The Boundary-Integral-Equation Method for Computing the Three-Dimensional Flow of Groundwater

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Summary

The boundary-integral-equation method for computing the three-dimensional steady flow of groundwater is developed. Starting from the basic flow equations, a reciprocity theorem is derived from which source-type integral representations for the flow-field quantities are obtained. Utilizing these representations, the relevant boundary integral equations are arrived at. Their numerical handling is discussed in some detail.

1. Introduction

In this paper we analyze the three-dimensional steady flow of groundwater through piecewise homogeneous and anisotropic fluid-saturated subsoils with the aid of the boundary-integral-equation method. To locate position in R^3, we employ the coordinates $\{x_1,x_2,x_3\}$ with respect to an orthogonal Cartesian reference frame with origin O and three mutually perpendicular base vectors $\{\underline{i}_1,\underline{i}_2,\underline{i}_3\}$ of unit length each. Partial differentiation is denoted by ∂. The subscript notation for vectors and tensors is used and the summation convention applies. Occasionally, a direct notation will be used to denote vectors; for example, $\underline{x}=x_k\underline{i}_k$ denotes the position vector.

The flow state of the groundwater is characterized by the pressure p and the flow velocity v_i. These quantities satisfy the continuity equation [1a]

$$\partial_i v_i = q, \tag{1}$$

and Darcy's law [1b]

$$-\partial_i p - R_{ij}v_j = -\rho g_i - f_i, \tag{2}$$

where q is the volume source density of injection rate, f_i the volume source density of force, R_{ij} the tensorial resistivity of the fluid-saturated porous medium, ρ the volume density of fluidmass, and g_i the local (constant) acceleration of free fall. On each part of the surface bounding the relevant

Th. A. Cruse (Editor)
Advanced Boundary Element Methods
IUTAM Symposium San Antonio, Texas, 1987

subsoil, either the pressure, or the normal component of the flow velocity, or a linear combination of these has a prescribed value. Furthermore, across an interface of discontinuity in resistivity and/or volume density of fluid-mass, the pressure and the normal velocity are to be continuous.

2. The reciprocity theorem for steady ground-water flow

We start with deriving a reciprocity theorem that interrelates, in a specific way, the flow quantities of two admissible, but non-identical, ground-water flow states (to be denoted by the superscripts A and B, respectively) that can occur in one and the same bounded domain in R^3. To this end, we consider the following interaction quantity between the two states: $\partial_i(p^A v_i^B - p^B v_i^A)$. Using (1) - (2) for the two states, we are led to the local form of the reciprocity theorem:

$$\partial_i(p^A v_i^B - p^B v_i^A) = (R_{ij}^B - R_{ji}^A)v_i^A v_j^B + (\rho^A v_i^B - \rho^B v_i^A)g_i + f_i^A v_i^B - f_i^B v_i^A - q^A p^B + q^B p^A. \quad (3)$$

Integrating (3) over a bounded domain V in R^3, and using Gauss' theorem in the resulting left-hand side, we obtain

$$\int_{\partial V}(p^A v_i^B - p^B v_i^A)\nu_i dA = \int_V (R_{ij}^B - R_{ji}^A)v_i^A v_j^B dV + \int_V[(\rho^A v_i^B - \rho^B v_i^A)g_i + f_i^A v_i^B - f_i^B v_i^A - q^A p^B + q^B p^A]dV, \quad (4)$$

where ∂V is the boundary of V and ν_i is the unit vector in the direction of the outward normal to ∂V. Equation (4) is the global form, for the domain V, of the reciprocity theorem. The first term on the right-hand sides of (3) and (4) is characteristic for the difference in resistivity of the media present in the States A and B, while the remaining part represents the interaction between the sources and the accompanying fluid-flow states.

3. Source-type integral representations for p and v_i

To obtain the source-type integral representation for the pressure we take in (4): $\{p^A, v_i^A\} = \{p, v_i\}$, where p and v_i apply to the actual flow state. Further, we take $\{p^B, v_i^B\} = \{p^{Gq}, v_i^{Gq}\}$, where p^{Gq} and v_i^{Gq} satisfy

$$\partial_i v_i^{Gq} = a\delta(\underline{x} - \underline{x}'), \quad (5)$$

$$-\partial_i p^{Gq} - R_{ji} v_j^{Gq} = 0, \tag{6}$$

where a is an arbitrary constant, $\delta(\underline{x}-\underline{x}')$ the three-dimensional spatial unit pulse operative at $\underline{x}=\underline{x}'$, and R_{ji} is the transpose of the resistivity R_{ij} of the actual configuration. The quantities p^{Gq} and v_i^{Gq} are linearly related to the constant a; we express this by writing $\{p^{Gq},v_i^{Gq}\}=a\{G^q,-\Gamma_i^q\}$, where G^q and Γ_i^q are the injection-source Green's functions. With this, (4) leads to

$$-\int_{\partial V}(G^q\nu_i v_i + \Gamma_i^q \nu_i p)dA + \int_V[G^q q + \Gamma_i^q(\rho g_i + f_i)]dV = \chi_V(\underline{x}')p(\underline{x}'), \tag{7}$$

where χ_V is the characteristic function of V, defined as $\chi_V(\underline{x})=\{1,\frac{1}{2},0\}$ when $\underline{x}\in\{V,\partial V,V'\}$, in which V' denotes the complement of $\partial V\cup V$ in R^3. For $\underline{x}'\in\partial V$, (7) holds at points where ∂V has a unique tangent plane, provided that the surface integral is interpreted as its Cauchy principal value.

Similarly, to arrive at the source-type integral representations for the flow velocity, we take State A as above, while now: $\{p^B,v_i^B\}=\{p^{Gf},v_i^{Gf}\}$, where p^{Gf} and v_i^{Gf} satisfy

$$\partial_i v_i^{Gf} = 0, \tag{8}$$

$$-\partial_i p^{Gf} - R_{ji} v_j^{Gf} = -b_i\delta(\underline{x}-\underline{x}'), \tag{9}$$

where b_i is an arbitrary constant vector. Expressing the linear dependence of p^{Gf} and v_i^{Gf} on b_i by writing $\{p^{Gf},v_j^{Gf}\}=b_i\{-\Gamma_i^f,G_{ij}^f\}$, where Γ_i^f and G_{ij}^f are the force-source Green's functions, (4) now yields:

$$-\int_{\partial V}(\Gamma_i^f\nu_j v_j + G_{ij}^f\nu_j p)dA + \int_V[\Gamma_i^f q + G_{ij}^f(\rho g_j + f_j)]dV = \chi_V(\underline{x}')v_i(\underline{x}'). \tag{10}$$

The Green's functions occurring in (7) and (10) will be taken to apply to the "infinite medium" with the properties of the relevant domain, and are calculated analytically in Section 5.

4. Boundary-integral equations

Equations (7) and (10) for $\underline{x}'\in\partial V$ are now applied to each homogeneous subdomain of the configuration. Then, (7) leads to an integral relation between p and $\nu_i v_i$ at ∂V which is of the first kind in $\nu_i v_i$ and of the second kind in p, while (10) leads to an integral relation of the first kind in p and of the second kind in $\nu_i v_i$. At interfaces between two different media we enforce the continuity of p and $\nu_i v_i$; at the outer boundary we prescribe either p or

$\nu_i v_i$. In this way, we end up with a system of boundary-integral relations. Since the resulting number of equations equals twice the number of unknowns, there is a freedom in choice of equations to be employed in the calculations. We shall employ a complete system of the second kind, both in p and $\nu_i v_i$. It is observed that in the literature (see, e.g. [2]), the boundary-integral-equation formulation is usually based on (7); this leads to integral equations of the first kind in $\nu_i v_i$ and of the second kind in p. There is some indication that using integral equations of the second kind, the systems of linear, algebraic equations that result after discretization are better conditioned than the ones that result from integral equations of the first kind.

5. Evaluation of the Green's flow states in an unbounded homogeneous domain

The injection-source and force-source Green's flow states pertaining to a homogeneous medium of infinite extent are calculated with the aid of a three-dimensional spatial Fourier transformation method. Let the Fourier transform $\tilde{h}=\tilde{h}(\underline{k})$ over R^3 of a function $h=h(\underline{x})$ be defined by

$$\tilde{h}(\underline{k}) = \int_{\underline{x}\in R^3} \exp(-ik_n x_n) h(\underline{x}) dV, \tag{11}$$

where i denotes the imaginary unit and $\underline{k}\in R^3$ is the wave vector in Fourier-transform space. According to Fourier's theorem, we then inversely have

$$h(\underline{x}) = (2\pi)^{-3} \int_{\underline{k}\in R^3} \exp(ik_n x_n) \tilde{h}(\underline{k}) dV. \tag{12}$$

First, (11) is applied to (5) and (6). Applying the rule $\tilde{\partial}_i = ik_i$, the transformed equations lead to the expressions:

$$\tilde{p}^{Gq} = a\tilde{G}\exp(-ik_n x_n'), \tag{13}$$

$$\tilde{v}_i^{Gq} = -ik_j K_{ji} a\tilde{G}\exp(-ik_n x_n'), \tag{14}$$

where K_{ij} denotes the inverse of R_{ij} and $\tilde{G}$ is defined by

$$\tilde{G} = (k_i K_{ij} k_j)^{-1}. \tag{15}$$

Evaluation of the relevant inversion integral yields

$$G(\underline{x}) = [\det(K_{ij})]^{-1/2} / [4\pi (R_{ij} x_i x_j)^{1/2}]. \tag{16}$$

Elementary rules of the Fourier transformation then lead to

$$p^{Gq} = aG(\underline{x}-\underline{x}'), \tag{17}$$

$$v_i^{Gq} = -aK_{ji}\partial_j G(\underline{x}-\underline{x}'). \tag{18}$$

From (17) and (18) the Green's functions G^q and Γ_i^q immediately follow. In a similar way, p^{Gf} and v_i^{Gf}, are obtained as

$$p^{Gf} = -b_i K_{ij}\partial_j G(\underline{x}-\underline{x}'), \tag{19}$$

$$v_i^{Gf} = K_{ji}b_r K_{rs}\partial_j\partial_s G(\underline{x}-\underline{x}') + b_j K_{ji}\delta(\underline{x}-\underline{x}'), \tag{20}$$

from which the expressions for Γ_i^f and G_{ij}^f directly result.

6. Numerical aspects in solving the boundary-integral equations

To discretize the system of boundary-integral equations, we first subdivide ∂V into NT planar, triangular surface elements $S_T(n)$ whose vertices have the position vectors $\{x_i(n,q),\ q=1,2,3\}$ with $x_i(n,q+3)=x_i(n,q)$. Each two adjacent triangles have an edge in common; their orientation is such that the direction of circulation forms a right-handed system with the (constant) normal $\nu_i(n)$ to $S_T(n)$. Next, in each triangle, the surface source distributions are expanded in terms of linear interpolation functions. Let $L_i(n,q)$ further denote an outwardly directed vector along the q-th edge $C_T(n,q)$ in the plane of $S_T(n)$. Then, the linear function $\phi(\underline{x},n,q)$ that equals unity when $\underline{x}=\underline{x}(n,q)$ and is zero in the remaining two vertices can be written as

$$\phi(\underline{x},n,q) = {}^1/_3 - [x_i - b_i(n)]L_i(n,q)/2A(n) \text{ when } \underline{x}\in S_T(n), \tag{21}$$

where $b_i(n)$ is the position vector of the barycenter of $S_T(n)$ and $A(n)$ is the area of $S_T(n)$. $\phi(\underline{x},n,q)$ is used as expansion function in each triangle $S_T(n)$. To conclude the discretization procedure, we apply the method of collocation (point matching) at the vertices of the triangles, i.e. we take $\underline{x}'=\underline{x}(m,s)$ $(m=1,2,\dots,NT;\ s=1,2,3)$. At a vertex, ν_i is taken to follow from the weighted average of the vectorial areas of those triangles that have that vertex in common. Combining these steps, we are led to a system of linear, algebraic equations for the unknown values of either p or $\nu_i v_i$ at the nodes of the discretized boundary. In the matrix of coefficients and in the known right-hand side of this system of equations, the following surface integrals occur:

$\{I1,I2,I3_i,I4_i\}(n,q,m,s)=\int_{\underline{x}\in S_T(n)}\phi(\underline{x},n,q)\{G^q,\nu_i\Gamma_i^q,\Gamma_i^f,\nu_jG_{ij}^f\}(\underline{x};m,s)dA=$ $\{(22),(23),(24),(25)\}$. The contributions resulting from q and f_i in (7) and (10) can be evaluated once the sources have been specified. The remaining integrals associated with the gravity term ρg_i are evaluated analytically by employing the expressions for the relevant Green's functions.

7. Numerical results

As a first test of our computer code we have applied a simplified version of it to the given flow field $p=-3^{-1/2}(x_1+x_2+x_3)+x_3+3^{1/2}-1$ and $\underline{v}=3^{-1/2}(\underline{i}_1+\underline{i}_2+\underline{i}_3)$ in the source-free domain V: $0\le x_1,x_2,x_3\le 1$ with the homogeneous and isotropic medium $\rho=1$, $R=1$, and $\underline{g}=\underline{i}_3$. The boundary surface of V is denoted by $\partial V=\partial V_1\cup\partial V_2$, where p is prescribed on ∂V_1 and ν_iv_i on ∂V_2. Each face of the unit cube is divided into sixteen isosceles rectangular triangles, four triangles occupying a square region of dimension 0.5×0.5. On each triangle, p and ν_iv_i are approximated by their values at the barycenter. Collocation is now applied at the barycenters of the triangles. The resulting system of linear, algebraic equations is solved by a direct method. Three cases were considered: (i) $\partial V_1=\{x_1=0,0\le x_2,x_3\le 1\}$, (ii) $\partial V_1=\{x_1=0,0\le x_2,x_3\le 1\}\cup$ $\{0\le x_1,x_2\le 1,x_3=1\}\cup\{0\le x_1,x_3\le 1,x_2=1\}$, and (iii) $\partial V_2=\{0.5\le x_1,x_2\le 1,x_3=0\}$. The local error in the pressure is defined as $ERR(p)=|p_{com}-p_{ex}|/\max(|p_{ex,bary}|)$, where p_{com} and p_{ex} are the computed and exact values of the pressure, respectively, and $\max(|p_{ex,bary}|)$ denotes the maximum value of p_{ex} at the barycenters of all triangles. Similarly, the local error in the normal flow velocity is defined as $ERR(\nu_iv_i)=|\nu_iv_{i,com}-\nu_iv_{i,ex}|$ (note that $\max(|\underline{v}_{ex}|)=1$). Further, the global root-mean-square error in the pressure is defined as

$$RMSE(p) = \{\int_{\partial V_2}|p_{com} - p_{ex}|^2dA \;/\; \int_{\partial V_2}|p_{ex}|^2dA\}^{1/2}; \qquad (26)$$

a similar expression is used for the global root-mean-square error in the normal flow velocity $RMSE(\nu_iv_i)$. A summary of the results is presented in

Table I. Global and local errors in p and ν_iv_i.

test case	RMSE(p)	RMSE(ν_iv_i)	ERR(p) at $\{\frac{7}{12},\frac{3}{4},0\}$	ERR(p) at $\{\frac{11}{12},\frac{3}{4},0\}$	ERR(ν_iv_i) at $\{0,\frac{3}{4},\frac{5}{12}\}$	ERR(ν_iv_i) at $\{0,\frac{3}{4},\frac{1}{12}\}$
(i)	0.046	0.065	0.025	0.039	0.020	0.027
(ii)	0.017	0.092	0.003	0.012	0.027	0.037
(iii)	0.009	0.087	0.001	0.002	0.030	0.091

Table I. The results obtained for p are more accurate than the ones for $\nu_i v_i$. This is ascribed to the fact that p is solved from an integral equation of the second kind, while $\nu_i v_i$ is solved from an integral equation of the first kind. At points near edges the error increases; a finer discretization is expected to lead to more accurate results. The implementation of a complete system of the second kind as discussed in Section 4 is under development.

All computations have been performed on a IBM PC/AT. Programs have been written in Fortran 77. The CPU time for each test case was about 8 minutes.

Appendix. Evaluation of IL1(n,q,m,s) (isotropic case)

The integrals (22) - (25) can be evaluated analytically. As an example, we discuss IL1 for the isotropic case where $R_{ij}=R\delta_{ij}$. From (22) and (21) it follows that IL1 has the shape:

$$IL1(n,q,m,s) = (R/4\pi)[S1(n,m,s)/3 + S1Q(n,q,m,s)/2A(n)], \qquad (A1)$$

where

$$S1(n,m,s) = \int_{\underline{x}\in S_T(n)} |\underline{x}-\underline{x}(m,s)|^{-1} dA, \qquad (A2)$$

$$S1Q(n,q,m,s) = \int_{\underline{x}\in S_T(n)} [x_i-b_i(n)]L_i(n,q)|\underline{x}-\underline{x}(m,s)|^{-1} dA. \qquad (A3)$$

To calculate S1, we first decompose x_i-x_i' into a part normal to $S_T(n)$ and a part parallel to $S_T(n)$, i.e.

$$x_i - x_i(m,s) = \zeta\nu_i(n) + y_i \quad \text{with } \zeta=\nu_i(n)(x_i - x_i') \quad \text{when } \underline{x}\in S_T(n). \quad (A4)$$

Since $\underline{y}$ is a vector in the plane of $S_T(n)$, we can represent it with respect to some local two-dimensional orthogonal Cartesian reference frame in this plane. Let y_α with $\alpha=1,2$ denote the Cartesian coordinates in this reference frame, then (cf. (A2))

$$S1(\zeta) = \int_{\underline{y}\in S_T(n)} |\zeta^2 + y_\alpha y_\alpha|^{-1} dA. \qquad (A5)$$

We now assume $\zeta \neq 0$, differentiate (A5) on both sides twice with respect to ζ, and apply in the resulting right-hand side the relation:

$$-|\zeta^2 + y_\alpha y_\alpha|^{-3} + 3\zeta^2|\zeta^2 + y_\alpha y_\alpha|^{-5} = \partial_\alpha[y_\alpha|\zeta^2 + y_\alpha y_\alpha|^{-3}]. \qquad (A6)$$

Then, upon successively using the two-dimensional form of Gauss' theorem and rewriting $y_\alpha y_\alpha$ with respect to the original reference frame, we end up with

$$\partial^2 S1(\zeta) = \Sigma_{q=1}^{3} \nu_i^C(n,q) \int_{\underline{y}\in C_T(n,q)} y_i \; |\zeta^2 + y_j y_j|^{-3} ds, \qquad (A7)$$

where $\nu_i^C(n,q)$ is the outwardly directed unit vector along the edge $C_T(n,q)$ lying in the plane of $S_T(n)$. To solve $S1(\zeta)$ from (A7) we simply integrate either side twice with respect to ζ and evaluate the remaining line integrals. After some tedious but elementary calculations the final result follows (see [3]). Due to limitations in space, the results are not reproduced here. To evaluate S1Q, we observe that (cf. (A4))

$$x_i - b_i(n) = x_i(m,s) - b_i(n) + y_i + \zeta\nu_i(n) \quad \text{when } \underline{x}\in S_T(n), \qquad (A8)$$

after which S1Q can be evaluated along similar lines. The same techniques can be applied to the surface integrals IL2, $IL3_i$, $I3_i$, and $IL4_i$. Integrals of the type S1 have also been evaluated, in a slightly different manner, by [4] and [5].

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* This research has been carried out with the financial support from the Netherlands Technology Foundation (STW); this support is greatly acknowledged.