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High-order line elements in modeling two-dimensional groundwater flow

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Abstract

This paper presents a new Analytic Element formulation for high-order line elements in modeling two-dimensional groundwater flow. These elements are line-doublets, line-dipoles and line-sinks. The jump functions for line elements are expressed as Chebyshev series. The unknown coefficients are computed by applying the principle of overspecification to the boundary conditions. The use of the high-order elements and the principle of overspecification have resulted in high precision and significant improvements in computational efficiency compared to the existing collocation-based formulation. The new formulation is currently being used in the development of the Metropolitan Area Groundwater Model for Twin Cities, Minnesota, USA and for enhancements of the next release of National Groundwater Model for The Netherlands. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Groundwater; Analytic element method; Overspecification; Line element; Doublet; Dipole

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1. Introduction

This paper deals with line elements as used in the Analytic Element Method (Strack, 1989; Haitjema 1995). A technique is presented which makes it possible to apply these elements with far greater accuracy than was possible to date and makes it attractive to apply elements with many degrees of freedom (elements of high order). The interested reader is referred for more information on the analytic element method to Strack, 1999, where this technique is presented as a general approach to determine vector fields that exhibit both non-zero divergence and curl. The approach is based upon the superposition of special functions that are used to approximate the curl and the divergence in addition to harmonic functions that are forms of Cauchy integrals. The latter harmonic functions play an important role in the method, and are used for the following two reasons. The first one is to satisfy conditions along boundaries that enclose domains of non-zero divergence or curl. The second one is to model a variety of linear aquifer features, such as the boundaries of inhomogeneities inside polygons of straight line segments, head-specified boundaries (e.g. rivers), boundaries with given discharge, leaky and impermeable walls, and cracks.

Applications in the present paper deal with flow in shallow aquifers where the Dupuit–Forchheimer assumption may be adopted. The applications are presented for the case of the combined confined–unconfined flow. For confined conditions, the relation between discharge potential Φ and piezometric head

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ϕ is given in Strack (1989) as:

$$\Phi(z) = kh\phi(z) - \tfrac{1}{2}kH^2 \qquad (\phi \geq H;\ \Phi \geq \tfrac{1}{2}kH^2) \tag{1}$$

where $z = x + \mathrm{i}y$ is the complex variable defined in the physical plane, k is the hydraulic conductivity, and H is the aquifer thickness. For unconfined conditions, the relation is:

$$\Phi(z) = \tfrac{1}{2}k\phi^2(z) \qquad (\phi \leq H;\ \Phi \leq \tfrac{1}{2}kH^2) \tag{2}$$

The discharge vector is the gradient of the discharge potential,

$$Q_x = -\frac{\partial\Phi}{\partial x} \qquad Q_y = -\frac{\partial\Phi}{\partial y} \tag{3}$$

The contribution to the discharge vector that is presented in this paper is both irrotational and divergence-free. This vector may therefore be expressed by the use of a complex potential Ω, defined as

$$\Omega = \Phi + \mathrm{i}\Psi \tag{4}$$

where ψ is the stream function. The discharge vector fields presented in this paper may be expressed in terms of the complex derivative of Ω as follows:

$$Q_x - \mathrm{i}Q_y = W(z) = -\frac{\mathrm{d}\Omega}{\mathrm{d}z} \tag{5}$$

The Analytic Element Method is based upon the principle of superposition; the discharge potential due to each aquifer feature is represented using analytic expressions that possess a certain number of degrees of freedom which are used to meet the boundary conditions. The discharge potential at any location thus equals the sum of the discharge potentials due to individual elements. The influences of linear aquifer features are represented using line elements: line-doublets, line-dipoles and line-sinks.

The complex potential for a straight line-doublet, as presented in Strack (1989), is:

$$\Omega(Z_j) = \frac{1}{2\pi\mathrm{i}}\left(\lambda(Z_j)\ln\frac{Z_j - 1}{Z_j + 1} + p(Z_j)\right) \tag{6}$$

$$Z_j = \frac{z - \frac{1}{2}(\overset{1}{z}_j + \overset{2}{z}_j)}{\frac{1}{2}(\overset{2}{z}_j - \overset{1}{z}_j)}$$

where $\overset{1}{z}_j$ and $\overset{2}{z}_j$ are the end points of the element j, and Z_j is a position written in a local coordinate system associated with element j. The element is mapped onto the segment of the real axis in the plane of the dimensionless complex variable $Z_j = X_j + \mathrm{i}\,Y_j$ between $X_j = -1$ and $X_j = 1$. Function $\lambda(Z_j)$, referred to as a jump function, is represented as a polynomial that is real along the element. $p(Z_j)$ is the far-field correction polynomial, one order less than $\lambda(Z_j)$, included to ensure that $\Omega(Z_j)$ approaches $(1/Z_j)$ near infinity.

The complex potential is analytic in the cut plane with the cut defined by $-1 \leq X_j \leq 1$. The real part of the complex potential $\Omega(Z_j)$ given by (6) (the discharge potential) and the tangential component of the discharge vector jump across the element. The stream function and the normal component of the discharge vector are continuous across the element.

The complex potential for a line-dipole causes a jump in the stream function and normal component of the discharge vector across the element. The discharge potential and the tangential component of the discharge vector for a line-dipole are continuous across the element. A line-sink is a line-dipole without logarithmic singularities in complex potential at the end points (Strack, 1989).

The expression for the complex potential for a straight line-dipole differs from discharge potential (6) only in the factor outside the parenthesis, which is i times that shown in (6). For brevity, in this presentation the analysis is performed for the case of a line-doublet only.

2. Overspecification principle

Strack and Haitjema (1981) express the jump function $\lambda(Z_j)$ as first and second order polynomials, while Fitts (1985) uses a second order polynomial. Strack (1989) presents expressions for polynomials of higher order and demonstrates that orders up to nine may be used for double-root elements but reports difficulties when applying higher orders.

The coefficients of the polynomial $\lambda(Z_j)$ were computed by requiring that the boundary condition be met exactly at a number of points that are referred to as the collocation points. For example, the contribution of a line-sink that represents a section of a river of specified head is computed so that the combined discharge potential of all elements gives the specified head value at collocation points.

Accurate results with this method require that the boundary be subdivided in many elements with $\lambda(Z_j)$ for each element a polynomial of order 1 or 2. The computationally most intensive part of (6) is the term $\ln((Z_j - 1)/(Z_j + 1))$ which has to be computed for all line elements. Hence, the precision is increased at the expense of the computational efficiency.

More importantly, this approach often forces a departure from the basic property of the Analytic Element Method, that one aquifer feature is represented by one element. This motivates the development of formulations for analytic elements where high precision can be achieved without dividing a feature into a number of elements, unless required for geometrical reasons.

The attempts to increase the precision by increasing the order of the $\lambda(Z_j)$ polynomial, rather than dividing a feature into a number of elements, were not successful. This is because the unknown coefficients could not be computed using the existing collocation method. This paper does use high order polynomials for $\lambda(Z_j)$ (orders of up to 40), but the unknown coefficients are computed using the principle of overspecification, developed by Janković and Barnes (1999). That is, the coefficients are computed by applying the boundary condition at a set of control points. The number of control points is greater than the number of degrees of freedom, and the coefficients are computed so as to satisfy the boundary condition in the least squares sense over the set of control points.

The benefit of the principle of overspecification is illustrated in Fig. 1, which also demonstrates that the problem cannot be solved by the use of the collocation method with a single high-order element for each straight segment. The overspecification fold is defined as the ratio of the number of control points to the number of degrees of freedom, and for this example equals three. The control points are distributed uniformly along the elements. The picture of the same visual quality as ones obtained using the overspecification may be obtained if each segment is divided into a number of line elements of low order (e.g. order 2) and collocation is used to compute the unknown coefficients. The remaining part of this paper presents this new formulation for line elements in details and a few examples.

3. Chebyshev representation

In this paper the jump function $\lambda(Z_j)$ is represented as a Chebyshev series with real coefficients:

$$\lambda(Z_j) = \sum_{n=0}^{N_j} a_{jn} T_n(Z_j) \tag{7}$$

where a_{jn} are real coefficients, T_n are Chebyshev polynomials (e.g. Press et al., 1986) and N_j is the order of this Chebyshev series. Computation of the unknown coefficients beyond order 20 is hampered by numerical inaccuracies when standard polynomials are used rather than Chebyshev polynomials. This is true even if overspecification is applied (Janković, 1997).

The expression (7) is real along the element:

$$\lambda(X_j) = \sum_{n=0}^{N_j} a_{jn} T_n(X_j) \tag{8}$$

The definition of Chebyshev polynomials $T_n(\cos\theta_j) = \cos(n\theta_j)$ is used to interpret (8) as an expansion of the jump function $\lambda(X_j)$ in a Fourier cosine series in terms of θ_j where $X_j = \cos\theta_j$. Hence, the order of the Chebyshev series may be viewed as a truncation level in this expansion.

The correction function may also be represented as a Chebyshev series of one order less. The expression for the complex potential due to the line-doublet j is now written as:

$$\Omega(Z_j) = \frac{1}{2\pi i}\left(\sum_{n=0}^{N_j} a_{jn} T_n(Z_j) \ln\frac{Z_j - 1}{Z_j + 1} + \sum_{n=0}^{N_j - 1} b_{jn} T_n(Z_j)\right) \tag{9}$$

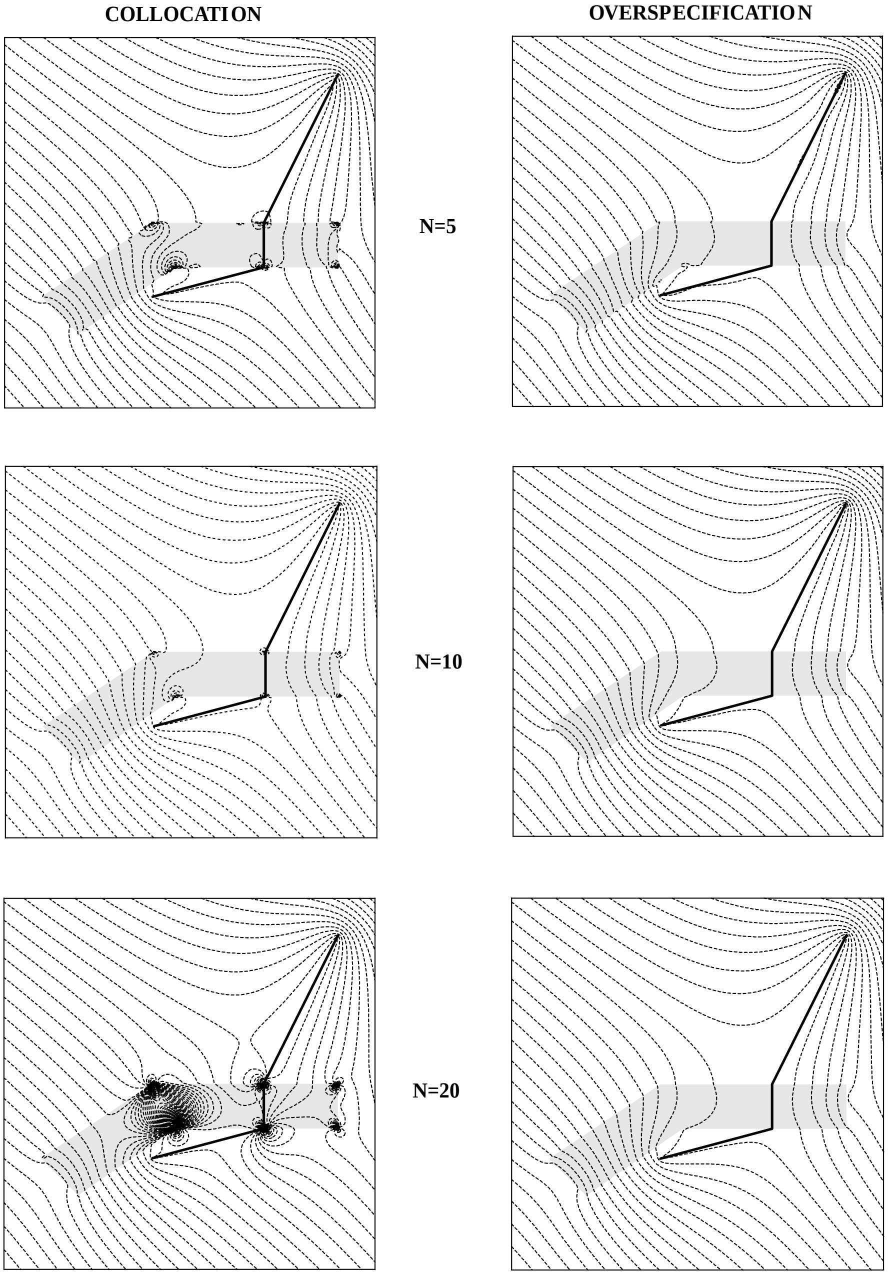

Fig. 1. Piezometric contours for an inhomogeneity ten times less conductive than the background and a constant head line sink. Each straight segment is modeled using a single line element. *N* is order of elements. Overspecification fold was 3.

The coefficients $\underset{j}{b}_{n}$ are computed so that the discharge potential (9) behaves as $(1/\underset{j}{Z})$ near infinity. This is accomplished by expanding the term $\text{In}((\underset{j}{Z} - 1)/(\underset{j}{Z} + 1))$ in a Laurent series, following the approach presented in Strack (1989). This yields the relation between $\underset{j}{a}_{n}$ and $\underset{j}{b}_{n}$ coefficients:

through:

$$\mathbf{b}_j = \mathbf{B}\,\mathbf{a}_j \tag{10}$$

where $\mathbf{a}_j$ is the vector of size $N_j + 1$ that contains $\underset{j}{a}_n$ coefficients, $\mathbf{b}_j$ is the vector of size N_j that contains the coefficients of the correction Chebyshev series and **B** is a matrix of $(N_j + 1)$ columns and (N_j) rows. The generic term in this matrix can be obtained as:

$$\mathbf{B}(m,n) = \begin{cases} \dfrac{4}{n-m} & \text{for } 0 < m < n \text{ and } m+n \text{ is odd} \\ \dfrac{2}{n} & \text{for } m = 0 \text{ and } n \text{ is odd} \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

The expression for the discharge potential (9) may be written in a form where the influence of each coefficient $\underset{j}{a}_n$ is explicitly represented by the use of (11)

$$\Omega(Z_j) = \frac{1}{2\pi \mathrm{i}} \left(\sum_{n=0}^{N_j} \underset{j}{a}_n \sum_{m=0}^{n} f(n,m;Z_j) T_m(Z_j) \right) \tag{12}$$

where:

$$f(n,m;Z_j) = \begin{cases} \ln \dfrac{Z_j - 1}{Z_j + 1} & \text{for } m = n \\ \dfrac{4}{n-m} & \text{for } 0 < m < n \text{ and } m+n \text{ is odd} \\ \dfrac{2}{n} & \text{for } m = 0 \text{ and } n \text{ is odd} \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

Hence, the influence of each coefficient is expressed as a Chebyshev series. The highest order terms of these series are used to create the jump in complex potential across the element, and all other terms are the correction terms. On the element itself, the function $\ln((Z_j - 1)/(Z_j + 1))$ is:

$$\ln \frac{Z_j - 1}{Z_j + 1} = \begin{cases} \ln \left| \dfrac{X_j - 1}{X_j + 1} \right| + \mathrm{i}\pi & \text{for } -1 < X_j < 1,\ Y_j = \overset{+}{0} \\ \ln \left| \dfrac{X_j - 1}{X_j + 1} \right| - \mathrm{i}\pi & \text{for } -1 < X_j < 1,\ Y_j = \overset{-}{0} \end{cases} \tag{14}$$

where + denotes the left side of the element *j* when going from the first to the second point of the element, and − denotes the right side of this element. All the correction terms are real along the element and do not contribute to the discharge potential due to the element *j* on the element itself:

$$\begin{aligned} \Phi(X_j, \overset{+}{0}) &= \frac{1}{2} \sum_{n=0}^{N_j} \underset{j}{a}_n T_n(X_j), \\ \Phi(X_j, \overset{-}{0}) &= -\frac{1}{2} \sum_{n=0}^{N_j} \underset{j}{a}_n T_n(X_j) \end{aligned} \tag{15}$$

The jump in the discharge potential is:

$$\Delta\Phi(X_j) = \Phi(X_j, \overset{+}{0}) - \Phi(X_j, \overset{-}{0}) = \sum_{n=0}^{N_j} \underset{j}{a}_n T_n(X_j) \tag{16}$$

which is the jump function $\lambda(X_j)$, as given by expression (8). The stream function from expression (12) is continuous across the element, as the term $\ln|(X_j - 1)/(X_j + 1)|$ does not jump across the element.

The discharge function *W*, defined in Eq. (5), due to the element *j* is obtained by differentiating the expression for the complex potential Eq. (12) with respect to *z*:

$$\begin{aligned} W(Z_j) &= -\frac{\mathrm{d}\Omega(Z_j)}{\mathrm{d}z} = -\frac{\mathrm{d}\Omega(Z_j)}{\mathrm{d}Z_j} \frac{2}{\overset{2}{z}_j - \overset{1}{z}_j} \\ &= -\frac{2}{\overset{2}{z}_j - \overset{1}{z}_j} \frac{1}{2\pi \mathrm{i}} \left(\sum_{n=0}^{N_j} \underset{j}{a}_n \sum_{m=0}^{n} g(n,m;Z_j) T_m(Z_j) \right) \end{aligned} \tag{17}$$

where:

$$g(n,m;\underset{j}{Z}) = \begin{cases} \dfrac{2}{(\underset{j}{Z}-1)(\underset{j}{Z}+1)} & \text{for } m = n \\ 2n \ln \dfrac{\underset{j}{Z}-1}{\underset{j}{Z}+1} & \text{for } 0 < m < n \text{ and } m+n \text{ is odd} \\ 8 \displaystyle\sum_{l=1}^{\frac{n-m}{2}} \dfrac{n-2l+1}{2l-1} & \text{for } 0 < m < n \text{ and } m+n \text{ is even} \\ n \ln \dfrac{\underset{j}{Z}-1}{\underset{j}{Z}+1} & \text{for } m = 0 \text{ and } n \text{ is odd} \\ 4 \displaystyle\sum_{l=1}^{\frac{n}{2}} \dfrac{n-2l+1}{2l-1} & \text{for } m = 0 \text{ and } n \text{ is even and } n \neq 0 \end{cases} \tag{18}$$

The derivatives of all correction terms and $2/((\underset{j}{Z}-1)(\underset{j}{Z}+1))$ are real along the element and do not contribute to the tangential component of the discharge vector along the element. This tangential component may be expressed as:

$$Q_{\underset{j}{X}}(\underset{j}{X},\overset{+}{0}) = -\frac{1}{\underset{j}{L}} \sum_{n=0}^{\underset{j}{N}-1} \underset{j}{d}_n T_n(\underset{j}{X}),$$
$$Q_{\underset{j}{X}}(\underset{j}{X},\overset{-}{0}) = \frac{1}{\underset{j}{L}} \sum_{n=0}^{\underset{j}{N}-1} \underset{j}{d}_n T_n(\underset{j}{X}) \tag{19}$$

where $\underset{j}{L} = \left|\underset{j}{\overset{2}{z}} - \underset{j}{\overset{1}{z}}\right|$ is the length of element j, and the coefficients $\underset{j}{d}_n$ are obtained using the recursive relation (e.g. Press et al., 1986):

$$\underset{j}{d}_n = \begin{cases} 0 & \text{for } n > \underset{j}{N}-1 \\ \underset{j}{d}_{n+2} + 2(n+1)\underset{j}{a}_{n+1} & \text{for } n = \underset{j}{N}-1, \underset{j}{N}-2, \underset{j}{N}-3, \ldots, 1 \\ \underset{j}{d}_2/2 + \underset{j}{a}_1 & \text{for } n = 0 \end{cases} \tag{20}$$

4. Far-field representations

Roundoff errors hamper computation of (12) and (17) for large $|\underset{j}{Z}|$. The complex potential and the discharge function are commonly evaluated for large $|\underset{j}{Z}|$ using asymptotic expansions,

$$\Omega(\underset{j}{Z}) = \frac{1}{2\pi \mathrm{i}} \sum_{n=1}^{\underset{j}{NF}} \underset{j}{e}_n \underset{j}{Z}^{-n},$$
$$W(\underset{j}{Z}) = \frac{2}{\underset{j}{\overset{2}{z}} - \underset{j}{\overset{1}{z}}} \frac{1}{2\pi \mathrm{i}} \sum_{n=1}^{\underset{j}{NF}} n\, \underset{j}{e}_n \underset{j}{Z}^{-n-1} \tag{21}$$

Expressions for coefficients $\underset{j}{e}_n$ are obtained by expanding the term $\ln((\underset{j}{Z}-1)/(\underset{j}{Z}+1))$ about $1/\underset{j}{Z} = 0$ and retaining a finite number of the terms ($\underset{j}{N}F$) that do not cancel with correction terms. The far field representations (21) are not used in the remaining part of this paper. The expressions for the coefficients $\underset{j}{e}_n$ are presented in Janković (1997).

The number of terms that needs to be retained, $\underset{j}{N}F$, has to be larger if the modulus $|\underset{j}{Z}|$ is smaller and fewer terms are needed for larger values of the modulus. The transition between (12) and (21) was successful for up to order 40 if representation (21) was used starting at about $|\underset{j}{Z}| = 1.02$.

5. The boundary conditions

The unknown coefficients of a line element are computed so as to satisfy the boundary condition assigned along the line element. For notational brevity it is convenient to express a whole class of boundary conditions using the following general equations:

$$c_1\Delta\underset{j}{\Phi}(\underset{j}{X}) + c_2\Delta\underset{j}{Q_X}(\underset{j}{X}) + c_3\underset{j}{Q_Y}(\underset{j}{X}) + c_4\underset{j}{\Psi}(\underset{j}{X}) = \alpha(\underset{j}{X}) \tag{22}$$

and

$$c_5\Delta\underset{j}{\Psi}(\underset{j}{X}) + c_6\Delta\underset{j}{Q_Y}(\underset{j}{X}) + c_7\underset{j}{Q_X}(\underset{j}{X}) + c_8\underset{j}{\Phi}(\underset{j}{X}) = \beta(\underset{j}{X}) \tag{23}$$

Constants c_1 through c_8 cannot be arbitrarily selected: these constants (and their dimensions) must be chosen so that (22) or (23) represents a physical boundary condition. The physical boundary conditions that can be satisfied using line elements are presented in Strack (1989). The first type of boundary condition (Eq. (22)) can be satisfied by placing a line-doublet along the element *j*, while the second type (Eq. (23)) with a line-dipole or a line-sink.

The influence of element *j* is isolated on the left-hand side of these expressions for the purpose of computing the unknown coefficients of element *j*. Hence, the right-hand side ($\alpha(\underset{j}{X})$ or $\beta(\underset{j}{X})$) equals the boundary value minus the influence of all other elements. For example, if the element is a line-sink of specified head, c_8 was set to the value of 1 and all the other constants (c_5, c_6 and c_7) to zero. Value $\beta(\underset{j}{X})$ is set to the value of the discharge potential that gives the specified head (according to (1) or (2)) minus the discharge potential due to all elements other than element *j*.

The conditions at the boundary of an inhomogeneity are that both head and the normal component of the discharge vector are continuous across the boundary. The discharge potential jumps because the hydraulic conductivity jumps and the head is continuous across the boundary (compare (1) and (2)). The jump is created using line-doublets, and the boundary condition can be expressed using Eq. (22) with $c_1 = 1$ and all other constants equal to zero. The detailed derivation for the desired value of the jump in the discharge potential is presented later in this paper.

Another example is an impermeable wall which is modeled using a line-doublet such that $\underset{j}{Q_Y}(\underset{j}{X})$ is zero on the element. A crack is modeled using a line-dipole such that $\underset{j}{Q_X}(\underset{j}{X})$ is zero. The boundary conditions for other leaky and drainy objects are presented in Strack (1989).

For the case of a line doublet, expressions (12), (15), (17) and (19) are substituted into (22):

$$\begin{aligned}
&c_1\sum_{n=0}^{\underset{j}{N}}\underset{j}{a}_n T_n(\underset{j}{X}) - c_2\frac{2}{\underset{j}{L}}\sum_{n=0}^{\underset{j}{N}-1}\underset{j}{d}_n T_n(\underset{j}{X})\\
&- c_3\frac{1}{\pi\underset{j}{L}}\sum_{n=0}^{\underset{j}{N}}\underset{j}{a}_n\sum_{m=0}^{n}\mathscr{R}[g(n,m;\underset{j}{X})]T_m(\underset{j}{X})\\
&- c_4\frac{1}{2\pi}\sum_{n=0}^{\underset{j}{N}}\underset{j}{a}_n\sum_{m=0}^{n}\mathscr{R}[f(n,m;\underset{j}{X})]T_m(\underset{j}{X})\\
&= \alpha(\underset{j}{X})
\end{aligned} \tag{24}$$

This expression can be represented symbolically as:

$$\sum_{n=0}^{\underset{j}{N}}\underset{j}{a}_n u_n(c_1, c_2, c_3, c_4, \underset{j}{L}, \underset{j}{X}) = \alpha(\underset{j}{X}) \tag{25}$$

where $u_n(c_1, c_2, c_3, c_4, \underset{j}{L}, \underset{j}{X})$ represents the terms in

(24) that contain the coefficient $\underset{j}{a}_n$:

$$\begin{aligned} u_n(c_1,c_2,c_3,c_4,\underset{j}{L},\underset{j}{X}) &= c_1T_n(\underset{j}{X}) \\ &- c_2\frac{2}{\underset{j}{L}}\sum_{m=0}^{n-1} d_{n,m}T_m(\underset{j}{X}) - c_3\frac{1}{\pi\underset{j}{L}}\sum_{m=0}^{n}\mathscr{R}[g(n,m;\underset{j}{X})] \\ &\times T_m(\underset{j}{X}) - c_4\frac{1}{2\pi}\sum_{m=0}^{n}\mathscr{R}[f(n,m;\underset{j}{X})]T_m(\underset{j}{X}) \end{aligned} \tag{26}$$

The coefficients $d_{\mathrm{n,m}}$ are obtained from (20) for a unit value of the coefficient $\underset{j}{a}_n$ and all other coefficients equal to zero:

$$d_{n,m} = \begin{cases} 0 & \text{for } m = n \\ 2n & \text{for } m = n-1 \\ d_{n,m+2} & \text{for } m = n-2, n-3, n-4, \ldots, 1 \\ \dfrac{d_{n,2}}{2} & \text{for } m = 0 \end{cases} \tag{27}$$

The benefit of the representation (25) is that the influence of the each coefficient is explicitly shown, which is important in the estimation of the unknown coefficients $\underset{j}{a}_n$.

6. Adding constraints

It is often necessary for special constraints to be satisfied in addition to the boundary conditions. For example, when line elements are combined into strings, it is advantageous to constrain the complex potential to be finite at nodes. For a string which is not intersected by other elements, this will be satisfied if the jump function is continuous at nodes.

Chebyshev polynomial $T_n(\underset{j}{X})$ at $\underset{j}{X} = -1$ equals $(-1)^n$ and at $\underset{j}{X} = 1$ equals 1. Hence, the value of the jump function at the end points is:

$$\lambda(-1) = \sum_{n=0}^{\underset{j}{N}} (-1)^n \underset{j}{a}_n, \qquad \lambda(1) = \sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \tag{28}$$

The constraint that the jump function is continuous at nodes may be represented as:

$$\sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \overset{1}{\underset{j}{\xi}}_n = \overset{1}{\underset{j}{\omega}}, \qquad \sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \overset{2}{\underset{j}{\xi}}_n = \overset{2}{\underset{j}{\omega}} \tag{29}$$

where $\overset{1}{\underset{j}{\xi}}_n = (-1)^n$ and $\overset{2}{\underset{j}{\xi}}_n = 1$. $\overset{1}{\underset{j}{\omega}}$ is the value of the jump function at $\underset{j}{X} = -1$ from the preceding element in the string:

$$\overset{1}{\underset{j}{\omega}} = \lambda(\underset{j-1}{X} = 1) \tag{30}$$

and $\overset{2}{\underset{j}{\omega}}$ is the value of the jump function at $\underset{j}{X} = 1$ from the next element in the string:

$$\overset{2}{\underset{j}{\omega}} = \lambda(\underset{j+1}{X} = -1) \tag{31}$$

Other constraints (such as continuity of the derivative of the jump function) may be expressed using the constraint equations (such as (29)) in the similar fashion. The constraints will be matched exactly.

7. Overspecification principle and least squares

The unknown coefficients $\underset{j}{a}_n$ will be computed, using the overspecification principle, by requiring the best approximation in a least squares sense over $\underset{j}{M}$ control points, but subject to the specified constraints. This is achieved using the method of Lagrange multipliers (e.g. Press et al., 1986). That is, the objective function that needs to be minimized is:

$$\begin{aligned} &\sum_{m=1}^{\underset{j}{M}} \left(\sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \overset{m}{\underset{j}{u}}_n - \overset{m}{\underset{j}{\alpha}} \right)^2 + 2\overset{1}{\underset{j}{\rho}} \left(\sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \overset{1}{\underset{j}{\xi}}_n - \overset{1}{\underset{j}{\omega}} \right) \\ &\quad + 2\overset{2}{\underset{j}{\rho}} \left(\sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \overset{2}{\underset{j}{\xi}}_n - \overset{2}{\underset{j}{\omega}} \right) \\ &\quad \rightarrow \mathrm{MIN} \end{aligned} \tag{32}$$

where $2\overset{1}{\underset{j}{\rho}}$ and $2\overset{2}{\underset{j}{\rho}}$ are Lagrange multipliers, $\overset{m}{\underset{j}{\alpha}} = \alpha(\overset{m}{\underset{j}{X}})$, $\overset{m}{\underset{j}{u}}_n = u_n(c_1,c_2,c_3,c_4,\underset{j}{L},\overset{m}{\underset{j}{X}})$ and $\overset{m}{\underset{j}{X}}$ is the location of the *m*th control point, which is on the element *j*. Differentiating expression (32) with respect to the unknown coefficients ($\underset{j}{a}_s$) and the Lagrange multipliers ($2\underset{j}{\overset{1}{\rho}}$ and $2\underset{j}{\overset{2}{\rho}}$), and setting the value of the derivatives to zero yields a system of linear equations:

$$\sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \sum_{m=1}^{\underset{j}{M}} \underset{j}{\overset{m}{u}}_n \underset{j}{\overset{m}{u}}_s + \underset{j}{\overset{1}{\rho}}\, \underset{j}{\overset{1}{\xi}}_s + \underset{j}{\overset{2}{\rho}}\, \underset{j}{\overset{2}{\xi}}_s = \sum_{m=1}^{\underset{j}{M}} \underset{j}{\overset{m}{\alpha}}\, \underset{j}{\overset{m}{u}}_s, \qquad (33)$$

$$s = 0, 1, 2, \ldots, \underset{j}{N}$$

$$\sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \underset{j}{\overset{1}{\xi}}_n = \underset{j}{\overset{1}{\omega}}, \qquad \sum_{n=0}^{\underset{j}{N}} \underset{j}{a}_n \underset{j}{\overset{2}{\xi}}_n = \underset{j}{\overset{2}{\omega}} \qquad (34)$$

Note that the constraint equations (29) are exactly satisfied.

8. Selecting the control points

The locations of control points are selected according to:

$$\underset{j}{\overset{m}{X}} = \cos\left(\frac{\pi(m - 0.5)}{\underset{j}{M}}\right), \qquad m = 1, 2, \ldots, \underset{j}{M} \qquad (35)$$

These locations yield near optimal approximations for a large number of functions (as explained in Cheney, 1966). That is, if locations (35) are used, the errors along the line element will be oscillatory with approximately constant amplitudes. If the control points are selected according to (35), the required value of the overspecification fold, $\underset{j}{M}/(\underset{j}{N} + 1)$, is smaller than for the case where the control points are distributed uniformly along the element. Increase of the overspecification fold beyond $\underset{j}{M}/(\underset{j}{N} + 1) = 3$ did not significantly improve the precision in any of the investigated problems.

9. Implementation

The implementation algorithm used to solve the problem is iterative: when coefficients for one line element are evaluated, the coefficients for other elements are selected on the basis of the solution for the preceding iteration. The influence of other elements comes in the evaluation of $\alpha(\underset{j}{X})$ and $\beta(\underset{j}{X})$ functions. The coefficients of a particular line element are then obtained by solving the system of equations given by (33) and (34) using a Gaussian elimination algorithm. Once an element is solved, its coefficients are then used in evaluation of the coefficients for other elements. This combination of the globally iterative (Gauss–Seidel) and the locally explicit (Gaussian elimination) algorithm, originally introduced by Janković and Barnes (1999), converged for all examined cases.

Note that the matrix of the system of equations, for all presented cases, depends only on the type of the boundary condition, order of the element $\underset{j}{N}$ and the number of control points $\underset{j}{M}$. This means that the matrix can be set up and inverted only once for all elements of the same number of degrees of freedom and number of control points which share the same boundary condition.

Conversion of the Chebyshev representations for the functions $\lambda(\underset{j}{Z})$ and $p(\underset{j}{Z})$ to standard polynomial representations (Janković, 1977) increases the computational efficiency. This conversion requires that the coefficients $\underset{j}{a}_n$ are known. Computations were carried out in order to assess differences in speed for the example on Fig. 1. Computation using the Chebyshev representation (12) was four times faster than that using twenty elements of order 2. The difference in speed increased to a factor of ten after combining the Chebyshev polynomials to a single standard polynomial.

10. Examples

Several examples are presented that involve a inhomogeneity in the hydraulic conductivity. An inhomogeneity is defined here as an area, bounded by a polygon, where the hydraulic conductivity differs from the background conductivity. Following the relation between the discharge potential and piezometric head (Eqs. (1) or (2)), the head across the boundary of an inhomogeneity will be continuous if the ratio of the discharge potential and hydraulic

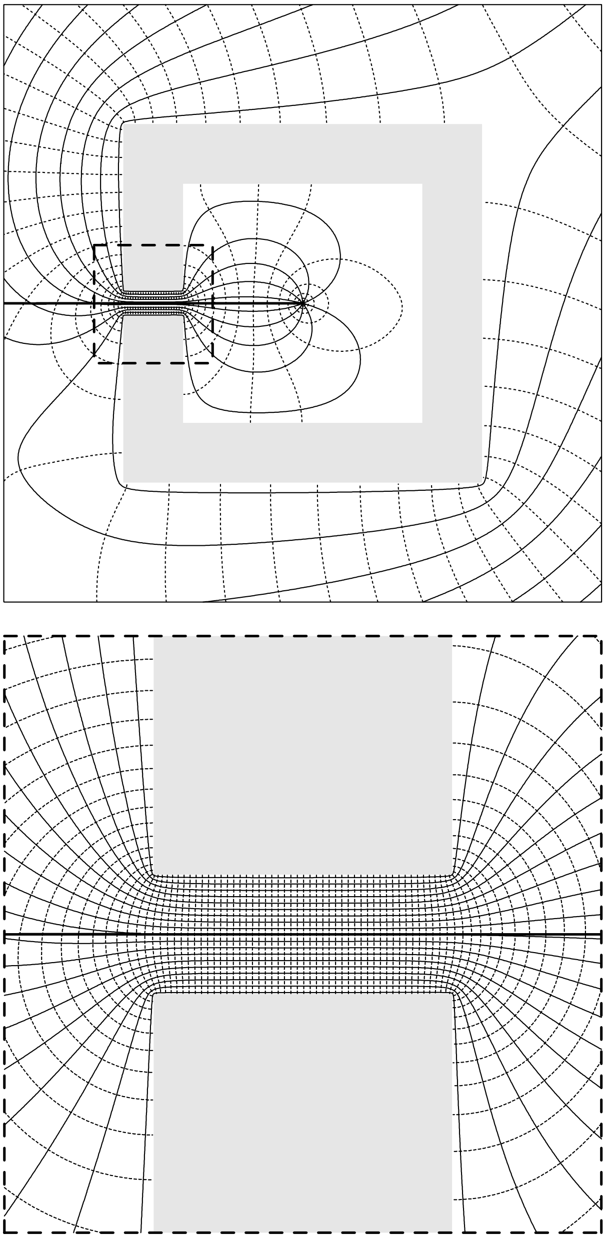

Fig. 2. An impermeable object with a gap and a well in a uniform flow field from northeast to southwest. The stream function contours are plotted as solid lines, piezometric contours are dashed.

conductivity is constant across the boundary:

$$\frac{\underset{\neq j}{\Phi}(\underset{j}{X}) + \Phi(\underset{j}{X}, \overset{+}{0})}{\underset{j}{\overset{+}{k}}} = \frac{\underset{\neq j}{\Phi}(\underset{j}{X}) + \Phi(\underset{j}{X}, \overset{-}{0})}{\underset{j}{\overset{-}{k}}} \qquad (36)$$

where $\underset{j}{\overset{+}{k}}$ is the hydraulic conductivity for the left side of the element j when going from the first to the second point of the element, and $\underset{j}{\overset{-}{k}}$ denotes the hydraulic conductivity for the right side of this element. $\underset{\neq j}{\Phi}(\underset{j}{X})$ denotes the discharge potential at

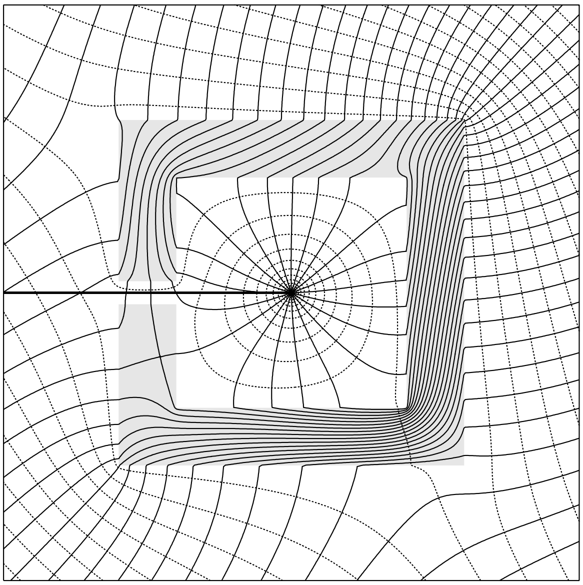

Fig. 3. The problem from Fig. 2 for an inhomogeneity one hundred times more conductive than the background. The stream function contours are plotted as solid lines, piezometric contours are dashed.

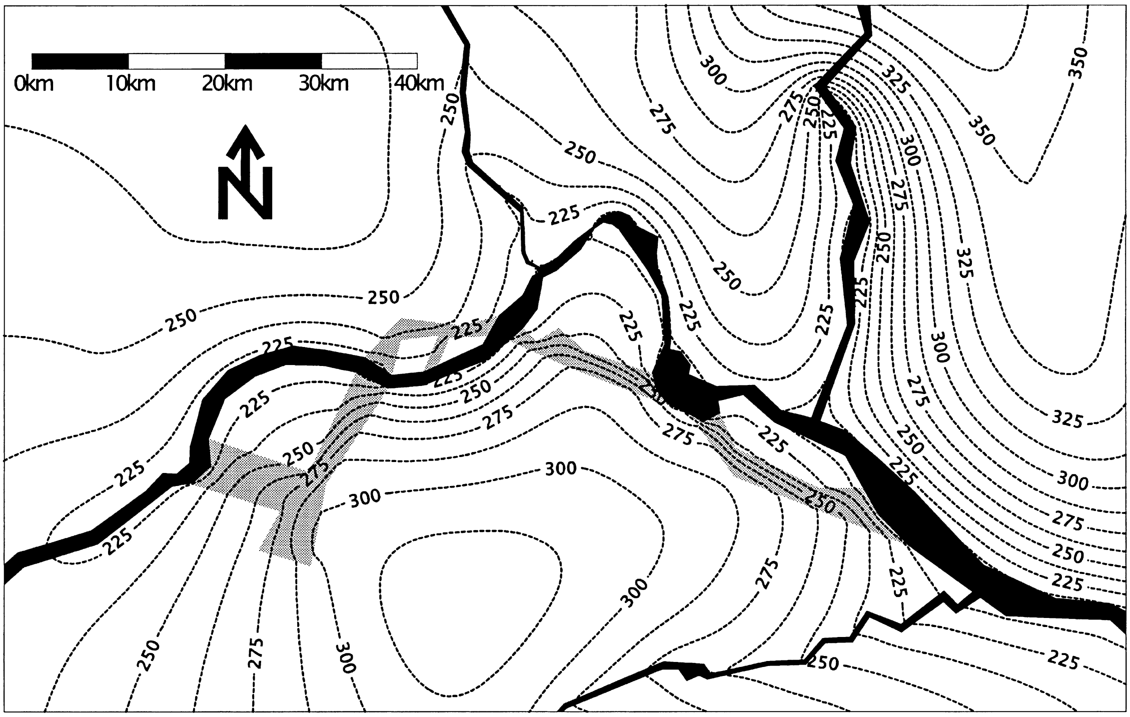

Fig. 4. Piezometric contours in meters for the Prairie Du Chien–Jordan aquifer from the METRO model, Twin Cities, Minnesota, USA. The major rivers (Mississippi River, Minnesota River and others) are presented as solid areas. The shaded area is an inhomogeneity that is modeled using line doublets with overspecification.

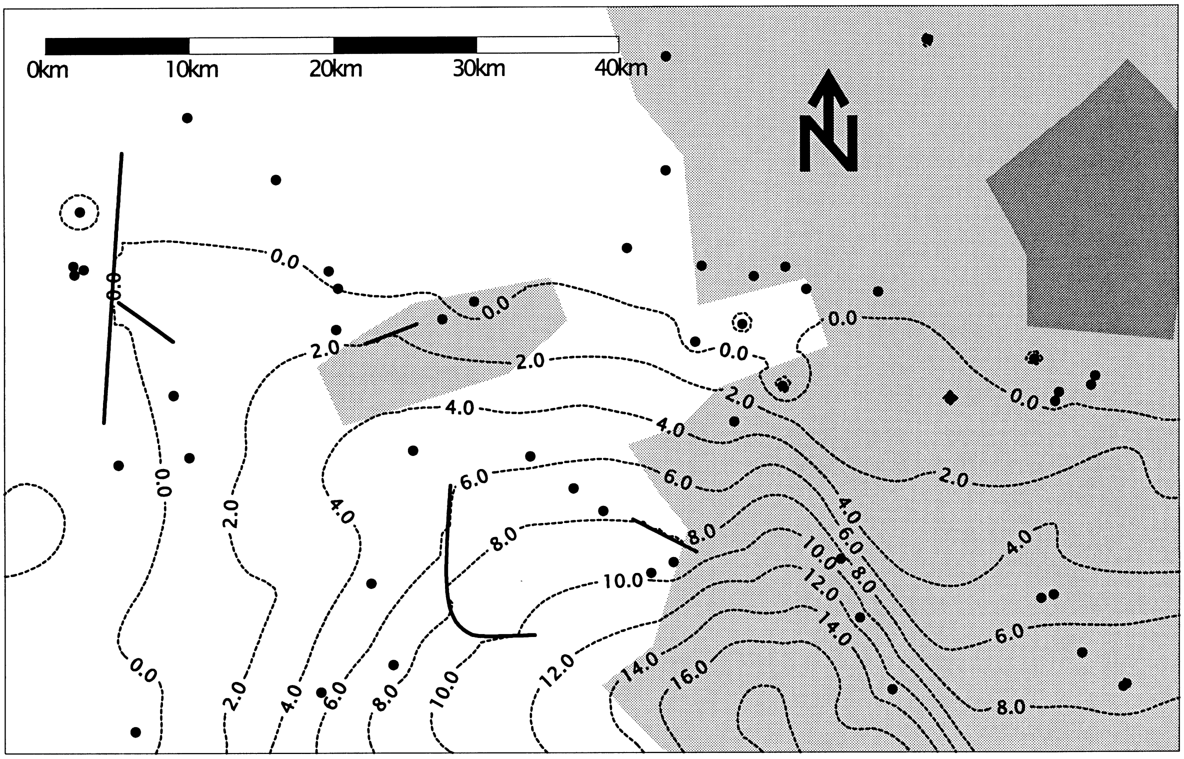

Fig. 5. Piezometric contours in meters for a northern region in The Netherlands. The shaded areas are inhomogeneities that are modeled using line doublets with overspecification. The linear features are leaky walls that are also modeled using line doublets.

location ($\underset{j}{X}$) along the element j due to all elements other than element j itself. The condition can be satisfied with a string of straight line-doublets placed along the boundary of the inhomogeneity. The required jump in the discharge potential can be expressed as:

$$\Phi(\underset{j}{X}, \overset{+}{0}) - \Phi(\underset{j}{X}, \overset{-}{0}) = (\underset{\neq j}{\Phi}(\underset{j}{X}) + \Phi(\underset{j}{X}, \overset{-}{0}))\frac{\underset{j}{\overset{+}{k}} - \underset{j}{\overset{-}{k}}}{\underset{j}{\overset{-}{k}}} \quad (37)$$

Because the discharge potential due to the element j on the element itself along the right ('$-$') side of the element is minus one half of the jump (expression (15)), the expression that guarantees the continuity of head can be written as:

$$\Delta\Phi(\underset{j}{X}) = \left(\underset{\neq j}{\Phi} - \frac{\Delta\Phi(\underset{j}{X})}{2}\right)\frac{\underset{j}{\overset{+}{k}} - \underset{j}{\overset{-}{k}}}{\underset{j}{\overset{-}{k}}} \quad (38)$$

Finally, the required jump is:

$$\Delta\Phi(\underset{j}{X}) = 2\left(\frac{\underset{j}{\overset{+}{k}} - \underset{j}{\overset{-}{k}}}{\underset{j}{\overset{+}{k}} + \underset{j}{\overset{-}{k}}}\right)\underset{\neq j}{\Phi} \quad (39)$$

The examples involving inhomogeneities are presented in Figs. 1–3. The line elements for all examples (excluding Fig. 1) are of order 40. Note that for some of these examples, the singular behavior at end points could have been incorporated explicitly using tip elements (Strack, 1989). This was intentionally omitted from the formulation to demonstrate the power and the precision of the new formulation.

The new formulation has already been applied to all the boundary conditions mentioned before. Furthermore, it is being used in the development of the Metropolitan Area Groundwater Model (METRO Model) for Twin Cities, Minnesota (e.g. Fig. 4) and for enhancements of the next release of National

Groundwater Model for The Netherlands (NAGROM) (e.g. Fig. 5), de Lange (1996), using the computer code MLAEM developed by O.D.L. Strack.

11. Conclusions

The presented formulation for line elements, based on the principle of overspecification, significantly increases the efficiency of previous formulation that is based on collocation. A single aquifer feature can now be represented as a single line element, more often than was possible when using collocation. Hence, this new formulation also enhances the elegance of the original formulation. The use of this new formulation is not restricted to divergence-free irrotational flow. For example, the discharge vector may, and has been, combined with the discharge vectors that exhibits a non-zero divergence for the regional modeling of groundwater flow.

The following five new tools are introduced to the original formulation for line elements: (1) the principle of overspecification; (2) high order Chebyshev polynomials; (3) a combination of an iterative and an explicit algorithm; (4) a new scheme for selecting the locations of control points; and (5) the concept of Lagrange multipliers for explicitly incorporating coefficient constraints. The new formulation is not exact but has been shown visually to approach an exact solution to within machine accuracy for all cases investigated to date. For example, for the problem illustrated in Fig. 3, the piezometric head was continuous across the boundary of an inhomogeneity everywhere in 6 significant digits. The formulation combines the versatility of numerical techniques and the precision of analytic solutions.

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