Semi-analytical homogeneous anisotropic capture zone delineation

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Abstract

We present an algorithm for the quick delineation of capture zones using complex discharge potential. The flow is steady and two-dimensional in a homogeneous domain with anisotropic transmissivity. The procedure accommodates an arbitrary number of injection and extraction wells at any locations throughout the flowfield, as well as regional flow, in the form of a uniform flow component. Capture zones are delineated by finding stagnation points and using a particle tracking scheme to plot separation streamlines along trajectories upgradient or downgradient from the stagnation points as appropriate. Stagnation points are found exactly using a partial fractions expansion. Initial particle tracking directions are determined by evaluating the Hessian matrix of the potential at stagnation points. Streamline tracing is performed using a fourth-order Runge-Kutta particle tracking scheme. © 2005 Elsevier B.V. All rights reserved.

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1. Introduction

In many applications, capture zones are plotted to assist in the design of hydraulic containment systems, pump and treat systems, (Cohen, 1997), and recirculation zone remediation schemes (McCarty et al., 1998). This work was motivated by the need to understand both recirculation zone geometry and tracer losses in a recirculation tracer test conducted at the United States Department of Energy (DOE) Natural and Accelerated Bioremediation Research Program Field Research Center (NABIR FRC) in Oak Ridge, Tennessee, USA in an aquifer known to be anisotropic (Lozier et al., 1987). Pumping rates and well alignment can both greatly impact the geometry of recirculation cells. As a result, a method to quickly delineate capture zone geometry is useful in planning.

We present a semi-analytical method based on complex discharge potential (see Strack, 1989). Anisotropy is considered through a coordinate rotation followed by domain stretching (Muskat, 1937). In the transformed domain, stagnation points are found analytically. At these points, the Hessian second derivative matrix of the potential is evaluated. This matrix describes the curvature of the potential surface on which stagnation points are saddle points. The eigenvectors of the Hessian matrix indicate
the principal directions of minimum curvature (troughs or ridges) in the potential surface, thus indicating the trajectories of streamlines both into and out of the stagnation points. These streamlines, called separation streamlines, delineate discrete zones of flow. In the case of wells extracting from an aquifer with regional flow, the separation zones delineate capture zones, whereas in the case of multiple injection and extraction wells, the separation streamlines can also delineate recirculation zones. The separation streamlines, stagnation points, wells and equipotential lines are plotted in the original domain after backtransformation.

Previous work in delineation of capture zones has generally followed one of the following approaches: parametric equations for capture zone shape, particle tracking to and from pumping wells, typically using numerical models, or tracing separation streamlines between wells and associated stagnation points.

The parametric approach, often based on the work of Javendel and Tsang (1986), involves calculating the streamfunction for the separation streamline and rearranging the resulting equation into parametric form such that the ‘capture curve’ can be plotted and evaluated (see, e.g. Buscheck, 1990; Shan, 1999).

Semi-analytical and numerical particle tracking schemes have also been used to determine capture zones. A common approach is to track many particles from each injection well and examine visualizations of particle traces to determine the boundaries between assemblages of particles that end up in one or the other extraction well (e.g. Cole and Silliman, 2000).

Bakker and Strack (1996) present a method for delineation of capture zones in an isotropic, homogeneous aquifer with recharge with an analytic element model using stagnation points to determine particle tracking starting points. Stagnation points are found using a two-level numerical gradient-type search derived for a flowfield without recharge and extended, ad hoc, to a flowfield with recharge. The first level involves a coarse search for minima in discharge at discretized points throughout the velocity field, followed by a refined search using an iterative algorithm to converge to stagnation points. The method presented herein is more efficient and guarantees that all stagnation points are identified but is not extended to consider recharge.

Other researchers have employed analytical methods to solve for a limited number of stagnation points (e.g. Christ and Goltz, 2002; Shan, 1999, and others). Christ and Goltz (2002) indicate that, for more than four wells, a numerical root finding technique such as Newton-Raphson is needed to solve for the stagnation points. Naturally, convergence in such a case depends on reasonable initial estimates of the solution. We expand on previous work by explicitly and exactly solving for the stagnation points algebraically. We also present a novel method to identify origin points for tracing separation streamlines from near stagnation points using the Hessian matrix of potential.

The goal of this work is to consider a steady-state, two-dimensional, anisotropic homogeneous domain with regional flow to provide a preliminary evaluation of an aquifer. Computational power has allowed for increasingly complicated numerical three-dimensional models to be applied to various sites. Typically, however, in the beginning stages of any groundwater project, information about parameters is not sufficient to use a detailed numerical model. Analytical models such as this provide a fast alternative for preliminary remediation design.

Cole and Silliman (2000) examined the uncertainty in predicting capture zone geometry when a homogeneous model is applied to a heterogeneous aquifer. They suggest the three factors that most greatly impact uncertainty are the geometric mean of hydraulic conductivity ($K_G$), the direction ($\gamma$) and magnitude ($|J|$) of regional gradient, and the magnitude ($\beta$) and orientation ($\theta$) of anisotropy in transmissivity. These are the factors accounted for in the methodology presented here.

2. Governing equations

The governing equations are presented in terms of complex potential for the isotropic case. The extension to anisotropic problems is presented in Appendix A.

2.1. Complex potential

Complex potential is a convenient method for solving the Laplace equation in two dimensions (Eq. (1)) for horizontal flow in a homogeneous,
isotropic medium with no vertical gradients; for example, a confined aquifer or an unconfined aquifer under the Dupuit-Forchheimer assumption. Ground water flow can be modeled with the Laplace equation

$$\nabla^2 \Phi = 0$$

(1)

where: $\Phi = \phi T$ with $\Phi$ as discharge potential, $\phi$ as hydraulic head, and $T$ as transmissivity.

The notation and development presented below follows Strack (1989). The discharge potential ($\Phi$) and the streamfunction ($\Psi$) satisfy the Cauchy-Riemann conditions

$$\frac{\partial \Phi}{\partial x} = \frac{\partial \Psi}{\partial y}$$

(2)

and as a result, $\Psi$ also satisfies the Laplace equation. The spatial coordinates can be combined into a complex variable

$$z = x + iy$$

(3)

and the complex discharge potential is represented as an analytic complex function

$$\Omega(z) = \Phi(x, y) + i\Psi(x, y)$$

(4)

which is analytic by virtue of the Cauchy-Riemann conditions in Eq. (2).

### 2.1.1. Superposition

The Laplace equation (Eq. (1)), being linear and homogeneous, allows for superposition of multiple sources and sinks; in this case, injection and extraction wells, and uniform regional flow. The general equation for complex discharge potential under these conditions is therefore

$$\Omega(z) = -\bar{R}z + \sum_{j=1}^{N} \frac{Q_j}{2\pi} \ln(z - z_{w_j})$$

(5)

where: $R$ is the uniform discharge attributed to regional flow and the overbar indicates the complex conjugate, $N$ is the total number of extraction and injection wells, $Q_j$ is the flow rate of the $j$ th pumping well (positive values indicate extraction, and negative values indicate injection), $z = x + iy$ is the location at which $\Omega(z)$ is to be calculated, and $z_{w_j} = x_{w_j} + iy_{w_j}$ is the spatial location of the $j$ th injection or extraction well.

### 2.1.2. Uniform flow component

For a uniform flow component, regional flow over unit width in two dimensions is derived from Darcy’s law as

$$R_x = -T \frac{\partial \phi}{\partial x}$$

(6a)

$$R_y = -T \frac{\partial \phi}{\partial y}$$

(6b)

where: $R_x$ and $R_y$ are the components of the regional flow in the $x$ and $y$ directions, respectively, $T$ is transmissivity, and $\phi$ is hydraulic head.

As a complex function, the regional gradient vector is expressed as

$$J = -\frac{\partial \Phi}{\partial x} - i \frac{\partial \Phi}{\partial y}$$

(7)

Rather than specifying the components, the regional gradient can be expressed as the magnitude

$$|J| = \sqrt{\left(-\frac{\partial \phi}{\partial x}\right)^2 + \left(-\frac{\partial \phi}{\partial y}\right)^2}$$

(8)

and the phase angle

$$\gamma = \tan^{-1}\left(\frac{\text{imag} J}{\text{real} J}\right)$$

(9)

which is also the angle of $J$ from the easting.

### 2.1.3. Discharge function

Discharge can be determined by complex differentiation of the discharge potential. The discharge function ($W$) is defined as

$$W = -\frac{d\Omega}{dz}.$$ 

(10)

Evaluation of this derivative allows for the expression of discharge in the $x$ and $y$ directions as the real and complex components of $W$

$$W = Q_x - iQ_y.$$ 

(11)

The discharge function is used for particle tracking which, in turn, allows for the delineation of separation streamlines. In the next section, we present a method for the determination of starting points for particle tracking.
2.1.4. Anisotropic transmissivity

Anisotropic transmissivity may be present at various scales in many aquifers. For example, cross bedding, dipping bedding planes, and graded bedding in silt or sand (Boggs, 1987), or preferential joint orientations in fractured rock may contribute to anisotropy (USNRC, 1996). The fractured, steeply dipping saprolite and shale found at the NABIR FRC in the Appalachian mountains of Tennessee, USA is an example of a heterogeneous medium in which parallel fracture sets create strong anisotropy that can be approximated using an anisotropic homogeneous model. Another example is a dipping turbidite sequence in which heterogeneity on the particle size scale results in an effectively homogeneous anisotropic medium at the aquifer scale.

If such conditions or others are suspected at a site, several methods are available to determine the angle ($\theta$) and magnitude ($\beta = \sqrt{\frac{T_{\text{max}}}{T_{\text{min}}}}$) of anisotropy (for example, Hantush and Thomas (1966): excellent reviews are also available in Batu (1998); Kruseman and deRidder (1990)). It is also possible to apply an optimization model to data with the parameters $\theta$ and $\beta$ used as fitting parameters. The methods developed in this work are extended to cases with anisotropic transmissivity in Appendix A.

3. Terminal points for streamline tracing

Terminal points are near stagnation points and provide the locations to begin tracing separation streamlines. This section discusses stagnation points, and how terminal points are defined and located near them.

3.1. Stagnation points

Stagnation points are critical because they demarcate points that separate regions of flow. An intuitive interpretation of stagnation points is to view them as equilibrium points. For example, considering two extraction wells, the stagnation point between them is located at the point where the pull from each well is equal and opposite, so the net flow at that point is zero. Mathematically, stagnation points are points of zero discharge, $Q_x = Q_y = 0$. Since we are interested in potential flow, this condition is equivalent to

$$\frac{\partial \Phi}{\partial x} = 0, \quad \frac{\partial \Phi}{\partial y} = 0. \quad (12)$$

It is generally easiest to solve for the complex discharge potential

$$\frac{dQ}{dz} = 0 \quad (13)$$

with respect to the complex variable $z$. The coordinates of $z$ satisfying Eq. (13) are the stagnation points.

Consider the general potential of Eq. (5), the derivative of which is

$$\frac{dU}{dz} = \frac{K}{2C^2} \sum_{j=1}^{N} \frac{1}{(z - z_j)^2} \quad (14)$$

where $z$, in this case, is the location of a stagnation point.

The roots of this equation are the locations of the stagnation points. The first term corresponds to the regional flow and is constant in Eq. (14). Christ and Goltz (2002) present a solution for the roots of Eq. (14) by expressing the equation as a polynomial of order $N$. For four or fewer wells, the roots may be found analytically, whereas for more than four wells, numerical techniques are used. Erdman (2000) similarly used analytical methods for four or fewer wells, favoring numerical gradient methods for greater numbers of wells. In solving for many roots using Newton-Raphson or another root-finding numerical algorithm, sensitivity to starting estimates of the roots is a significant limitation. An explicit algebraic solution is more efficient and accurate.

We present an efficient method for finding the locations of stagnation points by expressing Eq. (14) as a ratio of polynomials of order $N$, and finding the roots of that polynomial. This method is an improvement over those of Christ and Goltz (2002) and Erdman (2000) in that there is no practical limit to the number of wells allowed in the problem.

In general, a partial-fraction expansion can be expressed as a ratio of two polynomials (Oppenheim and Schafer, 1975).

$$\frac{F(z)}{G(z)} = R(z) + \sum_{j=1}^{N} \frac{A_j}{z - z_j} \quad (15)$$
where: $F(z)$, $G(z)$, and $R(z)$ are polynomials in $z$, and $A_j$ and $z_j$ are constants. In the case of Eq. (14), $A_j \triangleq Q_j / 2\pi$, $z_j \triangleq z_m$, and $R(z) \triangleq -\bar{R}$. Once the expression is formulated, the roots of the polynomial in the numerator, $F(z)$, correspond to the zeros of the right hand side of Eq. (15). The roots of this polynomial are found using the eigenvalue method, as discussed in Press et al. (1992). The eigenvalue method is based on the analogue between eigenvalues of a matrix and a polynomial. Consider a general polynomial of the form

$$f(x) = \sum_{j=1}^{m} a_j x^j$$  \hspace{1cm} (16)

where: the $a_j$ are the coefficients, and $x^j$ are the roots of the equation to the $j$th power.

A companion matrix can be constructed as

$$A = \begin{bmatrix} -a_{m-1} & -a_{m-2} & \cdots & -a_1 & -a_0 \\ a_m & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$  \hspace{1cm} (17)

The eigenvalues of $A$ are found by finding $\lambda$ such that

$$\det[A - \lambda I] = 0$$  \hspace{1cm} (18)

where: $\det[\cdot]$ indicates a matrix determinant, $\lambda$ is a vector of the eigenvalues, and $I$ is an identity matrix.

This determinant can be solved as the following polynomial:

$$a_m \lambda^m + a_{m-1} \lambda^{m-1} + \cdots + a_1 \lambda + a_0 = 0$$  \hspace{1cm} (19a)

$$\sum_{j=1}^{m} a_j \lambda^j = 0$$  \hspace{1cm} (19b)

Immediately, we see that Eq. (19a) and (19b) is equivalent to Eq. (16). We may, thus, take advantage of efficient and robust numerical techniques that are available to compute the eigenvalues (the $\lambda_j$).

### 3.2. Terminal points

The stagnation points are saddle points in the potential field. Fig. 1 shows the shape of the discharge potential surface at the saddle point corresponding to a stagnation point. The orthogonal lines on the surface indicate streamlines entering and exiting the space infinitesimally close to the stagnation point.

In order to trace the streamlines, we must know the discharge at the starting point and at each subsequent point. However, as defined above, the discharge at the stagnation point itself is zero. Hence, we must start streamline tracing at terminal points which are offset slightly from the stagnation points.

The Hessian (second derivative) matrix is a useful tool both for finding the principal orientations of maximum positive and negative curvature, and for verifying that the stagnation point is, indeed, a saddle point and not a strict minimum or maximum. The Hessian matrix is constructed as follows

$$H = \begin{bmatrix} \frac{\partial^2 \Phi}{\partial x^2} & \frac{\partial^2 \Phi}{\partial x \partial y} \\ \frac{\partial^2 \Phi}{\partial x \partial y} & \frac{\partial^2 \Phi}{\partial y^2} \end{bmatrix}$$  \hspace{1cm} (20)

The complex derivative of $\Omega$ is easy to calculate and can be deconstructed as

$$\frac{d \Omega}{d z} = \frac{\partial \Phi}{\partial x} + i \frac{\partial \Psi}{\partial x} = \frac{\partial \Psi}{\partial y} - i \frac{\partial \Phi}{\partial y}$$  \hspace{1cm} (21)

because $\Omega$ is analytic, and thus its first and second derivatives are independent of the path. Now, differentiating one more time and rearranging terms, we find all of the terms of the Hessian contained in the complex second derivative of $\Omega$

$$\frac{d^2 \Omega}{d z^2} = \frac{\partial^2 \Phi}{\partial x^2} + i \frac{\partial^2 \Phi}{\partial x \partial y} = -\frac{\partial^2 \Phi}{\partial y^2} - i \frac{\partial^2 \Psi}{\partial x^2}$$

$$= \frac{\partial^2 \Psi}{\partial x \partial y} - i \frac{\partial^2 \Phi}{\partial x \partial y}.$$  \hspace{1cm} (22)

Therefore, the Hessian can be constructed as

$$H = \begin{bmatrix} \text{real} \left( \frac{d^2 \Omega}{d z^2} \right) & -\text{imag} \left( \frac{d^2 \Omega}{d z^2} \right) \\ -\text{imag} \left( \frac{d^2 \Omega}{d z^2} \right) & \text{real} \left( \frac{d^2 \Omega}{d z^2} \right) \end{bmatrix}.$$  \hspace{1cm} (23)
The eigenvalues of the Hessian matrix, $\lambda_1$ and $\lambda_2$, reveal the nature of the potential at the stagnation point. For the flow problems considered, $\Phi$ satisfies the Laplace equation, thus $\lambda_1\lambda_2 < 0$ indicates that the stagnation point is a saddle point. The eigenvector associated with the positive eigenvalue points in the direction along which $\Phi$ is the most convex ($\cup$). In other words, ground water flows toward the stagnation point along this direction. The eigenvector associated with the negative eigenvalue points in the direction along which $\Phi$ is the most concave ($\cap$). In other words, ground water flows away from the stagnation point along this direction.

Knowing these orientations allows us to start our streamline tracing intelligently within the active velocity field, rather than at the stagnation point where discharge is, by definition, zero. In the direction of maximum convexity of potential ($\cup$), we track the particle upgradient. In the direction of maximum concavity ($\cap$), we track the particle downgradient. Plotting the trajectories of these four particles for each stagnation point results in a full picture of the separation streamlines delineating regions of capture throughout the system.

4. Streamline tracing

Particle tracking is performed using the resultant of the $x$ and $y$ discharge vectors starting at terminal points and stepping in space toward a new point, where the discharge vectors are calculated again. The discharge vector is calculated using a fourth order Runge-Kutta scheme (Zheng and Bennett, 2002). This method is approximately fourth-order accurate, employing two predictors and two correctors (Ferziger, 1998).

We use the assumption that the discharge vector calculated using the Runge-Kutta scheme is tangent to the streamline. Therefore, we need only the angle of orientation of the resultant vector, and can determine the new position as

$$z_{n+1} = z_n + e^{i\alpha}ds$$

(24)

where: $z_{n+1}$ is the new spatial location, $z_n$ is the previous location, $\alpha$ is the angle the resultant
The angle $\alpha$ can be found in closed form with the Runge-Kutta technique as follows:

$$e^{i\alpha} = \left( \frac{W(z_n) + 2W(z_{n+1}) + W(z_{n+2}) + W(z_{n+3})}{W(z_n) + 2W(z_{n+1}) + 2W(z_{n+2}) + W(z_{n+3})} \right)^{1/2}$$

(25)

where: $z_{n+1}$ is the first midpoint location, $z_{n+2}$ is the second midpoint location, and $z_{n+3}$ is the final location. The midpoints are found as follows:

$$z_{n+1} = z_n + \frac{W(z_n)}{|W(z_n)|} \frac{dS}{2}$$

(26)

$$z_{n+2} = z_n + \frac{W(z_{n+1})}{|W(z_{n+1})|} \frac{dS}{2}$$

(27)

$$z_{n+3} = z_n + \frac{W(z_{n+2})}{|W(z_{n+2})|} \frac{dS}{2}$$

(28)

Naturally, $dS$ must be found ‘small enough’ that the massless particles do not stray significantly from the streamline. In other words, the tangent to the streamline must be calculated at a small enough discretization such that the curvature of the streamline is well-approximated by the series of tangents.

5. Example applications

Two representative sets of examples are shown below. The first set is a hypothetical hydraulic containment scheme. The second set is based on data from a recirculation tracer test conducted at the NABIR FRC in Oak Ridge, Tennessee, USA.

5.1. Hydraulic containment

An obvious application of capture zone analysis is in the design of hydraulic containment systems. Analytical solutions for the capture zone shape of individual wells already exist for isotropic aquifers. However, anisotropy and regional flow at an oblique angle of incidence make the capture zone geometry more difficult to predict. A simple three-well extraction system with wells aligned on the $y$-axis is considered in the following three variations: isotropic (case HC1), anisotropic with $\beta = \sqrt{5}$ and $\theta = 0^\circ$ (case HC2), and anisotropic with $\beta = \sqrt{5}$ and $\theta = 45^\circ$ (case HC3). In all three cases, $T_{max} = 5 \times 10^{-4}$ m$^2$/s, $|J| = 0.01$, $\gamma = 180^\circ$, and three wells on 4-meter spacing along the $y$-axis are each extracting at 4 LPM. The spacing and extraction rates were selected heuristically to result in a composite capture zone without gaps for this illustrative example.

5.1.1. Case HC1: isotropic transmissivity

First, consider the isotropic case. Fig. 2 shows the flowfield with $\beta = 1$ and $\theta = 0$. A case such as this where $T_{max}$ and regional flow are aligned with the $x$-axis and the wells are perpendicular to flow on an even spacing is also relatively easy to model with parametric solutions or symmetric assumptions.

5.1.2. Case HC2: anisotropic transmissivity coincident with $x$-axis and regional flow

Next, consider a similar case as HC1, but with anisotropy as $\beta = \sqrt{5}$, $\theta = 0^\circ$. Fig. 3 shows the resulting flowfield. The composite capture zone geometry is very similar to HC1, although the capture zone is extended along the major ($x$) axis, and it is compressed in the perpendicular direction.

Fig. 2. Case HC1: Example of composite capture zone in an isotropic aquifer. Parameters are outlined in the text. Circled ‘x’ marks are wells, diamonds are stagnation points, dashed lines are hydraulic potential $\Phi$, and dark solid lines are separation streamlines.
5.1.3. Case HC3: anisotropic transmissivity oblique to x-axis and regional flow

Finally, consider a case with the same anisotropy as HC2 \( (\beta = \sqrt{5}) \), but oriented at an angle of \( \theta = 45^\circ \). The regional flow gradient is still oriented with the x-axis \( (\gamma = 180^\circ) \). Fig. 4 shows the flowfield. The obliqueness of \( J \) with respect to the principal axis of transmissivity results in regional flow that is oblique to that axis. Furthermore, as the wells are aligned with the original axes, they are also oblique to the principal axes. The result is a composite of three capture zones which are asymmetric, wider than the set of HC2, and inclined at an angle between the incident regional flow and the major axis of anisotropy.

5.1.4. Discussion of hydraulic containment examples

These examples illustrate that, as symmetry breaks down in flowfield parameters, the capture zone geometry of a scheme as simple as a line of evenly spaced wells extracting at a uniform rate becomes difficult to predict. This could have serious consequences in determining which wells remove water from certain parts of a plume.

5.2. Recirculation scheme

This work was motivated by the need to understand the geometry of a nested recirculation scheme in an anisotropic aquifer. Two scenarios are presented: case RC1 is the ideal planned tracer test for which this work was initially intended, and case RC2 is the same planned setup, but with actual flowrates attained during the field implementation and considering lateral deviation of boreholes from planned locations.

5.2.1. Case RC1: ideal recirculation scheme

A recirculation tracer experiment was planned for a wellfield at the NABIR FRC. Wells were assumed to be in a horizontal line at the following coordinates (in meters): \( A = (-1.15,0) \); \( B = (0,0) \); \( C = (1.98,0) \); \( D = (3.42,0) \). Pumping rates were specified to be: extraction wells A and B extracting at 1.4 and 3 LPM respectively, and injection wells C and D injecting at 3 and 2.8 LPM respectively. Aquifer parameters were: \( \beta = \sqrt{5}, \theta = -10^\circ, T_{\max} = 5 \times 10^{-6} \text{ m}^2/\text{s}, |J| = 0.0001, \text{ and } \gamma = 180^\circ \). Four unlabeled monitoring wells are also shown for reference. Fig. 5 presents the flowfield. Note the formation of an inner cell and an outer cell, both of which are closed. Water from well D escapes the system because the injection rates were intentionally planned to be higher than extraction rates. The objective was to create the inner cell within a forced gradient for its containment.

5.2.2. Case RC2: actual recirculation scheme

The second case accounts for conditions actually encountered in the field implementation of the tracer
The two major changes are: borehole deviation measurements became available after the tracer test was completed, indicating that the wells were not perfectly aligned along the x-axis, and the actual flow rates differed from those planned and modeled in RC1. Other aquifer parameters are assumed to be the same as in RC1. The actual flowrates were: extraction wells A and B extracting at 1.4 and 3 LPM respectively, and injection wells C and D injecting at 4 and 2.36 LPM respectively. The deviated well locations are (again in meters): \(A = (-1.15, -0.09);\) \(B = (0,0);\) \(C = (1.98,0.07);\) \(D = (3.42,0.45).\) Fig. 6 presents the resulting flow field. Note three zones are formed, and the outermost is not closed, resulting in loss of containment of the inner cells. Loss of tracer injected at well C was, indeed, observed in the study.

5.2.3. Discussion of recirculation examples

For the recirculation schema, in the ideal case RC1, one expects the recirculation zones to be closed as they are shown to be. However, the shape of the recirculation zones is difficult to predict. The consequences of borehole deviation and flowrate changes explored in example RC2 are difficult to imagine a priori, and the loss of containment resulting is significant for design and interpretation of tracer tests.

5.3. Independent verification

Verification of ComCZAR was performed in three steps. First, test case HC1 was confirmed using the U. S. EPA public domain analytic element model CZAEM (Strack et al., 1994). CZAEM delineates separation streamlines by tracing through stagnation points, resulting in delineation of capture zones with geometry coincident with the results of ComCZAR. CZAEM only considers isotropic media, so further testing was required for anisotropic cases. Particle tracking was performed with no wells and regional flow nonparallel to the major axis of anisotropy. The predicted angle of particle traces was predicted using a Mohr’s circle approach (Bear, 1972), and the same angle was observed in ComCZAR particle traces. Finally, all cases were verified using particle tracking performed with MODFLOW (McDonald and Harbaugh, 1988) and MODPATH (Pollock, 1994). Particles were released and tracked forward from injection wells and in reverse from extraction wells. Separation streamlines are not explicitly defined in this case, but particle traces lie within capture and recirculation zones, and no traces cross separation streamlines. The location of stagnation points is inferred from loci of a paucity of particle traces, although their actual location is not found well by particle tracking along.
In all cases, excellent agreement was observed. Fig. 7 shows the verification of HC3 which includes regional flow oblique to the major axis of anisotropy, and three wells extracting as a representative case.

6. Discussion and conclusions

The semi-analytical method for the quick delinea-
tion of capture and recirculation zones in a homo-
genous aquifer with anisotropic transmissivity is
valuable for the intermediate stage of analysis where
some information is available, but not enough to
justify a full three-dimensional numerical model.

The analytical solution for stagnation point
location, with an application of the eigenvalues of
the Hessian matrix, provides a robust method for
finding the correct starting points of separation
streamlines (the terminal points). This method is an
improvement over previous methods in that efficient
and robust algorithms are used rather than numerical
search algorithms which require preliminary search-
ing to determine starting points required for the
algorithm to converge.

The value of a semi-analytical, anisotropic,
homogeneous streamline delineation model is appar-
ent when conducting preliminary planning or design
with limited aquifer information, or to provide
confirmation for numerical models. The efficiency of
the code allows for quick results which is amenable to
uncertainty analysis using Monte Carlo techniques.

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Appendix A. Anisotropy transmissivity

The complex potential approach to solving the
flowfield presented in the main body of this work is
based on an assumption of isotropic transmissivity.
Through a well-established method of coordinate
transformations (Muskat, 1937), this can be extended
to an anisotropic aquifer. This appendix provides a
brief summary of the steps taken to apply the
coordinate transformation needed to solve the flow-
field, and the backtransformation to display the results
in the original coordinate system.

To apply the method of Muskat (1937), we must
first rotate, and then stretch the coordinates of all
vector quantities in the problem. In this case, the
locations of sources and sinks, and the gradient of \( \phi \)
due to uniform regional flow are the vector quantities
to transform. Volumetric flow rates for the wells are
scalars and hence no transformation is required for
them.

A.1. Sources and sinks (wells)

Assuming that the angle between the \( x \)-axis and the
axis of maximum transmissivity, \( \theta \), is positive in
the counterclockwise direction, as shown in Fig. A1,
the wells are rotated

\[
\begin{bmatrix}
  x_r \\
  y_r 
\end{bmatrix} =
\begin{bmatrix}
  \cos(\theta) & \sin(\theta) \\
  -\sin(\theta) & \cos(\theta) 
\end{bmatrix}
\begin{bmatrix}
  x \\
  y 
\end{bmatrix}
\] (A.1)

where: \( x \) and \( y \) are coordinates in the original system, and \( x_r \) and \( y_r \) are coordinates in the principal-axes system.

Next, the \( y_r \) axis is stretched such that the final transformed coordinates are

\[
x_t = x_r
\] (A.2)

\[
y_t = \beta y_r
\] (A.3)

where: \( x_t \) and \( y_t \) are the transformed coordinates, and \( \beta = \sqrt{T_{\text{max}}/T_{\text{min}}} \).

In this transformed domain, the potential \( \Phi \) satisfies the Laplace equation so the scalar complex discharge potential field can be solved for analytically as discussed for the isotropic case above.

### A.2. Regional flow

Recalling from Eq. (6a) and (6b)

\[
R_{x_t} = -T_{\text{min}} \frac{\partial \phi}{\partial y_t}
\] (A.4a)

\[
R_{y_t} = T_{\text{max}} \frac{\partial \phi}{\partial x_t}
\] (A.4b)

where: \( R_{x_t} \) and \( R_{y_t} \) are the volumetric regional flows in the \( x_t \) and \( y_t \) directions, respectively, \( T_{\text{max}} \) and \( T_{\text{min}} \) are the principal values of transmissivity tensor, and \( \partial \phi/\partial x_t \) and \( \partial \phi/\partial y_t \) are the gradients of potentiometric head in the \( x_t \) and \( y_t \) directions, respectively. Dividing \( R_{x_t} \) by \( \beta \) accounts for domain stretching.

The gradients of \( \phi \) must be rotated

\[
\begin{bmatrix}
  \frac{\partial \phi}{\partial x_t} \\
  \frac{\partial \phi}{\partial y_t}
\end{bmatrix} =
\begin{bmatrix}
  \cos(\theta) & \sin(\theta) \\
  -\sin(\theta) & \cos(\theta)
\end{bmatrix}
\begin{bmatrix}
  \frac{\partial \phi}{\partial x} \\
  \frac{\partial \phi}{\partial y}
\end{bmatrix}
\] (A.5)

Finally, in the complex domain

\[
R_t = R_{x_t} + iR_{y_t}
\] (A.6)

### A.3. Backtransformation

Particle tracking is performed in the transformed domain. Sources, sinks, and particle locations in terms of \( x_t \) and \( y_t \) must be backtransformed to the \( xy \) domain. To backtransform, first the locations must be expressed in terms of \( x_r \) and \( y_r \) by reversing the stretching

\[
x_r = x_t
\] (A.7a)

\[
y_r = \frac{y_t}{\beta}
\] (A.7b)

Finally, the particle locations are rotated back through \( \theta \) as

\[
\begin{bmatrix}
  x \\
  y
\end{bmatrix} =
\begin{bmatrix}
  \cos(\theta) & -\sin(\theta) \\
  \sin(\theta) & \cos(\theta)
\end{bmatrix}
\begin{bmatrix}
  x_r \\
  y_r
\end{bmatrix}
\] (A.8)

### Appendix B. Implementation

The program developed in this work is general and may be applied to any configuration of wells pumping...
at arbitrary rates. The code called ComCZAR (Complex Capture Zone with Anisotropy Routine) was developed in MATLAB (Mathworks, 2002) and is available for download at http://www.stanford.edu/~fienen/software/. The decision to use MATLAB was driven by the existence of functions well-suited to the efficient coding of the problem. The algorithms of this work are presented in sufficient detail such that the program could be adapted into the language of a user's choice. Specific documentation for users, a compendium of test cases, and source code are available for review at the same URL.

References


Mathworks 2002. MATLAB.


