Journal of Hydrology 392 (2010) 22–30

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Error analysis of a multi-cell groundwater model

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ARTICLE INFO

Article history:
Received 12 June 2009
Received in revised form 30 June 2010
Accepted 27 July 2010

This manuscript was handled by Philippe Baveye, Editor-in-Chief

Keywords:
Finite difference method
Finite Volume Method
Integrated finite difference method
Multi-cell groundwater models
Representational error
Truncation error

SUMMARY

The basic advantages of the multi-cell groundwater models are the parsimony, speed, and simplicity that make them ideal for hydrological applications, particularly when data are insufficient and/or repeated simulations are needed. However, the multi-cell models, in their basic version, are conceptual models and their parameters do not have physical meaning. This disadvantage may be overcome by the Narasimhan and Witherspoon's integrated finite difference method, which, however, demands that the cells' geometry conforms to the equipotential and no-flow lines. This restriction cannot be strictly satisfied in every application. Particularly in transient conditions, a mesh with static geometry cannot conform constantly to the varying flow kinematics. In this study, we analyse the error when this restriction is not strictly satisfied and we identify the contribution of this error to the overall error of a multi-cell model. The study is experimental based on a synthetic aquifer with characteristics carefully selected so as to be representative of real-world situations, but obviously the results of these investigations cannot be generalized to every type of aquifer. Nonetheless these results indicate that the error due to non-conformity to the aforementioned restriction plays a minor role in the overall model error and that the overall error of the multi-cell models with conditionally designed cells is comparable to the error of finite difference models with much denser discretization. Therefore the multi-cell models should be considered as an alternative option, especially in the cases where a discretization with a flexible mesh is indicated or in the cases where repeated model runs are required.

1. Introduction

Multi-cell models are multi-dimensional extensions of the completely mixed reactor model of chemical engineering (e.g., Aris, 1994). Key properties of these models are: (i) that the density of mesh nodes can be easily adjusted to fit irregular geometries efficiently with polygonal cells and (ii) that the setting up of the relevant equations is straightforward. These two advantages, in combination with the assumption of steady flow, have made the multi-cell models popular in water quality modelling such as in the multi-box simulation method of lake water quality (Thomann and Mueller, 1987).

Multi-cell models are also applied, to a lesser extent, in groundwater hydrological applications. Bear (1979) suggests using streamlines as parts of cell boundaries, which is more or less the concept behind the graphical method of flow-nets. Flow-nets have been introduced since the beginning of 20th century by Philipp Forchheimer to calculate the leakages under dams (Ettema, 2006). Narasimhan and Witherspoon (1976), building on the work of others, especially in the field of heat transfer (MacNeal, 1953; Dusinberre, 1961; Edwards, 1972), have developed the method of integrated finite difference (IFD) that can be also considered as the mathematical background of the graphical flow-nets method. A particular requirement of this method is that it strictly demands continuous adjustment of the mesh geometry to the flow kinematics, so that the cell boundaries are equipotentials or no-flow lines. Narasimhan and Witherspoon (1976) express this (in a not so explicit fashion) as follows: "*For maximum accuracy, interfaces between elements should be perpendicular to the line joining the two nodal points and intersect that line at an appropriate mean position* (*arithmetic* mean of nondivergent coordinates, log mean of cylindrical radii, or geometric mean of spherical radii). *This ideal situation may be difficult to achieve in practice but should be approximated as closely as possible*." The application tests of Narasimhan and Witherspoon (1976) are chosen such that essentially the situation is ideal; however, in most real-world problems the situation is far from ideal.

Narasimhan and Witherspoon's study proves that the multi-cell models, with appropriately designed cells, are able of functioning as physically based models in steady state conditions. However, in transient conditions, a continuous adjustment of cells' geometry to the flow kinematics is required. This is a very constraining requirement, which is likely the main reason why the multi-cell models have not been used widely for flow simulations.

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0022-1694/$ - see front matter
doi:10.1016/j.jhydrol.2010.07.036

The overall simplicity of the multi-cell models has motivated us to explore their application in transient groundwater simulations in addition to steady flow conditions, where the latter serves as reference basis for comparison. We wish to identify whether and under what conditions this method could be an appealing alternative when the data are sparse, and thus elaborate methods may not be warranted, or when repeated model runs must be made in the context of complex water resources management simulations, where computing efficiency is important. To this end, we examined three type of errors related with the multi-cell models: (1) the error due to inexact conformity of the cells' geometry to the flow kinematics, (2) the truncation error and (3) the representational error; the last two errors are common in every distributed (hydrogeologic) model. We investigate the dependence of these three errors on the density and on the geometry of a multi-cell discretization mesh.

The investigation is not based on a classical mathematical analysis but rather on experiments performed on a synthetic aquifer with a stochastic hydraulic conductivity field that resembles field conditions. For this reason, and though the characteristics of this aquifer were carefully selected to be representative of typical conditions met in groundwater applications, the conclusions of this study cannot be applied to every aquifer transient simulation (with arbitrary temporal and spatial distribution of stresses and boundary conditions). Rather they can serve as a reminder of the existence of alternative modelling methods that can be advantageous in some applications.

The results of a coarse multi-cell representation are compared against those of a typical detailed representation using MODFLOW. The coarse multi-cell model used in this study is the 3dkflow model (Rozos et al., 2004; Rozos and Koutsoyiannis, 2006). 3dkflow is a model that supports meshes with arbitrary geometry, i.e., the cells can be rectangular or irregularly shaped. 3dkflow is using a hydraulic analogous for simulating the water flow. This analogous is a network of interconnected tanks through water pipes. All aquifer properties and processes related with storage are simulated by the tanks whereas all properties and processes related with water transfer are simulated by the pipes.

The paper begins with an introduction to the Narasimhan and Witherspoon's method. This method is a simplification (enabled by the flow-nets-like discretization) of the widely used nowadays Finite Volume Method (FVM) (Carrera, 2008). For this reason in this study we chose a term that simultaneously denotes the method's relation with the FVM and indicates its distinctiveness. This new term is Finite Volume Method with Simplified Integration (FVMSI) used in this study in the context of the flow-nets-like discretization required by the multi-cell models to function as physically based models.

Afterwards we present two case studies. In the first case study, four FVMSI meshes are used to simulate a synthetic aquifer under steady state conditions. Reference simulations are used to derive the overall error of the simulations with each FVMSI mesh. The second case study concerns the flow simulation in the synthetic aquifer under transient conditions, with the four FVMSI meshes, and the comparison of their accuracy with the accuracy achieved using the finite difference method (FDM) with four grids.

The paper closes with the summary of the methods and the findings of this study.

2. Multi-cell models and FVM

2.1. Finite Volume Method

The differential equation of the groundwater movement in a confined anisotropic aquifer is (Bear, 1979):

$$\nabla \cdot \mathbf{K}\,\mathrm{grad}\,h + \mathrm{G} = \mathrm{SS}\frac{\partial \mathrm{h}}{\partial \mathrm{t}} \tag{1}$$

where h is the hydraulic head [L], $\mathbf{K}$ is the tensor of the hydraulic conductivity [$\mathrm{L\,T^{-1}}$], G is the external stress [$\mathrm{T^{-1}}$], and SS the specific storage [$\mathrm{L^{-1}}$]. If the coordinate system coincides with the principal axes of anisotropy, then the off-diagonals terms of the tensor $\mathbf{K}$ are zero.

When the space derivatives of the hydraulic head in Eq. (1) are approximated with finite differences, it is common to discretize the domain on a rectangular grid. To avoid this restriction, an alternative technique is used in the FVM. Eq. (1) is integrated with respect to the volume V of the discretization cell:

$$\int_V (\nabla \cdot \mathbf{K}\,\mathrm{grad}\,h + G)dV = \frac{\partial}{\partial t}\int_V \mathrm{SS}h\,dV \tag{2}$$

According to the divergence theorem of Gauss, and assuming that SS is constant and G and h are space invariant inside the cell, Eq. (2) is written as (Knabner and Angermann, 2003):

$$\int_S \mathbf{K}\,\mathrm{grad}\,h \cdot \mathbf{n}\,d\mathbf{S} + GV = SSV\frac{\partial h}{\partial t} \tag{3}$$

The surface integral at the left side of Eq. (3) is the total discharge crossing the surface S that surrounds the volume V, and $\mathbf{n}$ is the unit vector normal to a surface element d$\mathbf{S}$ (positive outwards). The application of Eq. (3) to all cells of the grid, results in a system of linear equations. The hydraulic head in the centres of the cells is obtained from the solution of this system.

2.2. Simplified integration

The surface integral in the left side of Eq. (3) cannot be calculated analytically in every case, so numerical methods (e.g., the trapezoidal rule or Gauss integration) must be used. Several studies have been conducted on these numerical methods to achieve better accuracy with simpler algorithms (Wenneker et al., 2000; Moroney and Turner, 2004). A methodology that simplifies the calculation of this surface integral was implemented in the present work.

We focus our study on isotropic aquifers (anisotropic aquifers can be transformed to isotropic with the appropriate mapping; Strack, 1999). In this case $\mathbf{K}$ reduces to a scalar K. A condition that simplifies the calculation of the integral in (3) is met when the edges of the discretization cells are equipotential lines or no-flow lines (hereafter referred as the 1st FVMSI condition). In this case, the product grad $h \cdot \mathbf{n}$ along the perimeter of each cell is equal to ±|grad h| (on no-flow edges |grad h| = 0). Consequently, the calculation of the surface integral is reduced to a simple summation of terms of Darcian fluxes. In the example shown in Fig. 1, the cell m is surrounded by N neighbouring cells. By substituting finite

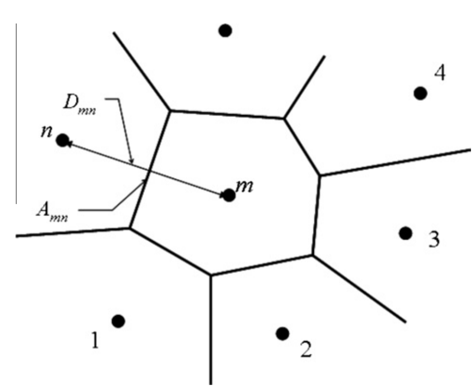

Fig. 1. Cell m surrounded by N neighbouring cells.