Streamline-oriented grid generation for transport modeling in two-dimensional domains including wells

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Flownets are useful tools for the visualization of groundwater flow fields. Using orthogonal flownets as grids for transport modeling is an effective way to control numerical dispersion, especially transverse to the direction of flow. Therefore tools for automatic generation of flownets may be seen both as postprocessors for groundwater flow simulations and preprocessors for contaminant transport models. Existing methods to generate streamline-oriented grids suffer from drawbacks such as the inability to include sources in the interior of the grid. In this paper, we introduce a new method for the generation of streamline-oriented grids which handles wells in the grid interior, and which produces orthogonal grids for anisotropic systems. Streamlines are generated from an accurate velocity field obtained from the solution of the mixed-hybrid finite element method for flow, while pseudopotentials, which are orthogonal to the streamlines, are obtained by a standard finite element solution of the pseudopotential equation. A comprehensive methodology for the generation of orthogonal grids, including the location of stagnation points and dividing streamlines, is introduced. The effectiveness of the method is illustrated by means of examples. A related paper presents a compatible formulation of the solution for reactive transport, while a second related paper gives a detailed quantitative assessment of the various forms of modeled mixing and their effect on the accuracy of simulations of the biodegradation of groundwater contaminants. © 1999 Elsevier Science Ltd. All rights reserved

1 INTRODUCTION

Flownets are classical tools for quantitative analysis and qualitative interpretation of two-dimensional flow fields such as for regional groundwater flow. They are useful for the visualization of flow fields, the delineation of capture zones and may be applied as streamline-oriented grids for contaminant transport models. Since standard flownets consist of potential-lines and streamlines, they may be constructed automatically by solving for the distribution of piezometric heads and streamfunction values. This approach, referred to as dual formulation, was introduced in the mid 80’s and refined in the following years.4,13,17,25 A specific purpose of this development was the use of streamline-oriented grids for the numerical simulation of contaminant transport in groundwater by the principal direction (PD) technique14,18,19 which was successfully applied in conservative and reactive transport studies.15,16,20,23,24,31

The main advantage of the PD technique is that the advective mass fluxes are always oriented into a principal direction of the grid. Additionally, in streamline coordinates the dispersion tensor is a diagonal matrix.
These two effects not only simplify the solution of the advection-dispersion equation but also suppress any numerical dispersion transverse to the direction of flow. The latter may be of specific significance in the context of multi-component reactive transport. In many set-ups insufficient mixing limits the (bio)reactive interaction of dissolved compounds. By using artificially dispersive schemes for reactive transport, mixing of the compounds may be overestimated in model calculations. This leads to unrealistically high reaction rates and consequently unrealistically short plumes of contaminants. Therefore, the most attractive application of streamline-oriented grids is for modeling of reactive transport controlled by transverse mixing.

The original dual formulation for construction of streamline-oriented grids was restricted to isotropic hydraulic conductivity fields in two-dimensional domains without interior sources or sinks such as wells. The restriction of isotropy was overcome by the introduction of pseudopotentials in the construction of flownets. However, since no unique streamfunction value can be defined for flow fields with interior sources and sinks, wells could only be handled if they were part of the exterior boundary. If a well was located within the domain, the latter had to be cut from the exterior boundary to the well, the well itself was excluded, and special transmission conditions had to be defined along the cut to ensure the continuity of the flow field. As a direct consequence of this approach, a jump in the streamfunction values by an amount of the well’s discharge occurred at the cut. This complicated the construction of streamline-oriented grids for transport modeling. Also no effort was made to automatically detect stagnation points and dividing streamlines which are crucial for the determination of capture zones. As a result of these complications, the authors are not aware of any practical application of the PD method on streamline-oriented grids to cases with interior wells, although the treatment of wells was already described in the first paper of Frind and Matanga.

In this paper we recast the conventional streamfunction formulation to obtain an efficient capability to generate flownets and flownet-oriented grids for the simulation of conservative and reactive transport in anisotropic 2-D heterogeneous media. The mixed-hybrid finite element method is used for the accurate calculation of velocities and the generation of streamlines. In contrast to the dual formulation, no global evaluation of the streamfunction is performed. Therefore, cutting the domain in order to handle wells is avoided. The method detects stagnation points and dividing streamlines and can thus efficiently handle multiple wells. This is a significant improvement over existing methods for automatic generation of flownets and streamline-oriented grids. Applying the grids to models for the transport of interacting compounds effectively removes the influence of numerical dispersion from the representation of the reactive process.

Two related papers complement this paper. The first, (Cirpka et al.), gives the theoretical development of a stabilized finite volume method for reactive transport based on the streamline-oriented grids. The second, (Cirpka et al.), presents a detailed quantitative exploration of the various causes and effects of modeled mixing, including the effect of grid orientation using the method developed in this paper. While the related papers focus on numerical dispersion due to insufficient grid orientation and its effect on the simulation of (bio)reactive transport, the grids constructed with the methods of the present paper may also be used for the visualization of groundwater flow fields independent of performing transport calculations.

2 GOVERNING EQUATIONS

This paper is restricted to two-dimensional saturated groundwater flow at steady state. All applications presented are for confined conditions.

For given boundary conditions and a given distribution of the hydraulic conductivity tensor $K$, piezometric heads $h$ and volumetric fluxes $\vec{q}$ can be evaluated from the continuity equation which is for steady-state conditions:

$$\nabla \cdot \vec{q} = q_s$$

with $q_s$ being a source/sink term representing e.g. wells. The volumetric flux can be evaluated by Darcy’s law:

$$\vec{q} = -K \nabla h.$$  

(2)

For two-dimensional domains free of sources and sinks, a streamfunction $\psi$ can be determined. Values of the streamfunction are constant along streamlines and therefore eqn (3) holds:

$$q_s = -\frac{\partial \psi}{\partial y}, \quad q_t = \frac{\partial \psi}{\partial x}.$$  

(3)

Considering that groundwater flow is irrotational one finds after some rearrangements:

$$\nabla \cdot (K_\psi \nabla \psi) = 0$$

(4)

with the conductivity for the streamfunction $K_\psi$ as defined by:

$$K_\psi = \frac{1}{\det(K)} K.$$  

(5)

Unfortunately the application of streamfunctions is restricted to source–sink-free domains. This restriction may be overcome by excluding the direct neighbourhood of wells by means of a cut. In this way the wells become part of the exterior boundary. Note that special transmission conditions must be defined along the cut in order to achieve conforming fluxes.

As an alternative to solving eqn (4) for the entire domain, streamfunctions may be evaluated by integra-
tion of eqn (3) which requires an accurate and conforming approximation of the velocity field.\textsuperscript{12,27} For the purpose of constructing streamlines, this may be done locally thus circumventing the non-uniqueness of streamfunction values in domains including wells. This approach is applied in the present study.

In case of isotropic hydraulic conductivities, streamlines and lines of equal piezometric head are orthogonal to each other. This does not hold for anisotropic hydraulic conductivities. For most applications orthogonality of streamlines and isopotentials is not required. However, if the results of flow calculations are used for the construction of streamline-oriented grids, a non-distorted, orthogonal grid will be preferred. For this purpose, pseudopotentials $\phi$ may be defined.\textsuperscript{25} Pseudopotential lines are always orthogonal to streamlines. Hence pseudopotentials satisfy:

$$\bar{q} = -K_\phi \nabla \phi$$

in which $K_\phi$ is the scalar pseudopotential conductivity discussed in Section 3.2. For steady-state flow, pseudopotentials $\phi$ satisfy the same type of elliptic partial differential equation [eqn (7)] as the streamfunction $\psi$ and the hydraulic head $h$:

$$\nabla \cdot (K_x \nabla \phi) = 0$$

and may therefore be solved by the same numerical methods. Note that the existence of pseudopotentials for anisotropic and heterogeneous hydraulic conductivities is guaranteed a priori only for two-dimensional flow fields. In three-dimensional applications such as those presented by Matanga\textsuperscript{26}, the existence of pseudopotentials requires the orthogonality of the specific discharge vector and its vorticity within the entire domain (see Chapter 3.4.1 of Bear’s textbook\textsuperscript{3}).

3 CALCULATION OF FLOW

For the construction of flownets both the distribution of hydraulic heads and the velocity field should be as accurate as possible. In order to achieve unique streamlines on an elemental basis, the mass balance must be met element by element and the normal components of the velocities must be conforming across the elemental interfaces. These requirements are not met by the standard FEM applied to the multi-dimensional groundwater flow equation followed by consistent postprocessing for the construction of streamlines.\textsuperscript{12} While the standard FEM solution for the groundwater flow equation is second-order accurate for the heads, the direct FEM solution for the streamfunction meets the requirement of high-order velocity approximation. The latter approach also correctly approximates the flow field in the vicinity of discontinuities. The combination of the FEM solutions for hydraulic heads and the streamfunction values is referred to as dual formulation\textsuperscript{17} and was used for the automatic construction of flownets.

In domains including interior wells, unfortunately, the direct FEM solution for the streamfunction is not possible. However, the same accuracy of the flow field can be achieved by using mixed or mixed-hybrid FEM for the original groundwater flow problem. Mosé \textit{et al.}\textsuperscript{27} as well as Durlofski\textsuperscript{12} presented comparisons for triangular meshes. The authors of the present study showed in unpublished tests that the velocity fields obtained by the direct FEM solution for the streamfunction and the mixed FEM for the original groundwater flow problem were identical on quadrilateral meshes.

In the present paper, the mixed-hybrid FEM is used to achieve accurate velocity fields. This accuracy is to be paid with an computational effort about twice as high as in the case of the standard FEM or the FVM.\textsuperscript{6} Since the results are used for the construction of flownets yielding grids for transport calculations, pseudopotentials need to be evaluated. Calculation of pseudopotentials by consistent postprocessing of the simulated flow field leads to non-conforming distributions.\textsuperscript{7} The latter may cause non-unique solutions for the construction of pseudopotential-lines and should therefore be avoided. As a consequence, a separate calculation of pseudopotentials using the standard FEM is performed. This guarantees a continuous pseudopotential distribution.

3.1 Mixed-hybrid finite element method for calculation of velocities

The principles of the mixed FEM are only briefly stated here; a more detailed description of the method and its underlying concept can be found e.g. in the review of Chavent.\textsuperscript{6} Note that only the simplest case of mixed FEM is discussed. This is the space of lowest order \textit{Raviart—Thomas} (RT$_0$) functions.\textsuperscript{28} Higher order approximations are discussed e.g. by Brezzi and Fortin.\textsuperscript{5}

In contrast to the standard FEM, in the mixed approach both volumetric fluxes $\bar{q}$ and hydraulic heads $h$ are taken as primary unknowns. For two-dimensional quadrilaterals, the four normal fluxes across the edges $a$–$d$ (see Fig. 1) and one head constant over the element are chosen in the RT$_0$ case.

The shape and weighting function $N_h$ for the piezometric head $h$ is simply the unity constant over the entire element, whereas the velocity components $q_1$ and $q_2$ inside the element are evaluated by interpolation of the normal fluxes across the edges $\bar{Q}$ by the shape function $N_q$.

For the continuity equation [eqn (1)] the hydraulic head $h$ is taken as the primary unknown, while for Darcy’s law [eqn (2)] the normal fluxes $\bar{Q}$ are taken as primary unknowns. In both cases, the Galerkin procedure and partial integration is applied. This leads to the following equations for each element with the volume $V$ and the boundary $B$: 

$$\bar{Q} = -K_q \nabla \bar{Q}$$

in which $K_q$ is the scalar pseudopotential conductivity discussed in Section 3.2. For steady-state flow, pseudopotentials $\phi$ satisfy the same type of elliptic partial differential equation [eqn (7)] as the streamfunction $\psi$ and the hydraulic head $h$:

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in which \( \nabla \cdot N_q \) is the divergence of \( N_q \). Note that with the introduction of \( Q_s \) in eqn (8) the recharge is homogeneously distributed over the element. This is of particular interest for the definition of wells.

\( \vec{h}_B \) is the vector of hydraulic heads at the edges. In case of constant normal fluxes across the edges, these edge heads are constant over the edges as well. However, they differ from the head in the interior of the element so that the spatial approximation of heads is discontinuous.

Under application of a discretization scheme in time, in the mixed FEM (eqn (8)) is used to solve for the interior hydraulic heads \( \vec{h} \). Additionally eqn (9) is taken to solve for the normal fluxes \( \vec{Q} \). For coupling of the equations related to each element, the following additional relations are valid:

- The normal flux \( \vec{Q} \) is equal for both elements sharing the edge \( i \). With \( \vec{Q} \) defined as positive in the outward direction, \( \vec{Q} \) has opposite signs at two elements sharing a common edge \( i \).
- The edge-related head \( h_B \) is equal for both elements sharing the edge \( i \). Hence the term containing \( h_B \) vanishes for all edges in the interior of the domain.

The applications presented in this paper are restricted to rectangular grids for flow calculation. In this case \( N_q \) is linear and the integrals of eqns (8) and (9) may be evaluated analytically.\(^7\) For arbitrarily shaped quadrilaterals, transformation of coordinates and the Gaussian quadrature rule may be applied.

The system of equations resulting from the mixed FEM is very ill-posed for steady-state groundwater flow. In the present study, therefore, the hybridization technique\(^2\) is applied in which the above equations are reordered, so that exclusively the boundary heads \( \vec{h}_B \) can be taken as primary unknowns. The resulting system of linear equations is symmetric and positive definite and can therefore be solved by a Conjugate Gradient solver.

In the present study diagonal scaling is used for preconditioning. The solver is taken from the SLAP library.\(^3^0\)

### 3.1.1 Postprocessing

Since the edge-related heads \( \vec{h}_B \) are the primary unknowns in the mixed-hybrid FEM, the other quantities of interest need to be evaluated by postprocessing. The normal fluxes \( \vec{Q} \) and the interior heads \( \vec{h} \) can be determined by reverting the hybridization procedure for each element. Local values of the stream function \( \psi \) can be determined additionally at the element corners. Setting the value of the streamfunction at node 1 arbitrarily to zero, the values at the other nodes can be determined by:\(^1^2\)

\[
\begin{align*}
\psi_1 &= 0, \\
\psi_2 &= \psi_1 + \frac{Q_2}{\Delta z}, \\
\psi_3 &= \psi_2 + \frac{Q_3}{\Delta z} = \psi_4 - \frac{Q_4}{\Delta z}, \\
\psi_4 &= \psi_1 - \frac{Q_4}{\Delta z}.
\end{align*}
\]

This is illustrated in Fig. 1. eqn (10) requires that the sum of all outward directed normal fluxes \( Q_i \) at an element equals zero. This is satisfied for all elements without recharge. For elements with \( Q_i \neq 0 \), such as well elements, no local streamfunction can be defined.

The ability to construct a conforming distribution of streamfunctions which are bilinearly interpolated inside of quadrilateral elements is a great advantage of mixed and mixed-hybrid FEM over standard FEM. The superiority of velocity approximation by mixed FEM over standard FEM has been stated by various authors.\(^1^2, 2^7\)

Cordes and Kinzelbach\(^1^0\) presented a postprocessing
approach for standard-oriented FEM which yields conforming bilinearly interpolated streamfunctions as well. However, if hydraulic conductivities are defined element by element, even this improved method suffers from inaccurate approximations of velocities around discontinuities.

Conversely it must be stated that the hydraulic heads, resulting from the mixed FEM, are non-conforming. Since the hydraulic heads are superconvergent at the centers of the elements, a second-order approximation could be retrieved by interpolation between these centers. A conforming second-order approximation can not be constructed for single elements. Anyway, in the case of anisotropic hydraulic conductivities, the piezometric head distribution is of minor significance for the construction of orthogonal flownets since the iso-contours of hydraulic heads are not orthogonal to the streamlines. As a consequence, in the study presented the velocity field is solved by mixed-hybrid FEM, whereas the field of pseudopotentials is solved subsequently by standard FEM.

3.2 Finite element method for calculation of pseudopotentials

Given a flow field evaluated by the mixed-hybrid FEM, the crucial point for the determination of the pseudopotential distribution is the appropriate choice of the pseudopotential conductivity \( K_\phi \). For a single quadratic element, a consistent local pseudopotential function would be:

\[
\phi = -\frac{Q_a}{\Delta y \Delta z} \xi + \frac{Q_a + Q_b}{2 \Delta x \Delta y \Delta z} \xi^2 - \frac{Q_a}{\Delta x \Delta z} \eta
+ \frac{Q_a + Q_b}{2 \Delta x \Delta y \Delta z} \eta^2 + C
\]

with the local coordinates \( \xi \) and \( \eta \). The corresponding pseudopotential conductivity \( K_\phi \) would be the unity constant. This choice is not unique. Any \( \phi = L(\phi_0) \) with an operator \( L \) independent of \( \xi \) and \( \eta \) would satisfy eqn (6); the related pseudopotential conductivity \( K_\phi \) would equal \( (\partial^2 \phi / \partial \phi_0)^{-1} \). Unfortunately, the resulting pseudopotential functions are non-conforming across elemental interfaces, and adopting the constant \( C \) and the operator \( L \) in order to minimize the corresponding error may be rather difficult for large domains.

Rather than following a consistent postprocessing approach, a physically reasonable approximation of \( K_\phi \) may be applied to a numerical solution of the pseudopotential distribution in the entire domain. For this purpose, Matanga\(^{25} \) used the conductivity in the direction of flow:

\[
K_\phi = \text{det}(K) \frac{q_i^2 + q_j^2}{K_{xq} q_i^2 - 2 K_{xq} q_i q_j + K_{yq} q_j^2}.
\]

Matanga\(^{25} \) claimed this to be an analytical solution for the pseudopotential conductivity. However, it is not consistent with the solution for the linear case given above.

In the present study, eqn (12) is applied to approximate \( K_\phi \) inside of each element. As the direction of flow may vary inside of an element, the corresponding pseudopotential conductivity varies as well. Therefore numerical integration of the mobility matrix is applied. The Gaussian quadrature rule using three integration points per coordinate axis is used.

The principle of Galerkin FEM is explained in many text books\(^{22} \) and need not be explained here in detail. Bilinear shape and weighting functions \( \bar{N}_s \) are used. Applying the Galerkin procedure to eqn (7) results in the following system of elementwise equations:

\[
\int_V (\nabla \bar{N}_s)^T K_\phi \nabla \bar{N}_s \, dV \, \phi = - \int_B \bar{N}_s^T \bar{n} \, dB
\]

in which \( M \) is the mobility matrix and the right-hand side contains the fluxes across the element’s boundary.

At all boundaries either with fixed piezometric head \( h \) or with fixed normal flux \( Q \), the mixed-hybrid FEM approach yields constant normal fluxes across the boundary. Substituting these fluxes into the right-hand side of eqn (13) yields that the normal flux of a boundary edge is to be distributed by equal parts to the two nodes describing the edge. This should not only be done for Neumann but also for Dirichlet boundaries of the original flow problem.

The elemental matrices at elements with recharge (well cells) are skipped. Instead, the normal fluxes across the edges of the well cells are determined and substituted as Neumann boundaries into the system of equations.

In order to obtain a regular system of equations, at least one nodal value of the pseudopotential \( \phi \) must be defined. This is done by giving the node at the lower left corner of the domain an arbitrary pseudopotential value equal to the hydraulic head. No other Dirichlet boundaries are defined for solving the pseudopotential problem. Similar to the system of equations from the mixed-hybrid FEM, the resulting system of linear equations is symmetric and positive definite. It is solved with a diagonally scaled Conjugate Gradient solver.

4 GENERATION OF STREAMLINE-ORIENTED GRIDS FOR TRANSPORT

4.1 General approach

The grid-generation procedure consists of the following steps:

- Determine all stagnation points in the domain.
- Track streamlines starting at the stagnation points.
- Trace streamlines starting at all inflow boundary sections. Distances of the starting points are chosen
so that the discharge is about equal in all stream-
tubes.

- Trace streamlines starting at all injection wells.
- Determine pseudopotential values for all points de-
scribing the streamlines.
- Detect the minimum and maximum pseudopoten-
tial values as well as the pseudopotentials of all
stagnation points and classify the range of pseudo-
potentials in approximately equal parts. Pseudopo-
tential values of the stagnation points must be
retained.
- Search for all required pseudopotentials along the
streamlines, using linear interpolation between
pseudopotentials at neighbouring points of the
streamlines.
- Select pairs of adjacent required pseudopotential
values in neighbouring streamlines and define
quadrilaterals by the intersection of isopotentials
and streamlines. If necessary, construct triangles
and/or pentagons at the ends of the streamtubes.

These steps are explained in more detail in the following
sections.

4.2 Detection of stagnation points

4.2.1 Regular stagnation points

Stagnation points are, by definition, points where both
velocity components equal zero. Therefore a stagnation
point inside of an element or at an element edge can
easily be detected, as the velocity components in mixed
FEM are evaluated by linear interpolation. The velocity
components at a stagnation point must equal zero as
well in local coordinates meaning for rectangular ele-
ments:

\[ \tilde{q}_n = (\xi - 1) \hat{Q}_n + \xi \hat{Q}_s = 0, \]
\[ \tilde{q}_g = (\eta - 1) \hat{Q}_g + \eta \hat{Q}_d = 0. \]

(14)

\( \xi \) and \( \eta \) are the local coordinates of the stagnation
point. Reordering eqn (14) yields the evaluation of their
values which may subsequently be transformed to global
coordinates:

\[ \xi = \frac{Q_n}{Q_n + Q_s}, \quad 0 \leq \xi, \leq 1, \]
\[ \eta = \frac{Q_d}{Q_d + Q_s}, \quad 0 \leq \eta, \leq 1. \]

(15)

Fig. 2 illustrates the possible configurations deter-
mining a stagnation point. For the cases (a)–(c) the
stagnation points can be detected by eqn (15). Besides
stagnation points inside of elements or at element edges,
there may be stagnation points at element corners or
nodes as well (case (d) in Fig. 2). At these points, ve-
locities are discontinuous since the normal fluxes are
constant along edges and differ from edge to edge.
However, at nodal stagnation points the sign of the

normal fluxes at parallel edges must switch for both
spatial directions.

Under strongly anisotropic conditions multiple stag-
nation points instead of one single point may be de-
tected due to discretization problems. In the current
implementation this cause of error is not yet corrected
for.

4.2.2 Stagnation points belonging to weak wells

For cells containing a well two cases may occur. A
strong well is a cell where all fluxes are oriented outward
in case of a injection well or inward in case of an ex-
traction well, respectively. For the definition of stagna-
tion points the strong well may be seen as the regular
case: The stagnation point related to the well is located
somewhere outside of the well cell. In case of a weak well
not all fluxes are oriented outward or inward, respec-
tively. Fig. 3(a) illustrates the situation. At weak wells
the related stagnation point must be somewhere inside
the well cell.

For particle tracking based on FD flow fields, Zheng\(^\text{33}\)
proposed a semi-analytical correction proce-
dure for weak sources and sinks. The scheme is based on
superposition of the analytical solution for the flow field
around a well in an infinite domain and the averaged
velocity inside the well cell based on the velocities at the
edges. Although this approach may be used for the
construction of reasonable pathlines of particles, it has
some serious disadvantages:
The proposed velocity field is non-conforming across the element edges. The detection of the stagnation point is not straightforward. A non-linear optimization routine would be necessary. The curved shape of the streamlines inside of the well cell requires numerical integration for the tracking procedure. This is not necessary for any other cell. Therefore a simplified approach for the detection of stagnation points and its connecting streamlines at weak wells is implemented:

- First the irregular edges or section of edges at the cell are searched for. In case of an injection well these are inflow edges.
- For each irregular edge or section of edges the stagnation point is supposed to be at the point dividing the specific discharge across the section into equal parts.
- Inside of the well cell the two dividing streamlines are linearized. The exit points are searched for at the connecting edges, so that the integrated normal flux across the edges from the stagnation point to the exit point equals zero. The latter is shown for a single irregular edge in Fig. 3(b).

Note that this ad hoc approach is not very accurate. The true location of the stagnation point is located inside the well cell rather than at the edge. Furthermore the edge center is an arbitrary choice for the location of the stagnation point. However, in most cases the absolute value of the irregular flux will be rather small compared to the regular fluxes at the well cell. Therefore the shift of the dividing streamlines due to the inaccurate detection of the stagnation point will be rather small.

4.3 Tracking of streamlines

4.3.1 Streamlines starting at stagnation points

In a domain containing wells the dividing streamlines are the most important streamlines of the domain. Bounding streamlines divide water originated from injection wells or flowing into extraction wells from background water. Bounding streamlines pass the stagnation point corresponding to the well of interest. Hence construction of the first streamlines starts at stagnation points.

Stagnation points inside of the domain require four corresponding streamlines. Stagnation points at the boundary of the domain require three corresponding streamlines. If the stagnation point is a corner of the domain only two corresponding streamlines are required.

Tracking of streamlines is based on the elementwise (local) evaluation of the streamfunction according to eqn (10). If the stagnation point is inside an element, the value of the local streamfunction is calculated for the stagnation point and the four points at the element edges where the value of the local streamfunction equals the value for the stagnation point are searched.

In the case where the stagnation point is at an element edge, the corresponding values are searched in both neighbouring elements. If the stagnation point is at a node, the search is to be done in all four neighbouring elements.

Once the first point of a corresponding streamline is found, tracking from one point of the streamline to the next is repeated until the boundary of the domain, an element containing a well (well cell) or another stagnation point is reached.

In order to achieve strict orientation of the streamlines in the flow direction, wrongly oriented streamlines indicated by increasing values of the hydraulic heads are reversed. Also streamlines constructed twice are deleted. The latter may occur if a streamline starting at a stagnation point ends in another stagnation point.

4.3.2 General tracking procedure

Given a streamline point at an edge or a node, the edges of the neighbouring elements are searched for the next streamline point. The entry point and the exit point of the streamline have equal local streamfunction values. The local streamfunction at the entry point is evaluated by linear interpolation along the edge. The exit point can be determined by linear interpolation along the adjacent edges.

In order to avoid that streamlines are tracked out of the domain due to small roundoff errors, the coordinates of an exit point are set to the coordinates of the corner \( n \) if the required value of the local streamfunction is in the range of \( \psi_n \pm 10^{-4} \max_{\delta}(\psi) \), where \( \psi_n \) is the nodal value of the local streamfunction and \( \max_{\delta}(\psi) \) is the maximum occurring value of the local streamfunction in the element.

If the last-determined point of a streamline is a node, more than one following point may be found in the three neighbouring elements. In this case the point leading to the smallest variation in the direction of the streamline is
assumed to be the most reliable continuation of the streamline.

4.3.3 Starting points at inflow boundaries and injection wells
The first step in the construction of streamlines starting at inflow boundaries, is to determine all inflow sections of the domain’s boundary. An inflow boundary section can be limited either by a change from inflow to outflow/no flow conditions or by the starting point of a dividing streamline. Fig. 4 illustrates the situation for the case of two injection wells in a parallel flow field.

For all inflow boundary sections the total discharge across the boundary section is determined by integration. Given a maximum discharge per streamtube \(DQ_m\) and the total recharge \(Q_t\) at the boundary section \(i\), the recharge per streamtube at the boundary section is calculated by:

\[
DQ_i = \frac{Q_t}{\text{INT} \left( \frac{DQ_m}{DQ_m + 1} \right)}
\]

in which INT is the integer function. All starting points of an inflow boundary section are chosen in such a way that the recharge of the streamtubes equals \(DQ_i\). The determination of starting points at injection wells is identical to that for the inflow boundary sections. The streamlines are tracked in the way described above.

4.4 Determining pseudopotential lines
For all points describing a streamline, the pseudopotential values are evaluated by bilinear interpolation of the nodal values.

After determination of the maximum and the minimum pseudopotential values \(\phi_{\text{min}}\) and \(\phi_{\text{max}}\) in the domain, and after determination of the pseudopotential values at the stagnation points \(\phi_j\), the range of occurring pseudopotentials is classified. The values of \(\phi_j\) are sorted and the pseudopotential subranges are divided into equal parts by:

\[
\Delta\phi_{j,j+1} = \frac{\phi_{j+1} - \phi_j}{\text{INT} \left( \frac{\phi_{\text{max}} - \phi_{\text{min}}}{\phi_{\text{max}} + 1} \right)}.
\]

\(\Delta\phi_{\text{max}}\) is the maximum difference in pseudopotentials between two pseudopotential lines prescribed by the user. \(\Delta\phi_{j,j+1}\) is the determined difference in pseudopotentials between two isolines within the range between \(\phi_j\) and \(\phi_{j+1}\). Notice that the classification must also be done for the pseudopotential ranges starting at \(\phi_{\text{min}}\) and ending at \(\phi_{\text{max}}\) respectively. Looping over all pseudopotential ranges yields the set of required pseudopotential values for the isolines.

In the following step all required pseudopotential values are searched along all streamlines. This is done by simple linear interpolation between existing points of the streamlines. \(\phi_r\) may be the required pseudopotential value. Then once a section of a streamline determined by the points \(i\) and \(i+1\) is found where \(\phi_i \leq \phi_r \leq \phi_{i+1}\), the coordinates \((x_r, y_r)\) of the intersection point between the streamline and the pseudopotential line corresponding to \(\phi_r\) are given by:

\[
x_r = x_i + \frac{\phi_r - \phi_i}{\phi_{i+1} - \phi_i} (x_{i+1} - x_i),
\]

\[
y_r = y_i + \frac{\phi_r - \phi_i}{\phi_{i+1} - \phi_i} (y_{i+1} - y_i).
\]
If the pseudopotential value of an existing point of a streamline is in the range of $\phi_i \pm 10^{-4} \Delta \phi_i$, the intersection point is set to the already existing point. In all other cases the intersection points are inserted into the streamline. All intersection points are marked for the construction of elements.

4.5 Construction of elements

A streamtube is described by two neighbouring streamlines. A list of streamtubes is generated in the procedure for inserting streamlines. The streamtubes are divided into elements by pseudopotential lines. Perfectly streamline-oriented grids would be curvilinear with broken lines at discontinuities of hydraulic conductivity. Based on the method for the construction of streamlines as explained above, this must be simplified at least to an approximation by polygons. In order to yield easy-to-handle grids for a Finite Volume method of transport, the elements are further simplified to quadrilaterals with the exception of a few triangles and pentagons at boundaries diagonally cutting a streamtube. For illustration see Fig. 5.

Starting at an inflow boundary or an injection well, the first intersection points of streamlines and pseudopotential lines are determined. If the pseudopotential values differ, the intersection between the streamtube and the boundary is not perpendicular. In this case the pseudopotential line of the higher pseudopotential value is crossing the boundary between the starting points of the two streamlines.

The intersection of this pseudopotential line and the boundary is evaluated by linear interpolation. As a consequence of the diagonal intersection of the streamtube and the boundary, the streamtube is cut into a triangle and a pentagon. The triangle is described by two edges perpendicular to flow (longitudinal interfaces) and one edge parallel to flow (transverse interface). The pentagon is described by three longitudinal interfaces and two transverse interfaces. Fig. 6 illustrates the situation.

All elements in the interior of the domain and most elements at the boundaries are described as quadrilaterals. The only information kept from the original streamlines are the locations of the intersection points. Once the element(s) at the inflow boundaries are determined the generation of the subsequent elements along the streamtube is straightforward. The intersection points to the following pseudopotential lines are searched one after another. At outflow boundaries of the domain or at withdrawal wells the element generation stops. If necessary, triangles and pentagons must be constructed at the end of the streamtube in the same manner as described for the start of the streamtube.

A special problem arises when one of the two streamlines describing a streamtube reaches a stagnation point. This occurs when the corresponding streamline is a reversed streamline, originally starting at the stagnation point. In contrast to all other points in the domain, at stagnation points the continuation of the streamline is non-unique as two streamlines intersect. From the three
possible continuing points, the one with the smallest
distance to the continuing point at the other streamline
is chosen.

The grid-generation is completed by writing a binary
output file containing the grid information.

4.6 Limitations and drawbacks

In the algorithmic implementation used for the present
study, a number of possible causes for errors are cor-
rected for. However, there’s still a possibility of failure
in the grid-generation, namely if the saddle points of the
detected local streamfunction and of the calculated
pseudopotentials lay in different elements which may be
the case for strongly anisotropic conditions.

The scheme is restricted to two-dimensional prob-
lems. The extension of the pseudopotential theory to
three-dimensional application and the introduction of
two families of orthogonal streamfunctions as supposed
by Matanga is debatable, at least for heterogeneous
and anisotropic aquifers. Also in three dimensions di-
viding surfaces must be considered rather than dividing
streamlines. The construction of these dividing surfaces
may be rather complicated under heterogeneous condi-
tions.

The limitation of the scheme to steady-state flow
fields cannot be overcome. Under transient flow condi-
tions a grid, preserving the dividing pathlines, would
have to be moved. Approaches based on moving or
grids this has been circumvented by applying a five-
partially moving grids can be found in Eulerian–La-

s

grangian schemes. However, the compounds in multi-
component reactive transport may differ in their mo-
bility, thus requiring a different grid movement for each
compound.

Simplifying the cells of the flownets by quadrilaterals
leads to minor non-orthogonality of the grid. This will
mainly occur in regions of very tortuous streamlines and
pseudopotential lines. Additionally, in such regions the
high variability of the pseudopotential conductivity $K_p$
will be averaged in the FEM context for solving the
pseudopotential function thus biasing the actual pseu-
dopotential value. As a consequence, the spatial dis-
cretization of both the flow problem and the related
transport problem should be fine enough to control the
error of non-orthogonality. Non-orthogonality causes the
dispersion tensor of the related transport calcula-
tions to contain off-diagonal entries if a strict transfor-
mation of coordinates is applied. In the method for
solving the transport equation on streamline-oriented
grids this has been circumvented by applying a five-
point differentiation stencil of the dispersive terms under
the definition of effective lengths and widths of the cells
as well as lengths of the interfaces. In principle, the
representation of the elemental interfaces of the flownet
could be extended to polygonal lines thus diminishing the
degree of non-orthogonality. In the opinion of the
authors, however, the computational effort for the re-
lated geometric analysis in the transport scheme is not
justified by the minor benefits.

5 APPLICATIONS

In the following, three application examples will be
given: a well couple with complete recovery of the in-
jected water by the extraction well, the same well couple
in a heterogeneous aquifer with uncomplete recovery
and a test case for a weak well in an anisotropic aquifer.
In the first two examples, calculations of conservative
transport will be presented.

The numerical methods used for the transport simu-
lation are described in detail in the accompanying
publication. For the calculation of advective transport
a Finite Volume scheme based on Roe’s superbee limiter
using explicit time-integration is used. Dispersion is solved
by the cell-centered FVM using implicit
time-integration.

5.1 Perfect well couple in parallel flow field

The first test case is a perfect well couple in a parallel
flow field. The domain is 80 m long, 21 m wide and 1 m
thick. Grid spacing for the flow calculation is 1 m × 1 m.
The cell at $x = 19.5$ m and $y = 10.5$ m contains an in-
jection well, the cell at $x = 60.5$ m and $y = 10.5$ m an
extraction well. The well discharge is $1.5 \times 10^{-4}$ m$^3$/s =
0.540 m$^3$/h. The top and bottom edges of the domain
are no-flow boundaries, the left and right edges are
Dirichlet boundaries for piezometric head. The head
difference is 0.6 m. The isotropic hydraulic conductivity
is homogeneously $10^{-3}$ m/s.

Fig. 7 shows the grid generated for the model prob-
lem. The maximum discharge per streamtube is set to
$5 \times 10^{-6}$ m$^3$/s, the maximum pseudopotential difference
per iso-pseudopotential is set to $5 \times 10^{-3}$ m. The grid
consists of 5378 elements in 48 streamtubes. Since the
extraction well is directly downgradient of the injection
well with respect to the background flow field, the well
couple forms a perfectly closed system for groundwater
flow. As a consequence, the dividing streamline is a
closed ellipse.

This grid is used for the transport simulation of a
conservative tracer. The longitudinal dispersivity is
0.01 m, the transverse dispersivity 0.001 m. The molecular diffusion coefficient is set to $10^{-9}$ m$^2$/s. The input concentration in the injection well is set to unity.

Fig. 8 shows the concentration distributions 1 day, 5 days and 20 days after the start of injection. Since transverse diffusion is the only process leading to a mass flux across the dividing streamline, the tracer is almost perfectly recovered in the extraction well. This behaviour can be obtained by the numerical method only because the streamline-oriented grid avoids artificial transverse diffusion due to the approximation of advective fluxes.

5.2 Well couple in a heterogeneous aquifer

The previous test case is now modified by using a heterogeneous distribution of the hydraulic conductivity. All other parameters and conditions remain unchanged. The stochastic distribution of hydraulic conductivity is generated by the software package GSLIB. The
standard deviation of logarithmic hydraulic conductivity $\sigma_{\ln k}$ is 1.0 which is a typical value for sandy aquifers. An exponential covariance model with a correlation length of 4 m is applied. Hydraulic conductivity is assumed to be locally isotropic. Fig. 9 shows the generated distribution of hydraulic conductivity.

Fig. 10 shows the streamline-oriented grid generated for a discharge of $5 \cdot 10^{-6}$ m$^3$/s per streamtube and a head difference of $5 \cdot 10^{-3}$ m per isopotential. The generated grid consists of 5031 elements in 45 streamtubes. The dividing streamlines are marked as bold lines. It is obvious that, due to the heterogeneity, the recovery of the injected water by the extraction well is incomplete.

This is illustrated by results simulated for a tracer injection shown in Fig. 11. Some streamtubes originating from the injection well pass the extraction well and, finally, reach the outflow boundary. As a consequence, the tracer transported along these streamlines is not recovered by the extraction well. Additionally, the shape of the tracer front is irregular due to the variability in the velocity within the streamtubes.

5.3 Weak well in an anisotropic aquifer

The third example illustrates how the scheme handles weak wells and hydraulic conductivity tensors, the principal directions of which differ from the grid orientation for the flow calculation.

The confined aquifer is $21 \text{ m} \times 21 \text{ m}$ with a thickness of 1 m. The grid spacing for the flow calculation is 1 m. The anisotropy factor is 20. Hydraulic conductivity is in the main direction $2 \cdot 10^{-3}$ m/s and in the transverse direction $1 \cdot 10^{-4}$ m/s, respectively. The principal direction points $20^\circ$ left of the $y$-direction. Constant-head boundary conditions are defined at the left and right boundaries, whereas no-flow boundary conditions are defined at the lower and upper boundaries. The head difference is 20 cm. Flow is from the left-hand to the right-hand side. An injection well with a recharge of $5 \cdot 10^{-6}$ m$^3$/s is located in the center-cell.

Fig. 12 shows lines of hydraulic heads and velocity vectors for the model problem, as constructed by the graphics software Tecplot. It is obvious that the contour lines are not perpendicular to the velocity vectors, instead, they are almost parallel to the principal direction of the conductivity tensor in most of the domain.

Fig. 13 shows the streamline-oriented grid generated for the model problem. The grid consists of 615 elements in 32 streamtubes. The well in the test case is weak as explained by Fig. 3. Obviously the use of pseudopotentials for the construction of the flownet guarantees approximately orthogonality of the net. At least for the given testcase, the pseudopotential conductivity determined by eqn (12) yields excellent results. This is of particular interest for the simulation of transport, since the principal directions of the dispersion tensor are...
parallel and orthogonal to the streamlines. Hence, a grid based on pseudopotentials rather than hydraulic heads is better adopted to transport simulations.

6 SUMMARY AND CONCLUSIONS

A new method has been developed for generating flownets for two-dimensional heterogeneous anisotropic aquifers. Because of their orthogonality these flownets may be used as streamline-oriented grids for transport modeling. The method presented eliminates one of the drawbacks of the conventional method in which the streamfunction equations were solved globally by means of finite elements, and which did not permit the inclusion of wells in the interior of the domain. By contrast, the new method generates streamlines by first applying the mixed-hybrid approach to create an accurate global velocity field, and then calculating streamlines locally. This approach yields streamfunction solutions of the same accuracy as the conventional dual formulation, while allowing multiple wells in the interior of the domain. In order to develop orthogonal grids for anisotropic conditions, pseudopotential contours are generated by solving the pseudopotential equation by means of conventional finite elements.

The comprehensive methodology for streamline-oriented grid generation includes the location of stagnation points and dividing streamlines which separate zones of different aqueous constituents that may react when mixed. This separation guarantees that transverse numerical dispersion, which would lead to fictitious mixing of the reactants and thus to unrealistically high transformation rates, is fully controlled. The orthogonal grid is generated by tracking regularly-spaced streamlines originating at stagnation points, wells, and inflow boundaries, and by determining the intersections of these streamlines with pseudopotential lines to form quadrilateral elements.

Applications demonstrate that the streamline-oriented grid effectively eliminates numerical dispersion in the case of a well couple, and that both heterogeneous and anisotropic conditions are handled competently by the grid generator. Consequences of inaccurate approximation of transverse mixing for reactive transport, which may be caused by conventional transport methods on regular grids, are shown in the related papers.8,9

The present scheme is limited to two-dimensional systems under steady-state flow conditions. The limitation to steady-state flow cannot be easily overcome, since the accommodation of transient flow conditions, perhaps due to seasonal flow variations, would require a movable grid, which is not very practical with the present approach. However, the steady-state flow limitation is not seen as a serious drawback in the context of the type of groundwater contamination problems addressed in this study, which generally have time scales of decades or centuries, over which seasonal flow variations can be averaged out.

REFERENCES


