INTERNATIONAL JOURNAL FOR NUMERICAL AND ANALYTICAL METHODS IN GEOMECHANICS
Int. J. Numer. Anal. Meth. Geomech., **23**, 1681–1699 (1999)

A BOUNDARY ELEMENT METHOD FOR ANALYSIS OF CONTAMINANT TRANSPORT IN POROUS MEDIA I: HOMOGENEOUS POROUS MEDIA

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SUMMARY

A boundary element method is developed for the analysis of contaminant migration in porous media. The technique involves, firstly, taking the Laplace transform with respect to time then followed by a co-ordinate transform and a mathematical transform of the well-known advection–dispersion equation. The series of transforms reduce the equation into the modified Helmholz equation and this greatly facilitates the formulation of the boundary integral equation and a system of approximating algebraic boundary element equations. The algebraic equations are solved simultaneously in the transform space before being inverted numerically to obtain the concentration of the contaminant in real time and space. The application of this technique is demonstrated by some illustrative examples. Copyright © 1999 John Wiley & Sons, Ltd.

KEY WORDS: boundary element method; contaminant migration; mass transport; homogeneous porous media

1. INTRODUCTION

In recent years, the Boundary Element Method (BEM) has been seen as an attractive numerical technique. While less powerful than some domain methods (such as the finite element method), it nevertheless has certain advantages. One particular feature of the BEM is that a set of boundary integral equations equivalent to the governing differential equations is formulated, instead of a set of domain integral equations used in most other methods. It leads to the possibility of reducing the dimensionability of the problem by one and in the number of approximating equations which must be solved. In the BEM data input preparation and mesh generation are regarded as simpler than domain methods, notwithstanding the availability of preprocessors nowadays for assisting in these tasks. Another advantage of the BEM involves problems with infinite boundaries; these are treated naturally in which the infinite boundaries are not formally included and so can result in potential savings in computational effort.

In order to develop the boundary element method however, it is necessary first to formulate an equivalent boundary integral equation to the governing equation. Different approaches have

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CCC 0363–9061/99/141681–19$17.50

Received 16 September 1997
Revised 9 April 1998

been adopted for the time-dependent advection–dispersion equation. The boundary integral formulation of Taigbenu and Liggett,[1] for instance, uses a finite difference scheme to treat the time derivative. This time discretization and the advection terms lead to a domain integral while the dispersion terms are cast into the form of a boundary integral. As the evaluation of a domain integral is required at each time step, this technique is potentially unattractive for problems with large domains.

Khanbilvardi *et al.*[2] studied the closely related problem of unsaturated moisture flow by formulating a boundary integral equation which employs the time-dependent fundamental solutions. With this technique, the space–time domain is divided up into elements with prescribed space and time interpolation functions. Since the approach requires that the temporal integration be evaluated from the commencement of the process to the time of interest, it will demand the storage and numerical integration of the complete solution history. For solutions at moderate or large time, this method will inevitably be computationally expensive.

An approach used by Rahman *et al.*[3] involves a Laplace transformation of the time variable enabling a boundary integral equation formulation of problems with isotropic hydrodynamic dispersion and uniformly zero initial background concentration while avoiding an undesirable domain integral. The use of Laplace transform technique in boundary element formulation is not new. For example, it was previously used by Cruse and Rizzo[4] to formulate boundary integral equations in transient thermoelasticity and by Smith[5] and Smith and Booker[6–9] in thermoelasticity. This is the first of two papers which will use the Laplace transform technique to develop a boundary element method for contaminant migration near a waste repository where hydrodynamic dispersion may or may not be anisotropic and the initial background concentration may or may not be uniformly zero. In this paper, the porous medium surrounding the waste source will be assumed to be homogeneous while the case in which the porous media is non-homogeneous will be discussed in the second paper.

2. DEVELOPMENT OF 2D BEM FOR HOMOGENEOUS POROUS MEDIA

In many practical situations, the longitudinal dimension of the waste repository or source under consideration is large relative to the dimensions of the other sides. For these cases, it is usually sufficient, in practice, to formulate the physical problem to be solved as a problem of two-dimensional plane contaminant transport. It will be assumed in this paper that the repository is long in the y direction and that contaminant transport is occurring in the two-dimensional x–z plane, that is, the BEM will be developed for problems in two spatial dimensions. As well, many of the cases to be dealt with involve engineered waste repositories where the surrounding groundwater flow occurring near the repositories is likely to remain fairly uniform. Therefore, in this discussion, the groundwater flow will be assumed to remain constant spatially and temporally in the porous media.

2.1. Governing equations

By considering a control area and applying the principle of conservation of mass, the governing equation of contaminant transport of a single species in the x–z plane of the porous media may be written as,[10–12]

$$\nabla \cdot \mathbf{f} + n\frac{\partial c}{\partial t} + g = 0 \tag{1}$$

where $\mathbf{\nabla} = [\partial/\partial x, \partial/\partial z]^{\mathrm{T}}$ is the gradient operator, $\mathbf{f} = [f_x, f_z]^{\mathrm{T}}$ the vector of mass flux components in the x, z directions, n the porosity of the porous media, c the concentration of the contaminant in the pore fluid, and g the rate at which the contaminant is lost from the groundwater due to adsorption onto the soil skeleton, radioactive decay, biodegradation and other sources and sinks per unit volume of porous media.

The mass flux is often assumed to be governed by a Fickian relationship given by

$$\mathbf{f} = n\mathbf{V}c - n\mathbf{D}\mathbf{\nabla}c \tag{2}$$

where $\mathbf{V} = [V_x, V_z]^{\mathrm{T}}$ is the vector of the components of the average groundwater velocity in the x, z directions, and $\mathbf{D}$ the tensor of hydrodynamic dispersion.

In isotropic porous media, the coefficients of hydrodynamic dispersion are commonly expressed in the form as,[10]

$$D_{kl} = (D_0 + \alpha_{\mathrm{T}} V)\delta_{kl} + (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}})\frac{V_K V_l}{V}$$

where $\alpha_{\mathrm{L}}, \alpha_{\mathrm{T}}$ are the longitudinal and tranverse dispersivities, D_0 is the coefficient of isotropic molecular diffusion, δ_{kl} is the Kronecker's delta and k, l range over the index set (x, z). In source or sink-free porous media, the quantity g can often be thought of as the sum of components, g_{A} (due to adsorption), g_{D} (due to radioactive decay) and g_{B} (due to biodegradation), i.e.

$$g = g_{\mathrm{A}} + g_{\mathrm{D}} + g_{\mathrm{B}} \tag{3}$$

A number of commonly occurring chemical reactions in groundwater may be approximated by either a linear equilibrium or a first-order non-equilibrium adsorption–desorption model.[13,14] In the case of linear equilibrium isotherm, the rate of adsorption onto the soil skeleton can be expressed as [15–17]

$$g_{\mathrm{A}} = \rho K_{\mathrm{d}} \frac{\partial c}{\partial t} \tag{4}$$

where ρ is the dry density of the soil. The relationship of equation (4) is applicable to sorption processes in which the contaminant concentrations are low.[18,19] The ratio at which contaminant is lost due to both biodegradation and radioactive decay is usually proportional to the concentration, thus

$$g_{\mathrm{D}} + g_{\mathrm{B}} = n\gamma c \tag{5}$$

where γ is the sum of the radioactive decay constant γ_{D} and the biodegradation constant γ_{B}, viz.

$$\gamma = \gamma_{\mathrm{D}} + \gamma_{\mathrm{B}}$$

Using the Fickian-type relationship between mass flux and concentration in equation (2) and combining with equations (1) and (3)–(5), it then follows that under isothermal conditions and assuming a steady advective flow field is occurring in a homogeneous saturated porous media, the equation of contaminant transport is given by

$$n(\mathbf{D}\mathbf{\nabla})\cdot\mathbf{\nabla}c - n\mathbf{V}\cdot\mathbf{\nabla}c = (n + \rho K_{\mathrm{d}})\frac{\partial c}{\partial t} + n\gamma c \tag{6}$$

In developing solutions of contaminant transport, it is sometimes preferred by investigators and also in this paper to define

$$\mathbf{D}_a = n\mathbf{D} \quad \text{the 'effective' tensor of hydrodynamic dispersion} \tag{7}$$

$$\mathbf{V}_a = n\mathbf{V} \quad \text{the Darcy velocity vector} \tag{8}$$

so that the mass flux may be written as

$$\mathbf{f} = \mathbf{V}_a c - \mathbf{D}_a \nabla c \tag{9}$$

and an alternative form to equation (6) may be represented as

$$(\mathbf{D}_a \nabla) \cdot \nabla c - \mathbf{V}_a \cdot \nabla c = (n + \rho K_\mathrm{d}) \left(\frac{\partial c}{\partial t} + \gamma^* c \right) \tag{10}$$

where $\gamma^* = \gamma/(1 + \rho K_\mathrm{d}/n)$.

2.1.1. Laplace transform. The boundary element solution techniques developed in this paper involve the use of a Laplace transform to eliminate the time variable. Thus, assuming that the initial background concentrations is c_0, a Laplace transform,

$$\bar{c} = \int_0^\infty c \mathrm{e}^{-st} \, \mathrm{d}t \tag{11}$$

of equation (10) yields

$$(\mathbf{D}_a \nabla) \cdot \nabla \bar{c} - \mathbf{V}_a \cdot \nabla \bar{c} = (n + \rho K_\mathrm{d})(s + \gamma^*) \left(\bar{c} - \frac{c_0}{s + \gamma^*} \right) \tag{12}$$

The Laplace transform equation of 2D plane contaminant migration for a single contaminant species in an infinite homogeneous saturated porous media, assuming that the principal directions of hydrodynamic dispersion are parallel to the x–z co-ordinate axes, reduces from equation (12) to the following form;

$$D_{axx} \frac{\partial^2 \bar{c}}{\partial x^2} + D_{azz} \frac{\partial^2 \bar{c}}{\partial z^2} - V_{ax} \frac{\partial \bar{c}}{\partial x} - V_{az} \frac{\partial \bar{c}}{\partial z} = (n + \rho K_\mathrm{d})(s + \gamma^*) \bar{c} \tag{13}$$

where in the first instance the background concentration in the domain, c_0, is assumed to be identically zero everywhere and D_{axx}, D_{azz} are the 'effective' coefficients of hydrodynamic dispersion in the x and z directions respectively, V_{ax}, V_{az} are the components of Darcy velocity in the x and z directions, respectively.

A more general case where the initial contaminant distribution is not identically zero everywhere will be discussed in a later subsection.

2.1.2. Co-ordinate transformation. Now, if the following co-ordinate transformation is introduced in the x–z plane.[20]

$$x = uX \tag{14}$$

$$z = wZ \tag{15}$$

where

$$u = \left(\frac{D_{axx}}{D_a}\right)^{1/2} \tag{16}$$

$$w = \left(\frac{D_{azz}}{D_a}\right)^{1/2} \tag{17}$$

$$D_a = (D_{axx} D_{azz})^{1/2} \tag{18}$$

It is found that

$$D_a \left(\frac{\partial^2 \bar{c}}{\partial X^2} + \frac{\partial^2 \bar{c}}{\partial Z^2}\right) - V_{aX} \frac{\partial \bar{c}}{\partial X} - V_{aZ} \frac{\partial \bar{c}}{\partial Z} = \Theta \bar{c} \tag{19}$$

where

$$\Theta = (n + \rho K_{\mathrm{d}})(s + \gamma^*) \tag{20}$$

$$V_{aX} = w V_{aX} \tag{21}$$

$$V_{aZ} = u V_{az} \tag{22}$$

The component of the contaminant flux normal to the boundary of the natural x–z space is given by

$$\bar{f}_{\mathrm{n}} = V_{an} \bar{c} - \left(D_{axx} \frac{\partial \bar{c}}{\partial x} l_x + D_{azz} \frac{\partial \bar{c}}{\partial z} l_z\right) \tag{23}$$

where l_x and l_z are the direction cosines of the normal to the natural boundary and V_{an} is the component of groundwater flow in the direction of the normal. This equation is transformed into

$$\bar{f}_N = V_{aN} \bar{c} - D_a \frac{\partial \bar{c}}{\partial N} \tag{24}$$

where $\bar{f}_N$, V_{aN} are, respectively, the component of the mass flux and groundwater velocity normal to the transformed boundary. It is shown in Leo and Booker[20] that this is related to $\bar{f}_n$ by

$$\bar{f}_N = (w l_x L_X + u l_z L_Z) \bar{f}_n \tag{25}$$

and that

$$V_{aN} = V_{aX} L_X + V_{aZ} L_Z \tag{26}$$

where L_X, L_Z are the direction cosines of the normal to the transformed boundary. Since the groundwater velocity is constant both spatially and temporally in the domain, the introduction of the second transform,

$$\bar{c} = \bar{c}^* \mathrm{e}^{(\varpi X + \lambda Z)} \tag{27}$$

where

$$\varpi = \frac{V_{aX}}{2D_a} \tag{28}$$

$$\lambda = \frac{V_{aZ}}{2D_a} \tag{29}$$

leads to a mathematically convenient transformed form of the contaminant transport equation in the X–Z space, viz. the Helmholtz equation

$$D_a \nabla^2 \bar{c}^* = S \bar{c}^* \tag{30}$$

where

$$S = \Theta + D_a(\varpi^2 + \lambda^2) \tag{31}$$

with

$$\bar{f}_N = \bar{f}_N^* \mathrm{e}^{(\varpi X + \lambda Z)} \tag{32}$$

$$\bar{f}_N^* = \frac{V_{aN}}{2} \bar{c}^* - D_a \frac{\partial \bar{c}^*}{\partial N} \tag{33}$$

2.2. Boundary integral equation

Equation (30) may be expressed more simply as

$$\mathbf{L}\bar{c} = 0 \tag{34}$$

where $\mathbf{L}$ is the modified Helmholtz operator which appears in equation (30). Suppose now that $\bar{c}^\sharp$ is a test function which satisfies the following adjoint equation in the presence of a singularity:

$$\mathbf{L}^\sharp \bar{c}^\sharp + \delta(\mathbf{r} - \mathbf{r}_0) = 0 \tag{35}$$

where $\mathbf{L}^\sharp$ is the adjoint differential operator, δ is the Dirac delta function, $\mathbf{r}_0$ is the position vector of the singularity and $\mathbf{r}$ is the position vector of the field point.
Since the modified Helmholtz operator is self-adjoint, the operators $\mathbf{L}$ and $\mathbf{L}^\sharp$ are identical. By integrating the inner product of $\bar{c}^\sharp$ and $\mathbf{L}\bar{c}^*$ by parts over the domain Ω, it is found that

$$\int_\Omega \bar{c}^\sharp \mathbf{L} \bar{c}^* \, \mathrm{d}\Omega = \int_\Gamma D_a \left(\bar{c}^\sharp \frac{\partial \bar{c}^*}{\partial N} - \bar{c}^* \frac{\partial \bar{c}^\sharp}{\partial N} \right) \mathrm{d}\Gamma + \int_\Omega \bar{c}^* \mathbf{L}^\sharp \bar{c}^\sharp \, \mathrm{d}\Omega \tag{36}$$

where $\partial \bar{c}^*/\partial N$, $\partial \bar{c}^\sharp/\partial N$ are the derivatives of $\bar{c}^*$ and $\bar{c}^\sharp$ respectively along the boundary normal. Combining equations (34)–(36) leads to

$$\int_\Omega \bar{c}^* \delta(\mathbf{r} - \mathbf{r}_0) \, \mathrm{d}\Omega = \int_\Gamma D_a \left(\bar{c}^\sharp \frac{\partial \bar{c}^*}{\partial N} - \bar{c}^* \frac{\partial \bar{c}^\sharp}{\partial N} \right) \mathrm{d}\Gamma \tag{37}$$

It follows from the properties of the Dirac delta function that

$$\varepsilon(\mathbf{r}_0) \bar{c}^*(\mathbf{r}_0) = \int_\Gamma D_a \left(\bar{c}^\sharp \frac{\partial \bar{c}^*}{\partial N} - \bar{c}^* \frac{\partial \bar{c}^\sharp}{\partial N} \right) \mathrm{d}\Gamma \tag{38}$$

where $\varepsilon(\mathbf{r}_0)$ is found to be

$$\varepsilon(\mathbf{r}_0) = \begin{cases} 1 & \text{if } r_0 \text{ is within domain } \Omega \\ 0 & \text{if } \mathbf{r}_0 \text{ is outside domain } \Omega \\ \frac{1}{2} & \text{if } \mathbf{r}_0 \text{ lies on a smooth boundary or} \\ & \text{the subtended angle } 2\pi \text{ if the boundary is not smooth} \end{cases} \tag{39}$$

The solution of the adjoint equation (35) is variously known as the fundamental solution, principal solution, elementary solution or free-space Green's function. Hence for the modified Helmholtz operator of equation (30), the solution of the adjoint equation (35) yields the fundamental solution in two spatial dimensions as

$$\bar{c}^{\#}(r^{\#}) = \frac{1}{2\pi D_a} K_0(\varrho r^{\#})$$

where $r^{\#} = |\mathbf{r} - \mathbf{r}_0|$ is the distance of the field point from the singularity, K_0 the modified Bessel function of the second kind, zero order, $\varrho = \sqrt{S/D_a}$ denotes the branch with the positive real part.

An alternative and equivalent boundary integral equation to (38) may be obtained by introducing the normal component of the transformed flux which is defined by equation (33) and it is found that

$$c(\mathbf{r}_0)\bar{c}^*(\mathbf{r}_0) = \int_\Gamma (\bar{c}^* \bar{f}_N^{\#} - \bar{c}^{\#} \bar{f}_N^*)\, \mathrm{d}\Gamma \tag{40}$$

where

$$\bar{f}_N^{\#} = \frac{V_{aN}}{2}\bar{c}^{\#} - D_a \frac{\partial \bar{c}^{\#}}{\partial N}$$

3. BOUNDARY ELEMENT APPROXIMATION

In the boundary element method, it is aimed to reduce equation (40) into a set of simultaneous algebraic equations by discretizing the boundary of the domain into a discrete number of elements $1, \ldots, N_e$. It will be necessary to adopt some approximating interpolation functions for the dependent variable $\bar{c}^*$ or $\bar{f}_N^*$ on the boundary surface. The boundary to the domain may also be approximated by elements in the form of straight line segments, quadratic, cubic polynomial curves (for 2D) or triangles, quadrilaterals (for 3D) and so forth. In the simplest case for a two-dimensional space problem, it is usually assumed that the boundary is approximated by straight line elements while the dependent variable remains a piecewise constant value over the length of the element. Thus in this case the position vector $\mathbf{r}_j$ on the jth element of the boundary may be defined in terms of nodal position vectors $\mathbf{r}_j^1, \mathbf{r}_j^2$ as follows (see Figure 1),

$$\begin{aligned} \mathbf{r}_j(\zeta) &= \tilde{N}^1(\zeta)\mathbf{r}_j^1(\zeta) + \tilde{N}^2(\zeta)\mathbf{r}_j^2(\zeta) \\ \tilde{N}^1(\zeta) &= \tfrac{1}{2}(1-\zeta) \\ \tilde{N}^2(\zeta) &= \tfrac{1}{2}(1+\zeta) \end{aligned} \tag{41}$$

where $\tilde{N}^1$ and $\tilde{N}^2$ are the shape functions for the straight line elements and the variable ζ represents the parametric distance measured from the local origin, usually located at the centre of the element. As the point moves from one end of the element to the other, its value ranges from -1 to 1. Since the continuous functions of $\bar{c}^*$ and $\bar{f}_N^*$ are assumed to be piecewise constant values on each of the line element, then an approximation of equation (40) is given by

$$\varepsilon(\mathbf{r}_0)\bar{c}(\mathbf{r}_0) = \sum_{j=1}^{N_e} \left\{ \bar{c}_j^* \int_{-1}^{1} \bar{f}_N^{\#}(\mathbf{r}_j(\zeta) - \mathbf{r}_0)\, \mathrm{d}\Gamma_j - \bar{f}_{N_j}^* \int_{-1}^{1} \bar{c}^{\#}(\mathbf{r}_j(\zeta) - \mathbf{r}_0)\, \mathrm{d}\Gamma_j \right\} \tag{42}$$

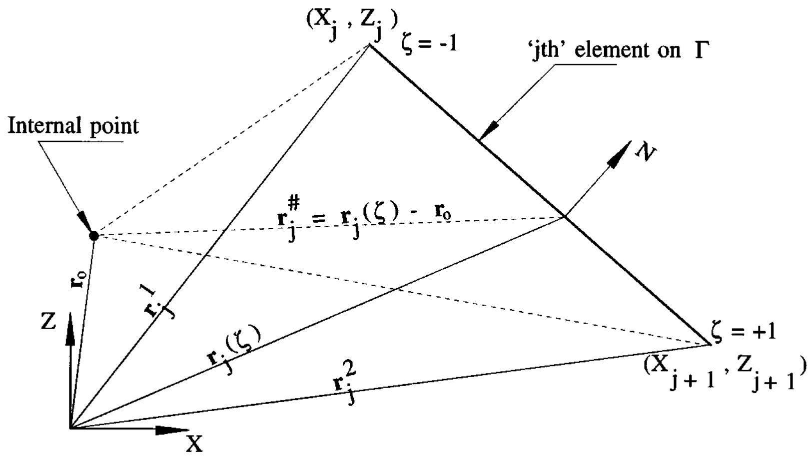

Figure 1. Straight line boundary element

where $d\Gamma_j = J_j d\zeta$ (J_j is the Jacobian of the 'jth' element), $J_j = [(X_{j+1} - X_j)^2 + (Z_{j+1} - Z_j)^2]^{1/2}$, $X_j, Z_j, X_{j+1}, Z_{j+1}$ are the co-ordinates of the end points of the 'jth', element in the X–Z co-ordinate space, and $\bar{c}_j^*, \bar{f}_{N_j}^*$ represent the known and unknown nodal values of the variables, at the centre of the boundary element j.

There is a conceptual advantage to now imagine that the singularity is 'applied' successively at each of the 'i' nodes, $\mathbf{r}_{0i}$, $i = 1, \ldots, N_e$, located at the centre of each boundary element, then the resulting system of simultaneous equations will develop into the matrix equation

$$\mathbf{H}^* \bar{\mathbf{c}}^* = \mathbf{G}^* \bar{\mathbf{f}}_N^* \tag{43}$$

where $\bar{\mathbf{c}}^*$, $\bar{\mathbf{f}}_N^*$ are the vectors of $\bar{c}_j^*$ and $\bar{f}_{N_j}^*$, $\mathbf{H}^*$, $\mathbf{G}^*$ are $N_e \times N_e$ influence matrices in which the general influence coefficients h_{ij}^* and g_{ij}^* for straight line elements are given by

$$h_{ij}^* = -\int_{-1}^{1} \bar{f}_N^{\#}(\mathbf{r}_j(\zeta) - \mathbf{r}_{0i}) J_j \, d\zeta \quad \text{if } i \neq j$$

$$h_{ii}^* = -\int_{-1}^{1} \bar{f}_N^{\#}(\mathbf{r}_i(\zeta) - \mathbf{r}_{0i}) J_i \, d\zeta + \frac{1}{2} \quad \text{if } i = j$$

$$g_{ij}^* = -\int_{-1}^{1} \bar{c}^{\#}(\mathbf{r}_j(\zeta) - \mathbf{r}_{0i}) J_j \, d\zeta \tag{44}$$

In contaminant transport problems, the boundary conditions which occur are usually that either the values of the contaminant concentration or the contaminant mass flux normal to the boundary are specified. These values are generally known in the original x–z space but in order to utilize them in equation (43), it is necessary to transform these values in an appropriate way. The values of the concentration are relatively straightforward to deal with since the transformed values can be found immediate by applying equation (27), viz.,

$$\bar{c}^* = \bar{c} e^{-(\varpi X + \lambda Z)} \tag{45}$$

so that if $\bar{c}$ is known on the natural boundary then $\bar{c}^*$ is also known. The relationship for the normal mass flux follows from equations (25) and (32), viz.

$$\bar{f}_N^* = (wl_x L_X + ul_z L_Z)\bar{f}_n \mathrm{e}^{-(\varpi X + \lambda Z)} \tag{46}$$

and so if the mass flux on the natural boundary, $\bar{f}_n$, is known then, $\bar{f}_N^*$, will also be known on the transformed boundary.

A problem is well opposed if either $\bar{c}^*$ or $\bar{f}_N^*$ (or a linear combination of both) is known at each node on the boundary. Thus there are only N_e unknown nodal values of either $\bar{c}^*$ or $\bar{f}_N^*$ which can be found by solving equation (43). Once the nodal values on the boundary are completely known, equation (40) can be used to evaluate $\bar{c}^*$ at any internal point in the domain. The value of $\bar{c}$ is found using the relationship in equation (40) and finally the concentration in the time domain is obtained using the Laplace inversion algorithm of Talbot.[21]

The value of the fundamental solution $\bar{c}^{\#}$ will depend on the relative positions of the point of singularity and the field point. As the field point approaches the singularity point of the fundamental solution, some care needs to be taken in evaluating the boundary integral. The overall accuracy of the numerical technique is contingent upon how accurately the various boundary integrals could be evaluated, particularly those involving singular or near singular fundamental solutions. Singular integrals occur when the field point coincides with the singularity point. Nearly singular integrals may also occur for the thin-body problem, for the case where the mesh contains a large element and a small element adjacent to each other, or for the case where the concentration is taken at a domain point which is very close to the boundary.[22] An efficient and accurate integration technique developed by Smith[5] is used in this paper.

3.1. Non-zero initial background concentration

Suppose, however, that the initial contaminant distribution is not zero, then the governing equation is

$$D_{axx}\frac{\partial^2 \bar{c}}{\partial x^2} + D_{azz}\frac{\partial^2 \bar{c}}{\partial z^2} - V_{ax}\frac{\partial \bar{c}}{\partial x} - V_{az}\frac{\partial \bar{c}}{\partial z} = \Theta\left(\bar{c} - \frac{c_0}{\mathbf{\Lambda}}\right) \tag{47}$$

where

$$\mathbf{\Lambda} = s + \gamma^* \tag{48}$$

and thus the presence of the initial concentration could lead to the necessity of evaluating a domain integral. One way of avoiding this undesirable integral is to find a particular solution of equation (47). Let such a particular solution be

$$\bar{c}_p = \sigma \tag{49}$$

Thus, if $\Delta\bar{c} = \bar{c} - \sigma$ is the value of concentration above σ then it satisfies the equation

$$D_{axx}\frac{\partial^2 \Delta\bar{c}}{\partial x^2} + D_{azz}\frac{\partial^2 \Delta\bar{c}}{\partial z^2} - V_{ax}\frac{\partial \Delta\bar{c}}{\partial x} - V_{az}\frac{\partial \Delta\bar{c}}{\partial z} = \Theta\Delta\bar{c} \tag{50}$$

and the corresponding initial distribution of the normal mass flux, $\bar{f}_{n\sigma}$, arising from the particular solution σ is

$$\bar{f}_{n\sigma} = V_{an}\sigma - \left(D_{axx} \frac{\partial \sigma}{\partial x} l_x + D_{azz} \frac{\partial \sigma}{\partial z} l_z \right) \tag{51}$$

so that the normal component of the mass flux above the initial distribution $\bar{f}_{n\sigma}$ is given by

$$\Delta \bar{f}_n = \bar{f}_n - \bar{f}_{n\sigma} \tag{52}$$

Equation (50), $\Delta \bar{c}$ and $\Delta \bar{f}_n$ transform in the same way as before into

$$D_a \nabla^2 \Delta \bar{c}^* = S \Delta \bar{c}^* \tag{53}$$

$$\Delta \bar{c}^* = \Delta \bar{c} \mathrm{e}^{-(\varpi X + \lambda Z)} \tag{54}$$

$$\Delta \bar{f}_N^* = (w l_x L_X + u l_z L_Z) \Delta \bar{f}_n \mathrm{e}^{-(\varpi X + \lambda Z)} \tag{55}$$

Once again it is possible to develop the boundary integral equation using equation (53) and the corresponding system of algebraic equations is

$$\mathbf{H}^* \Delta \bar{c}^* = \mathbf{G}^* \Delta \bar{\mathbf{f}}_N^* \tag{56}$$

where $\Delta \bar{c}^*$ and $\Delta \bar{\mathbf{f}}_N^*$ are the vectors of the nodal values of $\Delta \bar{c}^*$ and $\Delta \bar{f}_N^*$, respectively. The solutions may thus be obtained by proceeding formally in the same way as before. In the simplest case, when the background concentration, $\bar{c}_0$, is uniform then

$$\sigma = \frac{c_0}{\mathbf{\Lambda}} \tag{57}$$

is clearly a particular solution of the governing equation (47) and so for this case,

$$\Delta \bar{c}^* = \left(\bar{c} - \frac{c_0}{\mathbf{\Lambda}} \right) \mathrm{e}^{-(\varpi X + \lambda Z)} \tag{58}$$

$$\Delta \bar{f}_N^* = (w l_x L_x + u l_z L_z) \left(f_n - V_{an} \frac{c_0}{\mathbf{\Lambda}} \right) \mathrm{e}^{-(\varpi X + \lambda Z)} \tag{59}$$

3.2. Specification of boundary conditions for a waste repository

The presence of a waste repository in the porous media may be simulated by prescribing appropriate boundary conditions at the soil–repository interface. This is a matter which requires careful consideration. One possibility is to assume that the concentration in the repository remains constant spatially and temporally. This is however not very realistic since the mass of contaminant in a repository is finite and the concentration will diminish with time as the contaminant mass is transported outwards into the surrounding soil. A more realistic option is to use a lumped-parameter model, this has been applied successfully in other areas of water research (see e.g. Reference 23). In such a model, the concentration in the repository is assumed to be spatially constant but diminishing with time as the contaminant migrates into the surrounding soil. It may also be assumed that the contaminant undergoes radioactive decay and biodegradation, and adsorption but it is not sorbed. Thus, for a repository with spatially constant concentration, it follows from equation (5) that the repository mass change due to decay and biodegradation at time t is given by

$$m_\gamma = n_R U_R \int_0^t \gamma_R c_R \, d\tau \tag{60}$$

where n_R is the porosity of the repository, U_R is the true volume of the repository, γ_R is the sum of the biodegradation and decay constants in the repository and c_R is the repository concentration and mass change due to adsorption is

$$m_A = \rho_R K_{dR}(c_R - c_{Ro}) U_R \tag{61}$$

where ρ_R is dry density of the material in the repository, K_{dR} is the distribution coefficient in the repository, and c_{Ro} is the initial uniform background repository concentration.

From consideration of the principle of conservation of mass in the natural untransformed domain, the total mass change in the repository is the sum of mass loss due to decay, biodegradation, adsorption and outward mass flux into the porous media, thus it follows that

$$n_R U_R (c_R - c_{Ro}) = -U_R \rho_R K_{dR}(c_R - c_{Ro}) - n_R U_R \int_0^t \gamma c_R \, d\tau - \int_0^t \int_{\Gamma_R} f_n \, d\Gamma \, d\tau \tag{62}$$

where Γ_R is the repository boundary in the natural x–z space and f_n is the outward mass flux normal to the surface of the repository.

Taking the Laplace transform of equation (62) yields

$$n_R U_R \left(c_R - \frac{c_{R0}}{s} \right) = -U_R \rho_R K_{dR} \left(c_R - \frac{c_{R0}}{s} \right) - \frac{1}{s} n_R U_R \gamma \bar{c}_R - \frac{1}{s} \int_{\Gamma_R} \bar{f}_n \, d\Gamma \tag{63}$$

This leads to

$$(n_R + \rho_R K_{dR}) U_R \bar{c}_R = (n_R + \rho_R K_{dR}) U_R \frac{c_{Ro}}{s + \gamma_R^*} - \frac{1}{s + \gamma_R^*} \int_{\Gamma_R} \bar{f}_n \, d\Gamma \tag{64}$$

where

$$\gamma_R^* = \frac{\gamma_R}{1 + \rho_R K_{dR}/n_R} \tag{65}$$

Equation (64) will be applied in this paper at the boundary of the soil–waste repository interface to simulate the presence of the repository.

4. APPLICATION

4.1. Verification

In the test problem, a cylindrical contaminant source of 1 m radius is buried deeply in the porous medium (Figure 2(a)). The cases of infinite and finite contaminant mass in the cylinder are both considered. Initially ($t = 0$), it is assumed that the concentration of the contaminant in the cylinder has a spatially uniform concentration of 1000 mg/l and the concentration outside

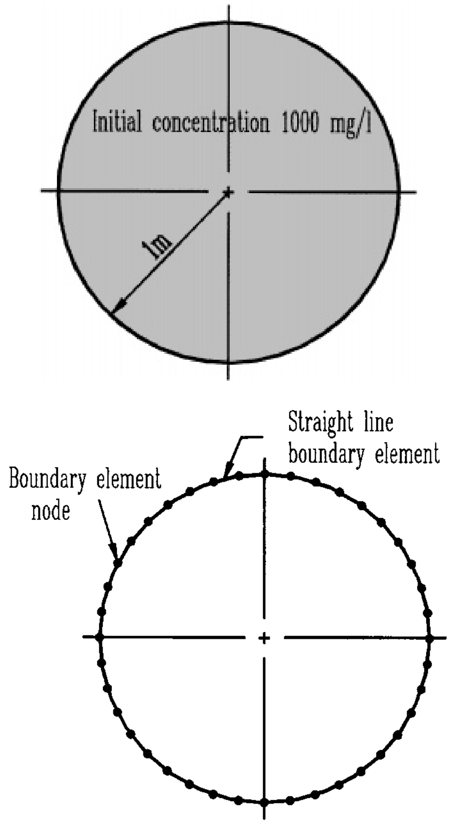

Figure 2. (a) Deeply buried cylindrical source; (b) Boundary element representation of deeply buried cylindrical source

Table I. Soil properties in Test Problem

n	ρK_d	D_{axx} (m^2/a)	D_{azz} (m^2/a)	V_{az} (m/a)	γ	(c^0 (mg/l)
0·4	0	0·002	0·002	0·002	0	0

the cylinder is uniformly zero. A general groundwater Darcy velocity of 0·002 m^2/a flows in the z-direction. Other relevant contaminant and soil properties are given in Table I. Semi-analytic solutions for this problem are given by Rahman and Booker.[25]

For the boundary element analysis, a total of 40 straight line constant-valued elements have been used to approximate the source as shown schematically in Figure 2(b). The interface between the source and porous medium is considered as an external boundary for which the boundary technique developed in Section 3.2 for a source with either a finite or infinite amount of contaminant mass is applied. At infinity, the contaminant concentration and concentration gradient vanish, thus the infinite boundary can be formally ignored whereas it must be approximated by a boundary far enough from the source in a domain method.

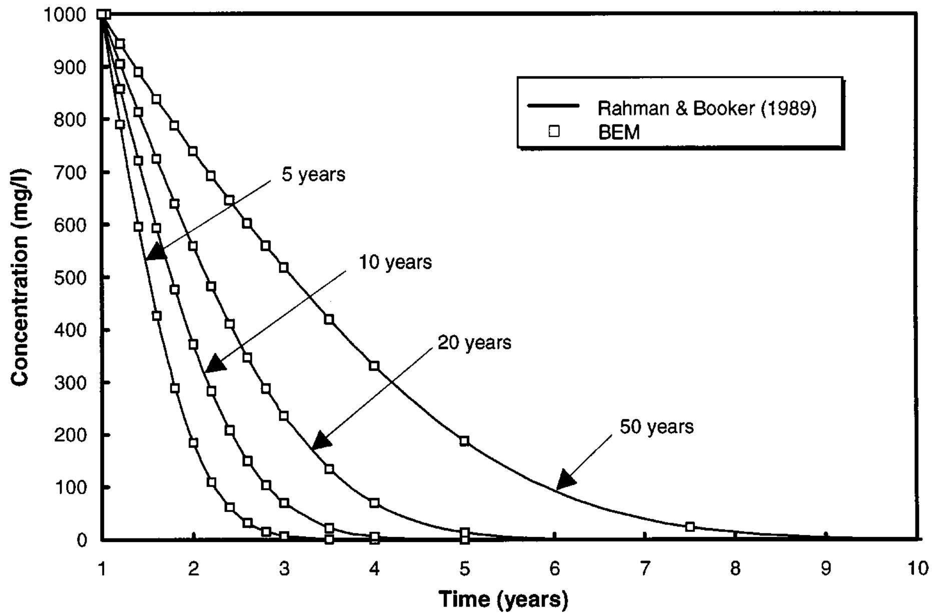

Figure 3. BEM vs. semi-analytic solutions for deeply buried cylindrical source with constant concentration

The concentrations in the radial direction of the advection velocity for various times are shown in Figure 3 (infinite contaminant mass in source) and Figure 4 (finite contaminant mass in source). The results show that there is excellent agreement between the boundary element solutions and the semi-analytic solutions.

4.2. Simulation of contaminant transport from waste repository

The solutions of the BEM are further illustrated in the following examples where concentration contours in the porous media due to the presence of a source are determined. Concentration may be evaluated at selected internal points within the domain at specified times of interest. The spacings between, and number of, selected observation points are entirely up to the discretion of the analyst hence there is considerable flexibility in applying the technique. When a high concentration gradient is found or is anticipated, a great number of points may be used to capture the rapid change in concentration. Conversely, the points need only be used sparsely at the locations where little change in concentration is expected to save on processing time. In the following analysis, concentration contours have been found for a hypothetical $20\ \text{m} \times 5\ \text{m}$ rectangular repository at 500, 1000 and 2000 years. The two different situations which have been examined are:

Simulation case 1 (Figure 5). A repository with initial concentration 1000 mg/l is buried at 2 m in a homogeneous half-space with z-direction advection and zero concentration boundary condition at the ground surface. The initial background concentration in the porous media is zero.

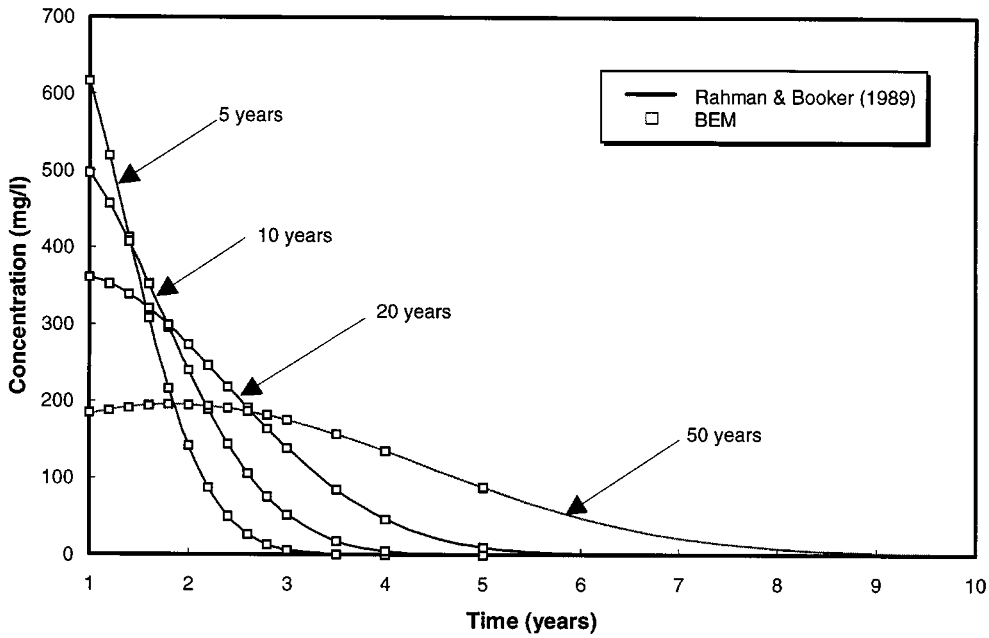

Figure 4. BEM vs semi-analytic solutions for deeply buried cylindrical source with diminishing concentration

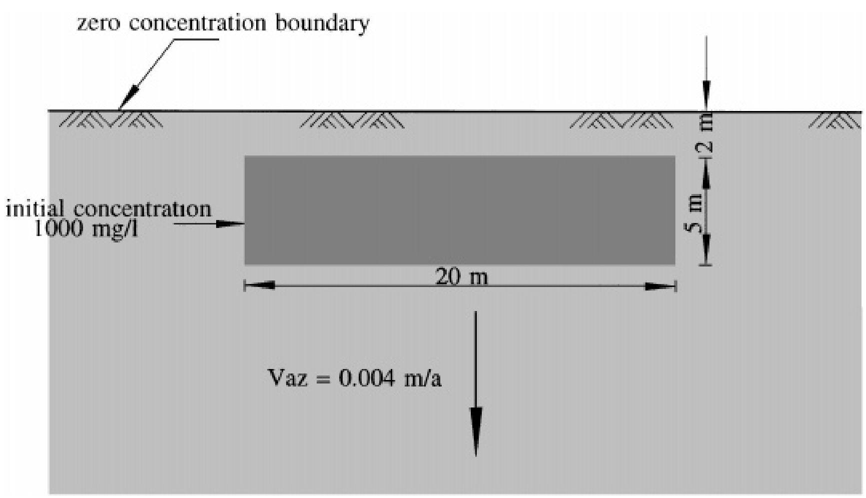

Figure 5. Schematic of simulation case 1

Simulation case 2 (Figure 6). A repository embedded in an 8 m clay layer with x-direction advection, zero flux boundary condition at the ground surface and at the 8 m interface (i.e. the underlying layer is assumed to be much more impermeable). The background concentration is 100 mg/l.

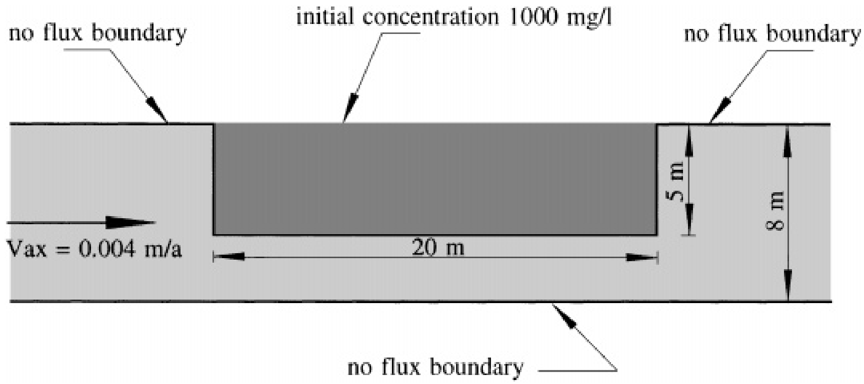

Figure 6. Schematic of simulation case 2

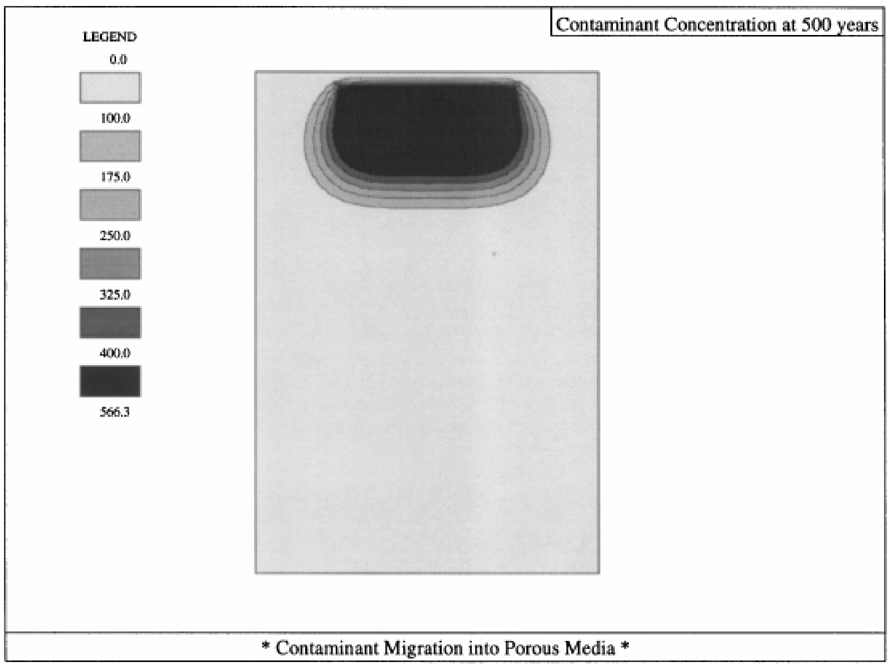

Figure 7. Simulation case 1: contaminant distribution at 500 years, advection in z direction

The contaminant is assumed to be conservative, the dispersion coefficients are $D_{axx} = D_{azz} = 0{\cdot}004\ \mathrm{m}^2/\mathrm{a}$, and the porosity of the porous medium is 0·4. The simulation results for this case are presented in Figures 7–9.

In case 2, the average groundwater velocity of magnitude 0·01 m/a is flowing in the x direction, $D_{axx} = 0{\cdot}004\ \mathrm{m}^2/\mathrm{a}$, $D_{azz} = 0{\cdot}0008\ \mathrm{m}^2/\mathrm{a}$, $n = 0{\cdot}4$, $\rho K_\mathrm{d} = 0$, $\gamma = 0$. In this problem, the coefficients of dispersion have been assumed to be anisotropic. The concentration contours are shown in Figures 10–12.

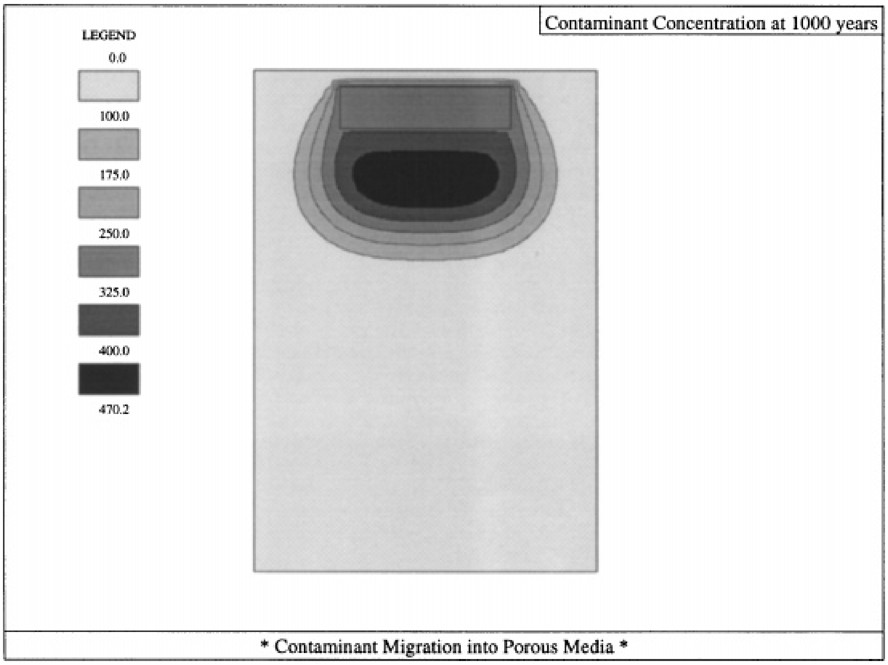

Figure 8. Simulation case 1: contaminant distribution at 1000 years, advection in z direction

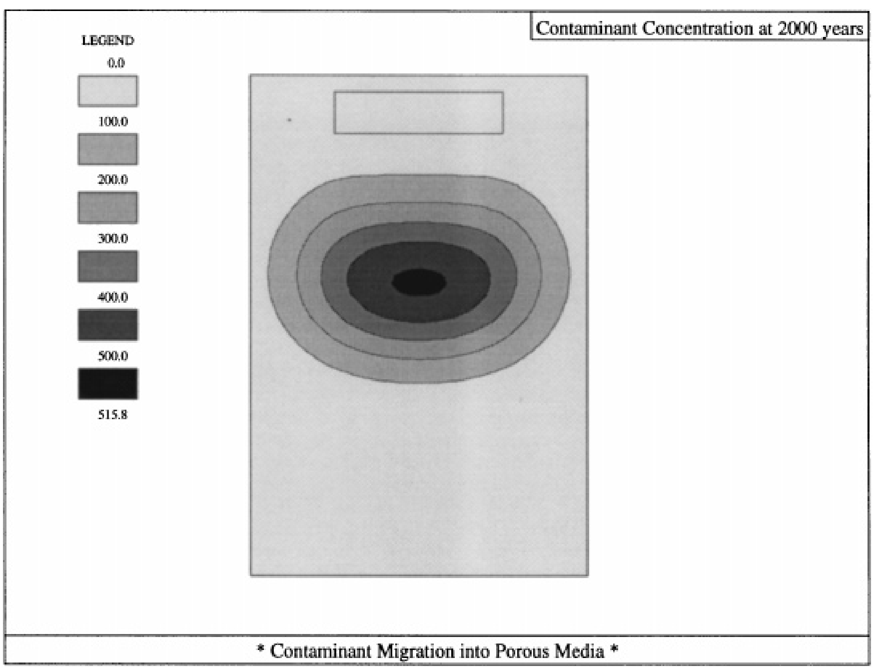

Figure 9. Simulation case 1: contaminant distribution at 2000 years, advection in z direction

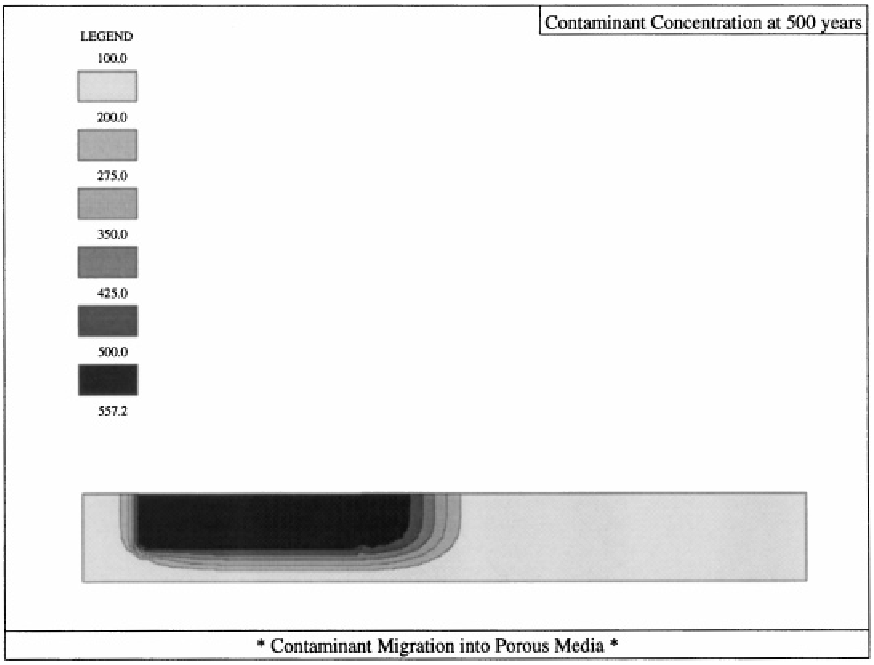

Figure 10. Simulation case 2: contaminant distribution at 500 years, advection in x direction

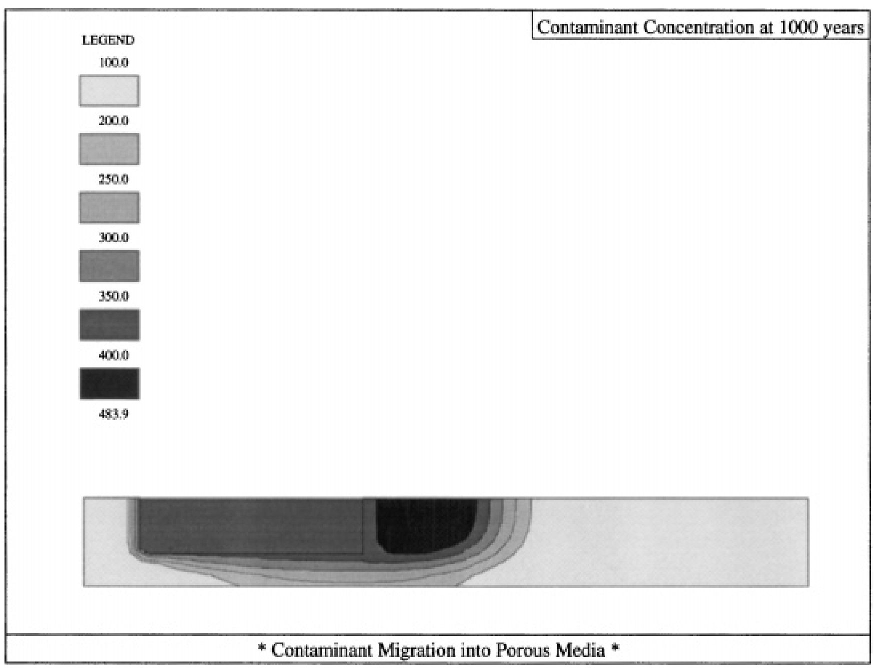

Figure 11. Simulation case 2: contaminant distribution at 1000 years, advection in x direction

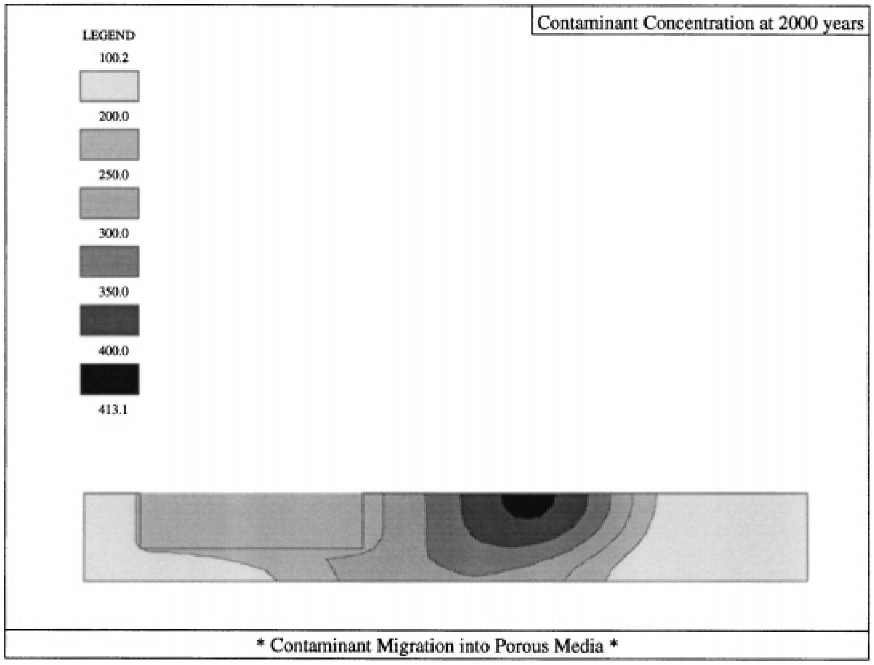

Figure 12. Simulation case 2: contaminant distribution at 5000 years, advection in x direction

Finally, it may be noted that in the above examples since no time discretization is used in the method, the solutions for large times can just as easily be obtained with the same computational effort as for smaller times of interest.

5. CONCLUSIONS

The boundary element method presented in this paper is found to be an efficient and accurate method for solving the advection–dispersion equation governing contaminant transport especially where problems of infinite or semi-infinite space are involved. One of the main advantages of using the BEM is of course its ability to potentially deal with such problems with ease since the fundamental solutions satisfy the boundary conditions at infinity naturally. This advantage can be maintained in this method as it is possible to avoid dealing with an undesirable domain integral. Essentially therefore, this method treats a problem as if its dimension is reduced by one. Illustrative examples have been used to demonstrate how the method can be applied to evaluate concentration contours of contaminant at specified times of interest.

REFERENCES

1. A. Taigbenu and J. A. Liggett, 'An integral solution for the diffusion-advection equation', *Water Resour. Res.*, **22,** 1237–1246 (1986).
2. R. M. Khanbilvardi, S. Ahmed and A. M. Sadegh, 'Boundary integral solutions to the unsaturated moisture flow equations', *Water Resour. Res.* **29**(5)**,** 1425–1434 (1993).

3. M. S. Rahman, J. R. Booker and C. W. Hwang, 'A boundary integral formulation for modelling pollutant migration in groundwater', *Proc. Int. Conf. 'Solving Groundwater Problems with Models*', Indianapolis, 1989.
4. T. A. Cruse and F. J. Rizzo, 'A direct formulation and numerical solution in the general transient elasto-dynamic problems I', *J. Math. Analyt. Appl.*, **22,** 244–259 (1968)
5. D. W. Smith, 'Boundary element analysis of heat flow and consolidation for geotechnical applications', *Ph.D. Thesis*, University of Sydney, 1990.
6. D. W. Smith and J. R. Booker, 'Boundary element analysis of time dependent thermoelasticity', *Proc. Conf. on Finite Element Methods in Engineering*, Melbourne, 1987, pp. 346–350.
7. D. W. Smith and J. R. Booker, 'Boundary element analysis of linear quasi-static coupled transient thermoelasticity', *Proc. 6th Int. Conf. on Numerical Methods in Geomechanics*, Innsbruck, 1988, pp. 1017–1022.
8. D. W. Smith and J. R. Booker, 'Boundary integral analysis of transient thermoelasticity', *Int. J. Numer. Analyt. Meth. Geomech.*, **13,** 283–302 (1989).
9. D. W. Smith and J. R. Booker, 'Applications of boundary integral analysis involving thermoporoelastic materials', *Proc. 2nd Asia Pacific Conf. on Computational Methods*, Sydney, 1983, pp. 627–633.
10. J. Bear, *Hydraulics of Groundwater*, McGraw-Hill, New York, 1979.
11. A. R. Freeze and J. A. Chery, *Groundwater*, Prentice-Hall, Englewood Cliffs, NJ.
12. R. K. Rowe, R. M. Quigley and J. R. Booker, 'Clayey barrier systems for waste disposal facilities', *E & FN Spon*, 1995.
13. C. C. Travis and E. L. Etnier, A survey of sorption relationships for reactive solutes in soils, *J. Environ. Qual.*, **10,** 8–17 (1981).
14. W. J. Weber, Jr., P. M. McGinley and L. E. Katz 'The nature and effects of sorption processes in subsurface systems', in J. Bear and M.Y. Corapcioglu, (eds), *Transport Processes in Porous Media*, Kluwer Academic Publishers, Dordrecht, 1991.
15. R. K. Rowe and J. R. Booker 'The analysis of pollutant migration in a non-homogeneous soil', *Geotechnique*, **34**(4)**,** 601–612 (1984).
16. R. K. Rowe and J. R. Booker, 'Two-dimensional pollutant migration in soils of finite depth', *Canadian Geotechn. J.*, **22,** 429–436 (1985).
17. R. K. Rowe and J. R. Booker, 'A Finite layer technique for solving general 3-D pollutant migration problems', *Geotechnique*, **36,** 205–214 (1986).
18. C. C. Travis, Mathematical description of adsorption and transport of reactive solutes in soil: a review of selected literature, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1978.
19. L. Luckner and W. M. Schestakow, *Migration Processes in the Soil and Groundwater Zone*, Lewis Publishers, 1991.
20. C. J. Leo and J. R. Booker, 'A note on co-ordinate transform and fundamental solutions of the equations of contaminant migration in porous media', *Working Paper*, University of Sydney, 1997.
21. A. Talbott, 'The accurate numerical integration of Laplace transforms', *J. Inst. Math. Appl.*, **23,** 97–120 (1979).
22. Q. Huang and T. A. Cruse, 'Some notes on singular integral techniques in boundary element analysis', *Int. J. Numer. Meth. Engng.*, **36,** 2643–2659 (1993).
23. L. W. Gelhar and J. L. Wilson, 'Ground-water quality modelling', *Groundwater*, **3,** 7–17 (1974).
24. S. Sharp and S. L. Crouch, 'Boundary integral methods for themoelastic problems', *J. Appl. Mech.*, **53,** 298–302 (1986).
25. M. S. Rahman and J. R. Booker, 'Pollutant migration from deeply buried repositories', *Int. J. Numer. Anal. Meth. Geomech.*, **13,** 37–51 (1989).

