XXXVIII IAH Congress

Groundwater Quality Sustainability Krakow, 12–17 September 2010

Extended Abstracts

Editors: Andrzej Zuber Jarosław Kania Ewa Kmiecik





University of Silesia Press 2010



abstract id: 472

topic: 5

Data processing in hydrogeology

5.2

Groundwater flow and solute transport modelling

title: The velocity oriented approach revisited

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keywords: groundwater flow modeling, velocity oriented approach, continuity of water flux

INTRODUCTION

Many hydro-geological situations require an extremely accurate quantification of the 3-dimensional groundwater flow velocity in the subsoil. Examples are: hydrology of wetlands, water balances of aquatic ecosystems depending on groundwater recharge, river-groundwater interaction, advective transport of pollution underneath waste disposal sites, particle trajectories in aquifer-aquitard systems with contrasting heterogeneities, and many others. A notoriously difficult problem is the numerical determination of the *vertical* component of the groundwater velocity. This component may be two or three orders of magnitude smaller than the horizontal velocity components. Application of Darcy's law to numerically calculated hydraulic heads may lead to a relatively inaccurate vertical velocity component. In cases where the Dupuit approximation—negligible vertical head gradient—holds, numerical differentiation of hydraulic head yields zero vertical velocity.

THE VELOCITY ORIENTED APPROACH IN THREE DIMENSIONS: STREAM FUNCTION BASED

In the 1980s Nawalany and Zijl started to consider 3-dimensional groundwater flow in the context of what they called Flow Systems Analysis (also see Tóth, 2009). In Flow Systems the small vertical velocity component plays an important role (Nawalany, 1986a, 1986b; Zijl and Nawalany, 1987, 1990). Similar to what was accepted practice for 2-dimensional flow, it was proposed to invert the order of calculating 3-dimensional flow by eliminating the hydraulic head from Darcy's law. This 3D extension was called the velocity oriented approach (VOA). Indeed, Darcy's law $\underline{k}^{-1} \cdot \vec{q} = -\nabla \varphi$ —in which the head occurs—is equivalent to $\nabla \times \underline{k}^{-1} \cdot \vec{q} = \vec{0}$ —from which the head is eliminated. In addition, the continuity equation $\nabla \cdot \vec{q} = 0$ is equivalent to $\vec{q} = -\nabla \times \vec{\psi}$, where vector $\vec{\psi}$ is the 3-dimensional stream function. Substitution into the equivalent of Darcy's law yields $\nabla \times \underline{k}^{-1} \nabla \times \vec{\psi} = \vec{0}$. After having solved this equation the Darcy velocity \vec{q} can be calculated. Finally, the head is calculated from the head equation $\nabla \cdot \underline{k} \cdot \nabla \varphi = 0$. The equation for the 3D stream function has not the same form as the equation for the head. This means that conventional finite element techniques for determination of the head cannot be applied to the stream function formulation.

THE VELOCITY ORIENTED APPROACH IN THREE DIMENSIONS: VELOCITY BASED

To overcome this disadvantage, not the three stream function components, but the two horizontal head gradients $e_x = q_x/k_h$, $e_y = q_y/k_h$ and the vertical Darcy velocity q_z have been chosen as the primary variables. For a perfectly layered aquifer-aquitard system in which the hydraulic conductivities $k_x = k_y = k_h(z)$ (horizontal) and $k_z(z)$ (vertical) vary only in the vertical *z* direction, the equations to be solved are

$$\nabla \cdot \underline{\mathbf{k}} \cdot \nabla e_i = \frac{\partial}{\partial x} k_h \frac{\partial e_i}{\partial x} + \frac{\partial}{\partial y} k_h \frac{\partial e_i}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial e_i}{\partial z} = 0, (i = x, y),$$
(1.1)

$$\nabla \cdot \underline{\kappa}^{-1} \cdot \nabla q_z = \frac{\partial}{\partial x} \frac{1}{k_z} \frac{\partial q_z}{\partial x} + \frac{\partial}{\partial y} \frac{1}{k_z} \frac{\partial q_z}{\partial y} + \frac{\partial}{\partial z} \frac{1}{k_h} \frac{\partial q_z}{\partial z} = 0$$
(1.2)

Indeed, the above equations have the same form as the equation for the head

$$\nabla \cdot \underline{\mathbf{k}} \cdot \nabla \varphi = \frac{\partial}{\partial x} k_h \frac{\partial \varphi}{\partial x} + \frac{\partial}{\partial y} k_h \frac{\partial \varphi}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial \varphi}{\partial z} = 0$$
⁽²⁾

which means that standard finite element techniques can be applied (Nawalany, 1987a, 1987b, 1990, 1992).

Good results have been obtained with this version of the velocity oriented approach (VOA) in combination with the conventional node-based finite element method. It has been proven to yield a high accuracy for all three components of the Darcy velocity, including the relatively small vertical component; see Figures 1a-b. In addition, this VOA version has successfully been used to analyze the Dupuit approximation in aquifer-aquitard systems (Zijl, Nawalany, 1993).

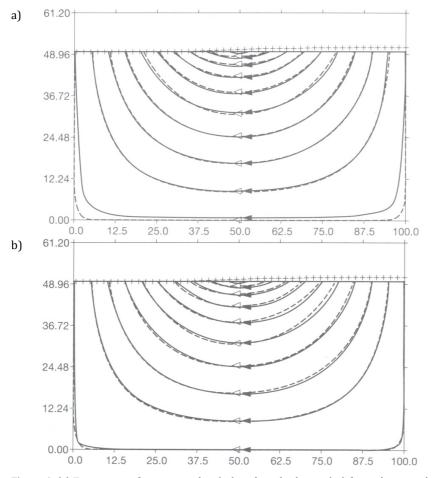


Figure 1. (a) Trajectories of water particles; (---) analytical solution, (—) finite element solution of velocity oriented approach; 605 nodes (121 horizontal × 5 vertical); (b) Trajectories of water particles; (---) analytical solution, (—) finite element solution of conventional head-based approach; 67240 nodes (1681 horizontal × 40 vertical).

It is important to note that equation (2) holds for all types of heterogeneity pattern of the hydraulic conductivity, while equations (1) hold only for perfectly layered patterns. To account for general heterogeneity additional terms can be added, but in these terms horizontal derivatives of the conductivities occur. This limits application of the velocity oriented approach to horizontally smoothly varying aquifer-aquitard systems. The remedy to overcome this disadvantage is the development of numerical techniques for the 3D stream function that differ from the techniques used for the head. In the 2000s Zijl and Nawalany (2004) found that a 3-dimensional stream function is feasible in the context of the finite volume method (FVM) and the mixed hybrid finite element method (MHFEM).

THE VELOCITY ORIENTED APPROACH IN THREE DIMENSIONS: STREAM FUNCTION BASED

Now we are in the right position to relate the velocity oriented approach (VOA) to the popular finite volume method (FVM) and its extension to non-rectangular grid volumes and general anisotropy, the mixed hybrid finite element method (MHFEM). In the velocity oriented approach the head is eliminated from Darcy's law. In addition stream functions $\Psi = (\Psi_{1},...,\Psi_{N_{c}})^{T}$

are introduced along the edges of the grid. The discretized system of algebraic equations for the stream function is $\mathbb{R}^T \Gamma \mathbb{R} \Psi = \mathbb{R}^T \Pi$. Matrix R is the grid's incidence matrix relating faces to edges. Array Π contains the head boundary conditions. Impedance matrix Γ contains the metrics of the grid combined with the inverses of the grid block conductivities. Using the simplest form of impedance matrix Γ the stream function equation is equivalent to the FVM (Mohammed, 2009; Mohammed et al., 2009). With a Galerkin-based Γ this equation is equivalent to the MHFEM. For details see the original introduction by Zijl and Nawalany (2004), who used the Galerkin-based VOA for generally shaped grid volumes and general anisotropy.

As an example we show 2-dimensional flow to a fully penetrating well. The 3-dimensional flow domain has a thickness of only one edge length (1 m) in the vertical direction. The grid consists of 225 grid blocks, 15 rows and 15 columns. The grid spacing in the horizontal directions equals 10 m. A well with a flow rate of $Q = 100 \text{ m}^3/\text{day}$ is situated in the central grid block (see Figure 2). Half of this flow rate is abstracted from the top face and half of it is abstracted from the bottom face of the well grid block.

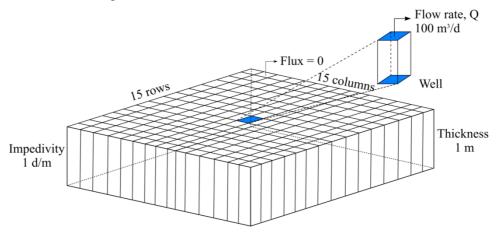


Figure 2. Illustration of the simulated system for the example.

Head boundary conditions were derived from the exact solution $\varphi = \gamma Q \ln r / 2\pi$, where $\gamma = k^{-1}$ is the impedivity (the inverse of the hydraulic conductivity), and $r = (x^2 + y^2)^{1/2}$. A stream function honors the continuity equation automatically, which means that for each internal grid block the inflow equals the outflow. Nevertheless, it is possible to apply a 2D stream function provided that the modeling domain is bounded by the positive *x* axis, with continuity of the Darcy velocity at y = 0 as boundary condition. Boundary conditions on such "cuts" in the modeling domain may be considered as a disadvantage of the stream function, especially if there are many wells in the modeling domain. This disadvantage is mitigated by introduction of the 3D stream function. In that case there is no need for cuts, because the nonzero flow into or out of the well grid block is arranged via the well grid block's top and bottom face. For more details of this particular example and of other examples see Mohammed (2009) and Mohammed et al. (2009).

SUMMARY, CONCLUSION AND FUTURE WORK

Although well developed, theoretically sound and applicable to complex subsoil conditions (3dimensional heterogeneity and anisotropy of rocks), the VOA method still does not find its way in general practice, as it possibly deserves. On one hand it promises to keep continuity and sufficient accuracy of the Darcy velocity in all three dimensions once the equations for the 3D stream function are solved. Applications that require a very accurate numerical estimation of relatively small vertical velocities, or require that the continuity equation is honored exactly, are becoming more and more important. Subtle water fluxes that need to be estimated in ecohydrological studies when assessing through-flows and mass transport within wetlands, or highly accurate calculations of inverse trajectories needed when trying to detect unknown sources of groundwater pollution are examples in which VOA might offer the expected solution. On the other hand, until recently the VOA, when applied to complex hydrogeological situations, has been considered "too complicated" even after (or, perhaps because of) adopting the existing (marketable) finite volume or finite difference software packages. It seems that, in order to get a breakthrough and to make VOA more popular, an appealing case study is needed (and financed). In this case study it can be clearly shown that that the accurate and continuous (exactly honoring the continuity equation) 3-dimensional estimate of the Darcy velocity is superior to the classical head-based approach. The superiority is to be well defined, either in terms of ultimate economics of the case, or just in terms of scientific accuracy of the physically estimated variables, or both.

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2-vol. set + CD ISSN 0208-6336 ISBN 978-83-226-1979-0