on the save side, but the in 7 the plume hits the second border in another place then in the deterministic case. But the additional dispersion caused by a disturbed flow field is large, so the question if a point above or below the plume of pollution calculated with the deterministic flow field is endangered would in many cases be answered incorrectly.

A further question that has to be considered is if the complexity of the finite element model is justified:

- The physical model of the aquifer is already simplified.
- Instead of the tensor of conductivity and the tensor for dispersion/dispersivity only a few scalar values are used.
- The information available is averaged in space.

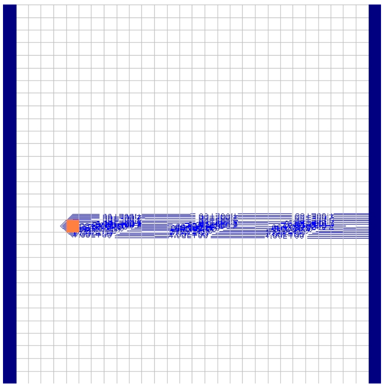

Fig. 5 Transport based on a flowfield computed with the average value of 10^{-3}

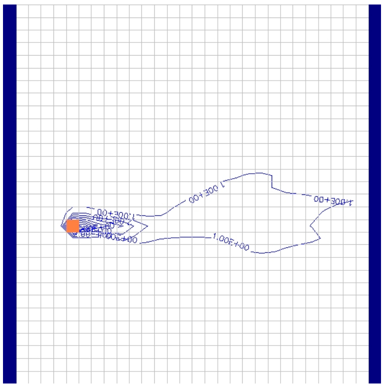

Fig. 6 Transport based on the flowfield shown in figure 1

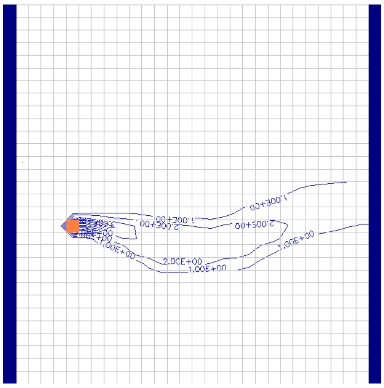

Fig. 7 Transport based on the flowfield shown in figure 1

- The information is averaged in time by using the steady state model.
- Other parameters are identified using an ill posed problem based on these averaged parameters.
- Either the transport problem already has to be incorporated when choosing the grid for the flow model, or the flow field used in the transport model has to interpolated in some places for the flow model.

This leads to a situation were the seemingly very precise and definite results FEM provides and which are desirable in most fields of engineering are often misguiding in groundwater engineering. On the other hand, a simple random walk model with a few thousand particles can be implemented in any programming or scripting language, an gives the user a coarse result without the deterministic character that often leads the users of geohydrological software into accepting the results of a FEM simulation as the real shape of the aquifer studied and the real level of groundwater in the aquifer.

For example Figures 8 and 9 shows two solutions for a groundwater remediation problem. Between the point where this concentration is calculated an a source of the pollution is a remediation plant. The plant is only operated in at night and during the weekends in order to run on cheap power.

The finite element solution was calculated using COMSOL, while the random walk method used custom code in MATLAB - the line in 9 corresponds to the part of the ”switched operation” curve in 8 where the fluctuation occur, and are on the same scale. In this case, the random walk is of course much more fluctuating then the COMSOL solution, and also shows an much higher level of concentration - almost 1.5 times as much as in the COMSOL solution. The explanation is on the one hand that the MATLAB code uses the approach of simulating a normal distributed random variable with 12 [0,1] equally distributed random variables which reduces the effective variance and the spread the therefore the spread of the pollution. But on the other hand the FEM solution only shows weekly fluctuation, while the daily fluctuations get smoothed out by the algorithm used. It is to be expected that under real world conditions the behaviour would be somewhere in the middle.

Furthermore, an aquifer is a system reacting very slow on changes, so most in most project after the calculation a very generous safety margin is added just in case and calculations to an arbitrary precision are ridiculed by this practice.

4 Conclusions

Given the amount of random fluctuations in the parameters used in groundwater modeling, one always has to as oneself if the complexity of a FEM model is justified. Especially in user oriented software aimed at groundwater engineers the formalism of FEM is often hidden beneath a graphical user interface, up to a point were

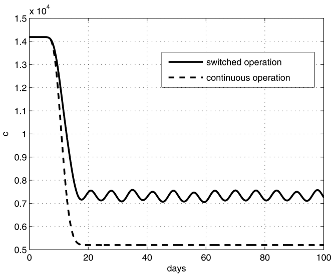

Fig. 8 Transport and remediation calculated with finite elements

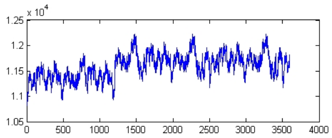

Fig. 9 Transport and remediation calculated with the random walk method

not even the the grid used is shown to the user. The challenge for the simulations is to produce reasonable results with a method appropriate to the data available, making the Random-Walk method a good choice if data is sparse, while the FEM is certainly better suited for well explored aquifers - but those are more like the exception that proves the rule then the every case.

5 References

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