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THE VELOCITY ORIENTED APPROACH REVISITED

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Abstract. A great deal of hydrogeological situations requires an extremely accurate calculation of the 3-dimensional groundwater discharge rates 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. Numerical determination of the *vertical* groundwater velocity is a notoriously difficult problem. In nature this component may be two or three orders of magnitude smaller than the horizontal velocity components. In such cases application of Darcy's law to the numerically calculated hydraulic heads obtained from a finite difference or finite element model may lead to relatively inaccurate vertical velocities. More specifically, when estimating vertical velocity components in cases where the Dupuit approximation – negligible vertical head gradient – holds, numerical differentiation of hydraulic heads yields zero vertical velocity. In the 1980s of the last century Zijl and Nawalany proposed to invert the order of calculating the velocity field by eliminating the head from Darcy's law and to consider the Darcy velocity as the primary variable. For 2-dimensional flow this was already common practice and the challenge was a 3-dimensional extension, which was called the Velocity Oriented Approach (VOA). In two dimensions such methods were conventionally based on a stream function as primary variable. However, at that time application of a 3D stream function was not feasible and, therefore, the Darcy velocity itself was considered as the primary variable. This approach has been proven to yield a high accuracy for all three components of the specific discharge, including the relatively small vertical component, especially in cases where the subsoil is smoothly heterogeneous in the horizontal directions. In the 1990s the mixed-hybrid finite element method was developed. The physical interpretation of this method shows the way how to liberate the VOA from its smoothness requirement by introduction of a practical applicable 3D stream function. In conclusion, the velocity oriented approach indicates a change in paradigm regarding the accurate calculation of specific discharge in groundwater flow.

Key words: velocity oriented approach, continuity of water flux, groundwater flow modeling.

INTRODUCTION

A great deal of hydrogeological situations requires an extremely accurate quantification of the 3-dimensional groundwater flow velocity (Darcy velocity, specific discharge, flux density) 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. In nature this component may be two or even three orders of magnitude smaller than the horizontal velocity components. In such cases application of Darcy's law to the numerically calculated hydraulic heads obtained from a finite element or finite difference model may lead to relatively inaccurate vertical velocity components. More specifically, when estimating the vertical flow component in cases where the Dupuit approximation – negligible vertical head gradient – holds, numerical differentiation of hydraulic head yields zero vertical flow rate.

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THE VELOCITY ORIENTED APPROACH IN TWO DIMENSIONS: STREAM FUNCTION BASED

Let us consider 2-dimensional groundwater flow through a vertical cross section of the subsurface. The relation between the specific discharge (Darcy velocity) and the hydraulic head is given by Darcy's law

$$q_x = -k_x \frac{\partial \varphi}{\partial x}, \tag{1.1}$$

$$q_z = -k_z \frac{\partial \varphi}{\partial z}, \tag{1.2}$$

where:
$\varphi(x,z)$ – hydraulic head,
$q_x(x,z)$, $q_z(x,z)$ – components of the Darcy velocity in respectively the horizontal x direction and the vertical z direction.

Darcy's law [1] is well known. It is less known that Darcy's law is mathematically equivalent to a formulation from which the head is eliminated

$$\frac{\partial}{\partial z}\frac{q_x}{k_x} - \frac{\partial}{\partial x}\frac{q_z}{k_z} = 0. \tag{2}$$

The mathematical equivalence of equation [2] – in which the head does *not* occur – to Darcy's law [1] – in which the head occurs – may be considered as the fundamental principle upon which the velocity oriented approach (VOA) is based.

In 2-dimensional flow the two Darcy velocities are conventionally eliminated by introduction of a stream function $\psi(x,z)$ defined as

$$q_x = -\frac{\partial \psi}{\partial z}, \tag{3.1}$$

$$q_z = +\frac{\partial \psi}{\partial x}, \tag{3.2}$$

Thanks to the stream function, the continuity equation (in which the head does not occur)

$$\frac{\partial q_z}{\partial x} + \frac{\partial q_x}{\partial z} = 0. \tag{4}$$

is honored automatically. This follows immediately from substitution of equations [3] into equation [4] using the identity $\partial^2 f / \partial x \partial y \equiv \partial^2 f / \partial y \partial x$ for $f = \psi$. (The equivalence of equation [1] to equation [2] is based on this identity for $f = \varphi$.) Substitution of equations [3] into the equivalent form of Darcy's law [2] yields the equation for the stream function

$$\frac{\partial}{\partial x}\frac{1}{k_z}\frac{\partial \psi}{\partial x} + \frac{\partial}{\partial z}\frac{1}{k_x}\frac{\partial \psi}{\partial z} = 0. \tag{5}$$

Equation [5] can be solved by a conventional finite element model, in which the stream functions are assigned to the nodes of a finite element mesh (grid), for instance a mesh with triangular 2-cells. After having determined the stream functions in the nodes, the Darcy velocities – and hence the groundwater flow rates (fluxes) through the edges connecting the nodes – can be determined using equations [3]. Knowing the Darcy velocities, the heads in the centers of the grid cells (e.g. in the centers of the triangles) can be determined by integration of Darcy's law [1]; see, for instance, (Mohammed, 2009; Mohammed *et al.*, 2009). However, for many practical applications it is preferable to know the heads in the nodes of the mesh. The nodal heads follow directly – without calculation of the Darcy velocities – from the following well known equation obtained from substitution of Darcy's law [1] into continuity equation [4]

$$\frac{\partial}{\partial x} k_x \frac{\partial \varphi}{\partial x} + \frac{\partial}{\partial z} k_z \frac{\partial \varphi}{\partial z} = 0. \tag{6.1}$$

In a number of situations the solution of equation [6.1] may be such that the head is almost independent from the vertical direction; i.e., $\partial\varphi / \partial z \approx 0$. In such cases the vertical Darcy velocity cannot be calculated accurately from Darcy's law [1.2]. However, determination by the VOA based on equations [2] and [4] will do the job correctly.

Equation [6] for the head has the same form as equation [5] for the stream function. In the 1980s the finite element method was already a well established – and at that time popular – technique for determination of the head by solving equation [6]. Therefore, the stream function formulation could be implemented in a relatively simple way.

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 referred to as "gravitational systems of groundwater flow" (Tóth, 2009). In 3-dimensional flow systems the small vertical velocity component plays an important role (Nawalany, 1986a, b; Zijl *et al.*, 1987; Nawalany, 1990). In order to focus on an accurate determination of the Darcy velocities, it was proposed to base 3-dimensional flow calculation on the equivalent form of Darcy's law from which the head is eliminated, similar to what was common practice for 2-dimensional flow (section 1.1). This extension to 3-dimensional flow was called the velocity oriented approach (VOA). In a more or less similar, but mathematically more complex way than presented in section 1.1, a 3-dimensional stream function can be introduced (see Appendix A). Moreover, like in the 2-dimensional case, it is "better" for a number of applications to determine the head directly from the 3-dimensional head equation

$$\frac{\partial}{\partial x} k_x \frac{\partial \varphi}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial \varphi}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial \varphi}{\partial z} = 0 . \qquad [6.2]$$

In section 1.1 we have shown the similarity between 2-dimensional stream function equation [5] and 2-dimensional head equation [6.1]. Unfortunately, such a similarity does not exist for 3-dimensional flow. The 3-dimensional stream function equation (Appendix A, equation [A.1]) has not the same form as the 3-dimensional head equation [6.2]. As a consequence, the well known finite element techniques for the determination of the head cannot be applied in a simple way to the stream function formulation.

THE VELOCITY ORIENTED APPROACH IN THREE DIMENSIONS: VELOCITY BASED

To overcome this disadvantage of the 3-dimensional stream function, not the three stream function components ψ_x, ψ_y, ψ_z, 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

$$\frac{\partial}{\partial x} k_h \frac{\partial e_x}{\partial x} + \frac{\partial}{\partial y} k_h \frac{\partial e_x}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial e_x}{\partial z} = 0 , \qquad [7.1]$$

$$\frac{\partial}{\partial x} k_h \frac{\partial e_y}{\partial x} + \frac{\partial}{\partial y} k_h \frac{\partial e_y}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial e_y}{\partial z} = 0 , \qquad [7.2]$$

$$\frac{\partial}{\partial x} \frac{1}{k_z} \frac{\partial q_z}{\partial x} + \frac{\partial}{\partial y} \frac{1}{k_z} \frac{\partial q_z}{\partial y} + \frac{\partial}{\partial z} \frac{1}{k_h} \frac{\partial q_z}{\partial z} = 0 . \qquad [7.3]$$

The above equations [7] have the same form as equation [6.2] for the head, which means that standard finite element techniques can be applied, not only to calculate the head (equation [6.2]), but also to calculate the "velocity components" e_x, e_y and q_z in the nodes of a finite element mesh (Nawalany, 1986a, b, 1990, 1992).

Good results have been obtained with this version of the velocity oriented approach (VOA) in combination with a conventional node-based finite element model (in which the head values are assigned the nodes of the mesh). It has been proven to yield a high accuracy for all three components of the specific discharge, including the relatively small vertical component; see Figures 1–3. In addition, this VOA version has successfully been used for asymptotic expansions to analyze the Dupuit approximation and its consequences for the relatively small vertical groundwater flow rates in aquifer-aquitard systems (Zijl, Nawalany, 1993).

It is important to note that equation [6.2] holds for all types of heterogeneity pattern of the hydraulic conductivity, while equations [7] hold only for perfectly layered patterns. To account for general heterogeneity additional terms can be added to equations [7]. However in these terms horizontal derivatives of the conductivities occur. This smoothness requirement limits application of the velocity oriented approach to aquifer-aquitard systems that vary smoothly in the horizontal directions. The remedy to overcome this disadvantage is the development of finite element or finite difference techniques for the 3D stream function that differ from the techniques used for the head. On the other hand, we want to use as much as possible the already available discretization techniques.

Until now we have tacitly assumed that quantities like head, stream function and velocity components have to be assigned to the nodes of a mesh (grid). In the 2000s the authors of this paper discovered that, if the values of the 3-dimensional stream function are not assigned to the

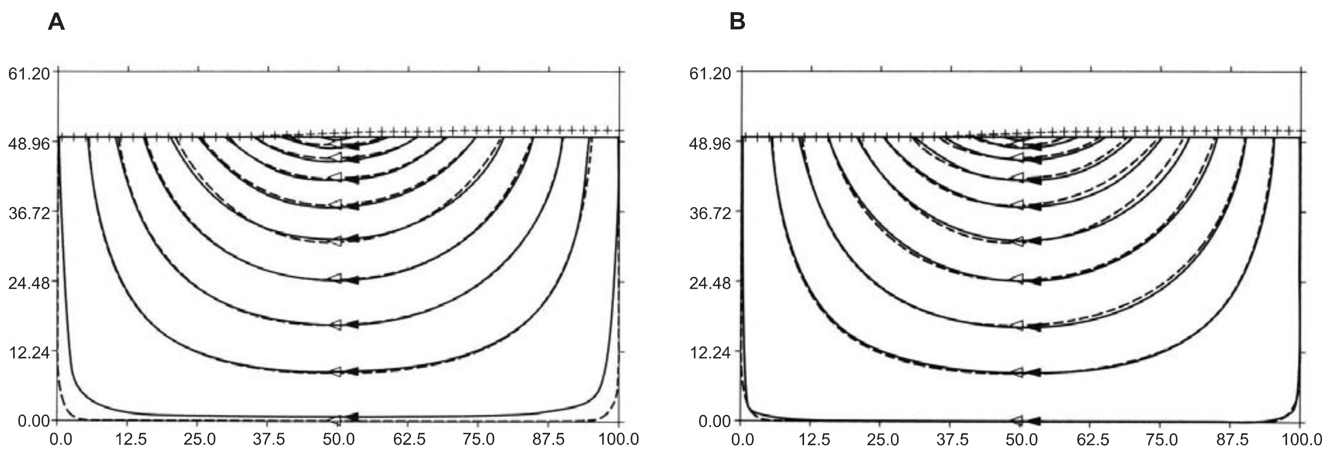

Fig. 1. Trajectories of water particles; (dashed line) analytical solution, (solid line) finite element solution of velocity oriented approach

A – 605 nodes (121 horizontal, 5 vertical); **B** – 67240 nodes (1681 horizontal, 40 vertical)

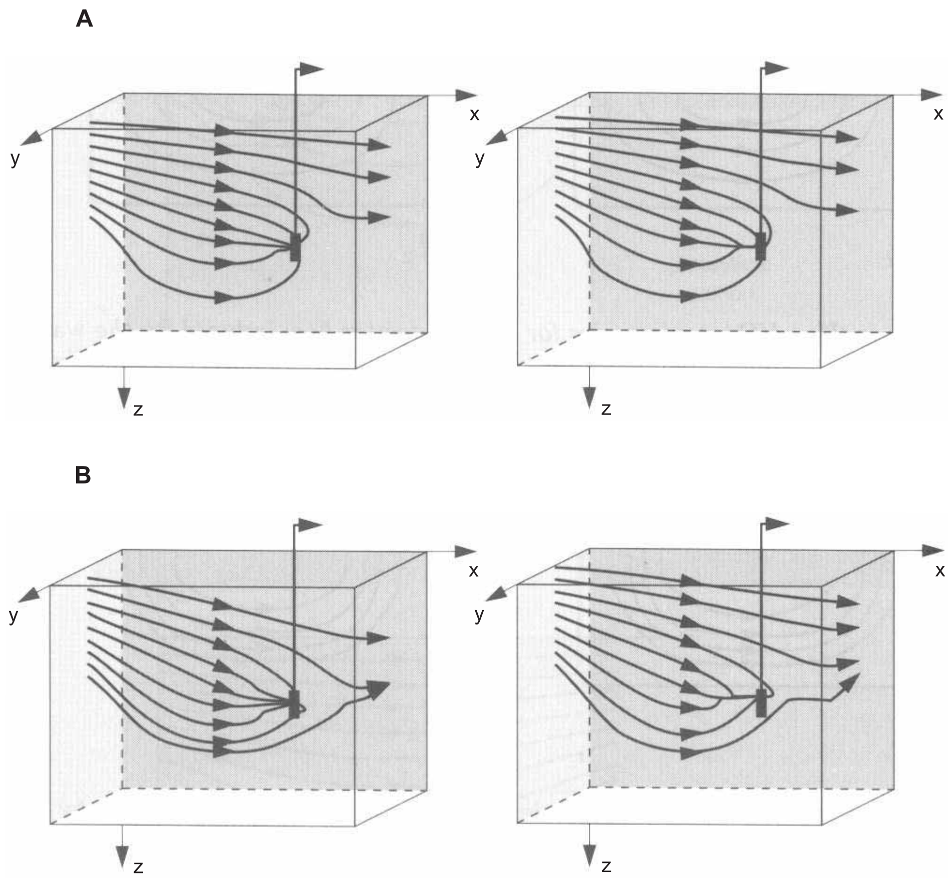

Fig. 2. A. VOA trajectories for groundwater flow partly induced by head differences between the vertical boundaries and partly induced by a pumping well. Left: finite element model with 300 nodes; right: finite element model with 1200 nodes. B. Classical head-based trajectories for groundwater flow partly induced by head differences between the vertical boundaries and partly induced by a pumping well. Left: FEM 300 nodes; right: FEM 1200 nodes. The classical approach is heavily dependent on the discretization, while the VOA is not (see Fig. 2A; also see Figures 1A, B)

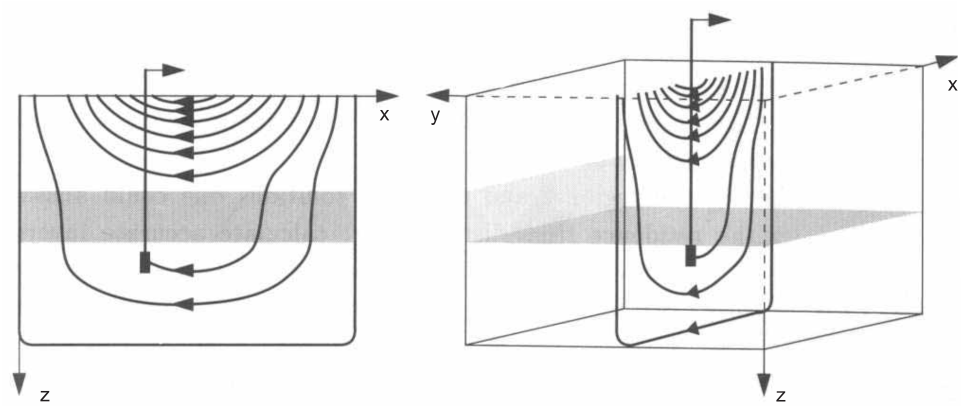

Fig. 3. Well located below a semi-pervious layer can intercept some trajectories (anisotropy ratio 1:100)

nodes, but to the edges (lines connecting nodes), they can be calculated in a relatively simple way. Moreover, it turned out that this edge based 3-dimensional stream function can be considered as a "missing links" in the well known block centered finite difference method (also called finite volume method) and in the (less known, but not unknown) mixed hybrid finite element method (Zijl, Nawalany, 2004).

However, before explaining this stream function version of the velocity oriented approach in section 3, we will first consider the finite volume method and the related mixed hybrid finite element method in section 2.

FINITE VOLUME AND FINITE FACE METHODS

During the 1990s the mixed-hybrid finite element method was introduced in hydrogeological practice (Kaasschieter, 1990; Kaasschieter, Huijben, 1992; Trykozko, 1997; Trykozko *et al.*, 2004). Unlike the block centered finite difference method (finite volume method), the mixed-hybrid finite element method can handle non-rectangular grid volumes and general anisotropy of the hydraulic conductivity (anisotropy in which the principal conductivities are not aligned with Cartesian grid block directions). Unfortunately, almost without exception, the mixed hybrid finite element method is explained in an overly mathematical way, which impedes its acceptance by the hydrogeological community. To "rehabilitate" this excellent method, an alternative introduction to the finite volume method and the mixed hybrid finite element method based on relatively simple algebra is presented in respectively sections 2.1 and 2.2.

FINITE VOLUME METHOD

We consider a grid (mesh) with volumes (not necessarily rectangular grid blocks), faces (each face connects two volumes), edges (connection two nodes) and nodes. On this grid the continuity equation is written as a matrix-vector equation (in short-hand notation $DQ = 0$; see Appendix B for more details). In a more or less similar way we can also write Darcy's law as a matrix-vector equation (in short-hand notation $D^T \Phi - \Pi = \Gamma Q$; for details see Appendix B). Vector Q contains the flow rates (fluxes) through the faces, vector Φ contains the heads in the centers of the grid volumes, and vector Π represents the heads on the boundary of the modeling domain (and in the wells). Matrix Γ is the impedance matrix (or resistance matrix) containing the hydraulic resistances experienced by the groundwater flux through the faces under the influence of the head differences between the faces.

In the block centered finite difference method (finite volume method), the grid volumes are rectangular blocks with edges in the x, y and z directions; also the principal axes of the conductivity matrix are in the x, y and z directions. In that case the hydraulic resistance experienced by the flux through a face is only influenced by the head difference between that face, not by head differences between other faces. As a result impedance matrix Γ is a diagonal matrix. Its inverse, Γ^{-1}, is also a diagonal matrix; each components is equal to the well known harmonic average of the two conductivities in the grid block joining a face. In that case we can easily determine system matrix $M = D\Gamma^{-1}D^T$ and right-hand side vector $B = D\Gamma^{-1}\Pi$ to find the system of algebraic equations $M\Phi = B$ (for more details see Appendix B). The solution of this system can be obtained by well established numerical techniques (for instance, preconditioned conjugate gradients; Kaasschieter, 1988). At present this method is extremely well known (although the derivation of the equations is generally presented in a different way). For instance, the popular groundwater flow package MODFLOW is based on it.

FINITE FACE METHOD

If the grid volumes are not rectangular, or if the principal directions of the conductivity are not aligned with the edge directions, impedance matrix Γ can be determined by a simple Galerkin method (Zijl, Nawalany, 2004; Zijl, 2005). However, in this case the impedance matrix is no longer a diagonal matrix. As a consequence, it is impossible from a computational point of view to determine system matrix M and right-hand side vector B, except if the modeling domain is partitioned into only a few volumes. For a domain with one grid volume the head in this volume center can be calculated in a simple way. This way we can find a relation between the six face-based fluxes and the six face centered heads (see Appendix B). Having found this relation we consider a domain partitioned into many such "one-grid – volume-domains". Requiring continuity of fluxes and heads at the faces, we end up with a linear system of algebraic equations for the heads in the face centers, from which the heads can be solved by well established numerical techniques (for instance, preconditioned conjugate gradients; Kaasschieter, 1988; 1990). For more details see Appendix B.

This method has successfully been applied in hydrogeology by Kaasschieter, Huijben (1992) and Trykozko (Trykozko, 1997; Trykozko *et al.*, 2004); see Figure 4.

Unfortunately, in the literature this method is, almost without exception, presented in an overly mathematical way, which impedes acceptation by the hydrogeological community. The generally accepted name of the method, "mixed hybrid finite element method", reflects its history of "mathematical discovery". To a hydrogeologist who wants to be able to communicate with the "mixed hybrid finite element community," it is advised read a clear introduction to the generally accepted mathematical framework; for instance the introduction presented by Kaasschieter (Kaasschieter 1990; Kaasschieter, Huijben, 1992). In fact, the name mixed hybrid finite element method is a misnomer, because a mixed method is a method that solves both the head and the Darcy velocity simultaneously. However, as we have seen above, the mixed hybrid finite element method solves the heads in the centers of the finite faces (in the conventional "mathematical presentation" these heads are called the "Lagrange multipliers"). Only after having solved the Lagrange multipliers (i.e., the heads) the velocities are determined from these heads. As has been shown by our above-presented much more simple alternative introduction

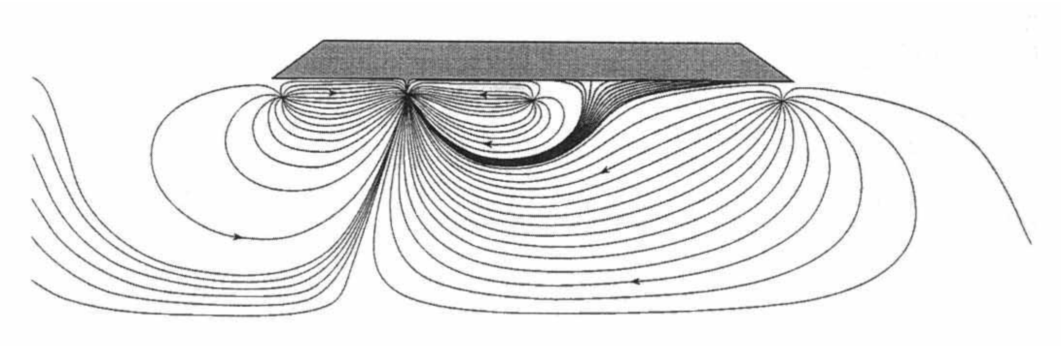

Fig. 4. Waste disposal with horizontal pumping and injection wells for hydraulic isolation (after Trykozko, 1997)

(also see Appendix B), a better name would be face centered finite element method, or finite face method.

If the grid volumes are rectangular blocks with edges in the x, y and z directions and if also the principal axes of the conductivity matrix are in the x, y and z directions, the finite volume method is generally applied. However, the finite face method could be applied as an alternative. The two methods are very different from an algorithmic point of view (block centered vs. face centered). Also from an algebraic point of view the two methods differ, because the finite volume method is based on a finite difference impedance matrix, while the finite face method (or mixed hybrid finite element method) is based on a Galerkin impedance matrix. However, it has been proven by Weiser and Wheeler (1988) that, if the grid volumes are rectangular blocks with conductivities along the x, y and z directions, the finite difference impedance is a good approximation of the Galerkin impedance. Therefore, in this case the finite volume method will yield almost the same solution as the finite face method.

VELOCITY ORIENTED APPROACH IN THREE DIMENSIONS: STREAM FUNCTION BASED

The above-presented interpretation of the finite volume method and the finite face method (mixed hybrid finite element method) brings us in the right position to base the velocity oriented approach (VOA) on the 3-dimensional stream function. As has been emphasized in section 1, the velocity oriented approach is based on elimination of the head from Darcy's law. To do so we need a matrix (denoted as R^T) with the property that it eliminates the head from the discretized version of Darcy's Law (see Appendix B). In addition we introduce a vector of edge based stream functions Ψ such that $Q = -R\Psi$(in analogy with equation [3]). Thanks to the stream function the continuity equation (inflow = outflow) is honored automatically for each grid volume. The "discovery" was that the stream function values had not to be assigned to the nodes of the grid, as conventional, but to the *edges*. Finally, the discretized equation for the edge based stream function is

$$R^T \Gamma R \Psi = R^T \Pi \ . \qquad [8]$$

For an explanation of the meaning of matrix R see Appendix C.

With a Galerkin-based impedance matrix this version of the VOA is equivalent to the finite face method (i.e., the mixed hybrid finite element method). For more details see the original introduction to the VOA by Zijl and Nawalany (2004). This VOA version has been used with the Galerkin-based impedance matrix by Zijl and Nawalany (2004) for generally shaped grid volumes and general anisotropy. This VOA version has also been used with the finite difference impedance matrix by Mohammed (2009); also see (Mohammed *et al.*, 2009). In this case the method is equivalent to the finite volume method (MODFLOW, say).

As an example we consider 2-dimensional flow to a fully penetrating well. The 3-dimensional flow domain has relatively large dimensions in the horizontal directions, but has a thickness equal to only one edge length in the vertical direction. The grid consists of 225 grid blocks in 1 layer with 15 rows and 15 columns. The layer thickness equals 1 m and the grid spacing in the horizontal directions equals 10 m. A well is situated in the central grid block with an assumed flow rate of Q = 100 m^3/day (see Fig. 5). Half of this flow rate is abstracted from the top face and half of is abstracted from the bottom face of the well grid block. Head boundary conditions were derived from the exact solution $\varphi = \gamma Q \ln r / 2\pi$, where $r = (x^2 + y^2)^{1/2}$. The system of linear algebraic equations was solved by a conjugate gradient method with diagonal preconditioning.

In section 1.1 authors have shown that a 2-dimensional stream function honors the continuity equation automatically. This means that for each internal grid block the inflow equals the outflow. Nevertheless, wells can be modeled by the 2-dimensional stream function $\psi = Q\theta / 2\pi$. Here θ is

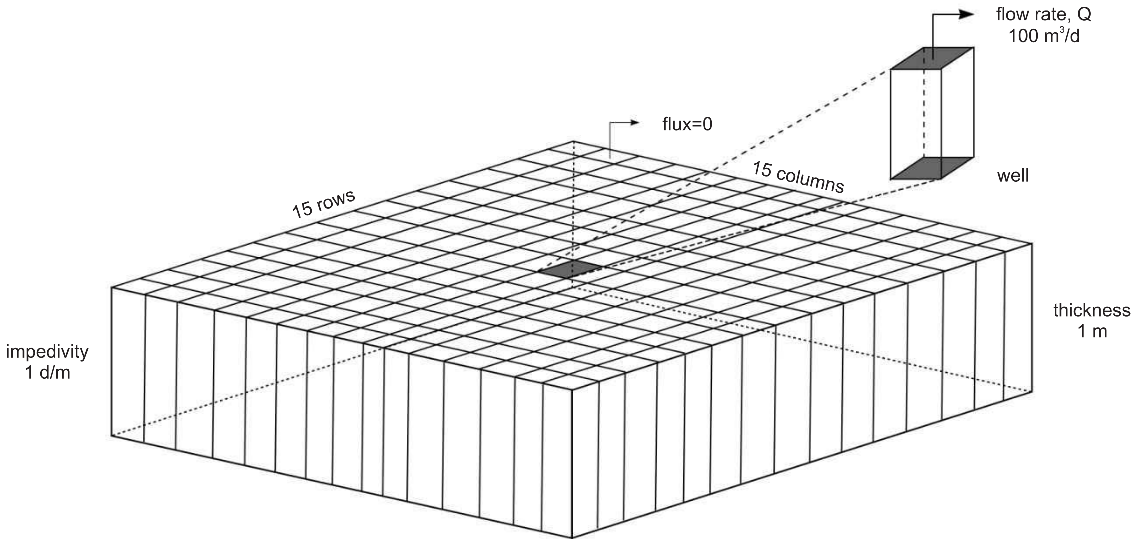

Fig. 5. Illustration of the simulated system

the angular coordinate of a circular coordinate system with $0 \leq \theta < 2\pi$. This stream function equals 0 (zero) at $\theta = 0$ and Q at $\theta \to 2\pi$. As a consequence, both from the side $y \downarrow 0$ and from the side $y \uparrow 0$ the modeling domain is bounded by the positive x axis, with continuity of the flow 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 method, especially if there are many wells in the modeling domain. This disadvantage is mitigated by the introduction of the 3D stream function. In this case there is no need for cuts (internal boundaries), because the nonzero flow into or out of the well grid block is arranged via the third dimension (via the well grid block's top and bottom face). This example also demonstrated that the 3D stream function differs from the 2D stream function, and that the stream function method can be used to simulate wells and other complex situations. 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 (3-dimensional heterogeneity and anisotropy of rocks), the velocity oriented approach (VOA) still does not easily find its way in general hydrogeological practice. One of the reasons might be that the mixed hybrid finite element method, to which the VOA is related, is generally presented in a mathematical terminology that is almost incomprehensible to practical hydrogeologists (see section 2.2). The authors have shown that a much more comprehensible explanation is possible, which open the way to greater acceptance: the VOA deserves it.

On one hand the VOA 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 eco-hydrological 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 the VOA might offer the expected solution.

An additional promise of the VOA is that its equations are linear in the impedivities (the inverses of the hydraulic conductivities). As has been shown and exemplified by Mohammed (2009) this offers possibilities for direct inverse modeling; that is determination of hydraulic conductivities by solving a linear system of algebraic equations for the impedivities.

Coming back to what has been mentioned above, 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 the accurate and continuous (exactly honoring the continuity equation) 3-dimensional estimate of the specific discharge 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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APPENDIX A: The 3-dimensional stream function

Darcy's law $\vec{q} = -\underline{k} \cdot \nabla\varphi$ – in which the head occurs – is mathematically equivalent to $\nabla \times k^{-1} \cdot \vec{q} = \vec{0}$ – from which the head is eliminated. In addition, the continuity equation $\nabla \cdot \vec{q} = 0$ – in which the head does not occur – is equivalent to $\vec{q} = -\nabla \times \vec{\psi}$, where vector $\vec{\psi}$, is the 3-dimensional stream function (or vector potential). Substitution into the equivalent form of Darcy's law yields

$$\nabla \times \underline{k}^{-1} \nabla \times \vec{\psi} = \vec{0}\,. \qquad [A.1]$$

After having solved $\vec{\psi}$ from this equation the Darcy velocity $\vec{q}$ can be calculated. Finally, using Darcy's law the head follows from integration of $\mathrm{d}\varphi = (k_x^{-1} q_x \mathrm{d}x + k_y^{-1} q_y \mathrm{d}y + k_z^{-1} q_z \mathrm{d}z)$ along an arbitrary path. Like in the 2-dimensional case, it is sometimes more practical (and "safer" from a numerical point of view) to determine the head directly from the 3-dimensional head equation

$$\nabla \cdot \underline{k} \cdot \nabla\varphi = 0\,. \qquad [A.2]$$

APPENDIX B: Alternative formulation of the mixed hybrid finite element method

We consider a grid (mesh) with N_V volumes, N_F faces, N_E edges and N_N nodes. On this grid the continuity equation (inflow = outflow) is represented by the matrix-vector equation

$$\begin{pmatrix} D_{11} & \dots & D_{1N_F} \\ . & . & . \\ D_{N_V 1} & \dots & D_{N_V N_F} \end{pmatrix} \begin{pmatrix} Q_1 \\ . \\ . \\ . \\ Q_{N_F} \end{pmatrix} = \begin{pmatrix} 0 \\ . \\ 0 \end{pmatrix}, \qquad [B.1]$$

in short hand notation written as matrix-vector equation DQ = 0. Q_f is the flux (flow rate) through face f; it is a component of flux vector Q. In a more or less similar way, on this grid we can write Darcy's law as

$$\begin{pmatrix} D_{11} & \dots & D_{N_V 1} \\ . & . & . \\ . & . & . \\ . & . & . \\ D_{1N_F} & \dots & D_{N_V N_F} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ . \\ \varphi_{N_V} \end{pmatrix} - \begin{pmatrix} \pi_1 \\ . \\ . \\ . \\ \pi_{N_F} \end{pmatrix} = \qquad \text{[B.2]}$$

$$= \begin{pmatrix} \Gamma_{11} & \dots & \Gamma_{1N_F} \\ . & \dots & . \\ . & \dots & . \\ . & \dots & . \\ \Gamma_{1N_F} & \dots & \Gamma_{N_F N_F} \end{pmatrix} \begin{pmatrix} Q_1 \\ . \\ . \\ . \\ Q_{N_F} \end{pmatrix},$$

in short hand notation written as matrix-vector notation $D^T\Phi - \Pi = \Gamma Q$. For an explanation of the meaning of matrix D see Appendix C. Here φ_v is the head in the center of grid volume v, while π_f is plus or minus the head on boundary face f; on internal faces $\pi_f = 0$. Γ_{fg} is a component of impedance (resistance) matrix Γ denoting the hydraulic resistance experienced by the flux through face f under the influence of the head difference between face g. If Γ is a diagonal matrix, its inverse, Γ^{-1}, can simply be determined. In that case substitution of equation [B.1] into equation [B.2] yields (in short-hand matrix-vector notation)

$$D\Gamma^{-1}D^T\Phi = D\Gamma^{-1}\Pi \,. \qquad \text{[B.3]}$$

Equation [B.3] is equivalent to the system of algebraic equations MΦ = B upon which the block centered finite difference method (e.g. the popular MODFLOW model) is based.

If Γ is not a diagonal matrix, its inverse cannot efficiently be determined numerically, except for a domain with only a few grid volumes. For one grid volume the head in the volume center can simply be determined as $\Phi = (D\Gamma^{-1}D^T)^{-1}D\Gamma^{-1}\Pi$. Substitution into equation [B.2] relates the six face-based fluxes to the six face centered heads $Q = \Gamma^{-1}[D^T(D\Gamma^{-1}D^T)^{-1}D\Gamma - I]\Pi$. Now we consider a domain partitioned into many such "one-grid-volume-domains". Requiring continuity of fluxes and heads at the faces, we end up with a system of linear algebraic equations for the heads in the face centers, from which the heads can be solved by well established numerical techniques (Kaasschietter, 1988; 1990). For more details see (Zijl, 2005).

APPENDIX C: Incidence matrices

Matrix D is the grid's incidence matrix relating volumes to faces. If volume v is not connected to face f, $D_{vf} = 0$. If there is a connection $D_{vf} = \pm 1$, the plus (+) sign holds if the orientation of face f points out of volume v, otherwise the sign is minus (–).

Matrix R is the grid's incidence matrix relating faces to edges. If face f is not connected to edge e, component $R_{fe} = 0$. If there is a connection $R_{fe} = \pm 1$, the plus (+) sign holds if the orientation of edge e matches with the orientation of face f, otherwise the sign is minus (–).