A boundary element method solution to spatially variable coefficients diffusion convection equation of anisotropic media

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Abstract. The diffusion-convection equation with variable coefficients and for anisotropic media which were previously considered by other authors are discussed again in this paper to find their numerical solutions by using the boundary element method (BEM). The numerical results obtained show the consistency and accuracy of the BEM solutions. Also, the solutions exhibit the impact of the anisotropy and inhomogeneity (spatial variability) of the media.

1. Introduction

The diffusion-convection equation with variable coefficients of the form

\[
\frac{\partial}{\partial x_i} \left[ d_{ij}(x) \frac{\partial c(x)}{\partial x_j} \right] - \frac{\partial}{\partial x_i} \left[ v_i(x) c(x) \right] = 0
\]

will be considered. Equation (1) is used to model physical phenomena involving anisotropic diffusion and convection processes in inhomogeneous media where both the diffusion coefficient and the velocity vary spatially and continuously. Among the physical phenomena of applications include pollutant transport and heat transfer.

In the context of pollutant transport problems, equation (1) is usually used as the dimensionless governing equation in which \(d_{ij} = D_{ij}/\hat{D}, c = C/\hat{C}, x_i = X_i/l, v_i = \left( l/\hat{D} \right) V_i, D_{ij}\) is the components of dispersion/diffusion coefficients \(L^2T^{-1}\), \(C\) is dissolved concentration of the pollutant \(ML^{-3}\), \(X_i\) is the component of the point coordinates \(X\) \((L)\), \(V_i\) is the component of the seepage velocity \(LT^{-1}\), \(\hat{D}\) is a reference dispersion coefficient, \(\hat{C}\) is a reference concentration of pollutant and \(l\) is a reference length (see for example Meenal and Eldho [5]).

A number of studies had been done on the initial/boundary value problems governed by diffusion-convection equation to find either analytical or numerical solutions. The previous studies can be classified, according to the anisotropy and inhomogeneity of the considered media, into those on isotropic and homogeneous, anisotropic homogeneous and isotropic inhomogeneous media. The anisotropy and inhomogeneity of the media are indicated by the coefficients \(d_{ij}\) and \(v_i\) involved in the governing diffusion-convection equation. Specifically, the medium is
inhomogeneous if the coefficients are spatially variable. And it is anisotropic when the diffusion in one geometrical direction is different to the diffusion in another direction.

Wu et al in 2012 [6], Hernandez-Martinez et al in 2013 [7], Wang et al in 2017 [8] and Fendo˘ glu et al in 2018 [9] had been working on the isotropic diffusion and homogeneous media. Yoshida and Nagaoka in [4], Meenal and Eldho in [5], Haddade et al in [10], Azis et al in [11, 12] and Azis [13] (with Helmholtz type governing equation) considered the case of anisotropic diffusion and homogeneous media. Whereas for the case of isotropic diffusion and variable coefficients (inhomogeneous media), studies had been done by Rap et al in 2004 [14], Ravnik and Škerget in 2013 and 2014 [1, 2], Li et al in 2015 [15] and Pettres and Lacerda in 2017 [3].

Equations (1) provides a wider class of problems since it applies for anisotropic and inhomogeneous media and nonetheless cover the case of isotropic diffusion that happens when \( d_{11} = d_{22}, d_{12} = 0 \) and also for homogeneous media occurring when the coefficients \( d_{ij} \) and \( v_i \) are constant. Apparently, there exists very few studies on problems governed by diffusion-convection equation (1) for the cases of simultaneous anisotropic diffusion and spatially variable coefficients. Zoppou and Knight [16] had been working on finding the analytical solution to the unsteady orthotropic diffusion-convection equation with spatially variable coefficients. The equation considered is almost similar to equation (1) but with limitation \( d_{12} = 0 \). Recent works considering the case of anisotropic diffusion and spatially variable coefficients were reported in [17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29] for different class of governing equations.

Referred to the Cartesian frame \( Ox_1x_2 \) we will consider boundary value problems governed by (1) where \( x = (x_1, x_2) \). The coefficient \( [d_{ij}] \) \((i,j = 1, 2)\) is a real positive definite symmetrical matrix. Also, in (1) the summation convention for repeated indices holds.

Given the coefficients \( d_{ij}(x) \) and \( v_i(x) \), a solution \( c \) to (1) is sought which is valid in a region \( \Omega \) in \( R^2 \) with boundary \( \partial \Omega \) which consists of a finite number of piecewise smooth curves. On \( \partial \Omega_1 \) the dependent variable \( c(x) \) is specified, and

\[
P = d_{ij}(\partial c/\partial x_i)n_j = l/(\hat{D}\hat{C})D_{ij}(\partial C/\partial X_i)n_j
\]

(2)
is specified on \( \partial \Omega_2 \) where \( \partial \Omega = \partial \Omega_1 \cup \partial \Omega_2 \) and \( n = (n_1, n_2) \) denotes the outward pointing normal to \( \partial \Omega \). The method of solution will be to obtain a boundary integral equation from which a BEM can be formulated by which then numerical values of the dependent variable \( c \) and its derivatives may be obtained for all points in \( \Omega \).

2. The boundary integral equation

The boundary integral equation is derived by transforming the variable coefficient equation (1) to a constant coefficient equation. We restrict the coefficients \( d_{ij} \) and \( v_i \) to be of the form

\[
d_{ij}(x) = \hat{d}_{ij}h(x)
\]
\[
v_i(x) = \hat{v}_ih(x)
\]

(3)

(4)

where \( h(x) \) is a differentiable function and \( \hat{d}_{ij} \) and \( \hat{v}_i \) are constant. Substitution of (3) and (4) into (1) gives

\[
\hat{d}_{ij}\frac{\partial}{\partial x_i}\left[h\frac{\partial c}{\partial x_j}\right] - \hat{v}_i\frac{\partial (gc)}{\partial x_i} = 0
\]

(5)

Assume

\[
c(x) = h^{-1/2}(x)\varsigma(x)
\]

(6)

therefore equation (5) can be written as

\[
\hat{d}_{ij}\frac{\partial}{\partial x_i}\left[h\frac{\partial (h^{-1/2}\varsigma)}{\partial x_j}\right] - \hat{v}_i\frac{\partial (h^{1/2}\varsigma)}{\partial x_i} = 0
\]
which can be further written as
\[
\hat{d}_{ij} \left[ \left( \frac{1}{4} h^{-3/2} \frac{\partial h}{\partial x_i} \frac{\partial h}{\partial x_j} - \frac{1}{2} h^{-1/2} \frac{\partial^2 h}{\partial x_i \partial x_j} \right) \hat{\varsigma} + h^{1/2} \frac{\partial^2 \varsigma}{\partial x_i \partial x_j} \right] - \hat{v}_i \frac{\partial (h^{1/2} \hat{\varsigma})}{\partial x_i} = 0 \quad (7)
\]

Use of the identities
\[
\frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} = - \left( \frac{1}{4} h^{-3/2} \frac{\partial h}{\partial x_i} \frac{\partial h}{\partial x_j} - \frac{1}{2} h^{-1/2} \frac{\partial^2 h}{\partial x_i \partial x_j} \right)
\]
\[
\hat{h} \frac{\partial (h^{-1/2} \hat{\varsigma})}{\partial x_i} = h^{1/2} \frac{\partial \varsigma}{\partial x_i} - \hat{\varsigma} \frac{\partial h^{1/2}}{\partial x_i}
\]
allows equation (7) to be written in the form
\[
\hat{h}^{1/2} \left( \hat{d}_{ij} \frac{\partial^2 \varsigma}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \varsigma}{\partial x_i} \right) - \varsigma \left( \hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + \hat{v}_i \frac{\partial h^{1/2}}{\partial x_i} \right) = 0 \quad (8)
\]

So that if \( h \) satisfies
\[
\hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + \hat{v}_i \frac{\partial h^{1/2}}{\partial x_i} = 0 \quad (9)
\]
then the transformation (6) brings the variable coefficients equation (1) into a constant coefficients equation
\[
\hat{d}_{ij} \frac{\partial \varsigma}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \varsigma}{\partial x_i} = 0 \quad (10)
\]
Moreover, substitution of (3) and (6) into (2) gives
\[
P = -P_h \varsigma + P_h^{1/2} \quad (11)
\]
where \( P_h(x) = \hat{d}_{ij} \left( \frac{\partial h^{1/2}}{\partial x_j} \right) n_i \) and \( P_h(x) = \hat{d}_{ij} \left( \frac{\partial \varsigma}{\partial x_j} \right) n_i \).

One possible form of function \( h \) satisfying (9) is \( h(x) = |A \exp (\alpha_m x_m)|^2 \) with \( \hat{d}_{ij} \alpha_i \alpha_j + \hat{v}_i \alpha_i = 0 \) where \( A \) and \( \alpha_m \) are constant. When the material under consideration is a layered material consisting of several layers where each layer is a specific type of material of specific constant coefficients \( d_{ij} \) and \( v_i \) then the discrete variation of the constant coefficients from layer to layer may certainly accommodate the determination of a continuous variation of the variable coefficients \( d_{ij}(x) \) and \( v_i(x) \) by interpolation, that is to determine the parameters \( \alpha_m \) of function \( h(x) \).

By using Gauss divergence theorem equation (10) can be transformed in a boundary integral equation (see for example [30])
\[
\eta(x) \varsigma(x) = \int_{\partial \Omega} \left\{ P_v(x) \Phi(x, \chi) - [P_v(x) \Phi(x, \chi) + \Gamma(x, \chi)] \varsigma(x) \right\} ds(x) \quad (12)
\]
where \( P_v(x) = \hat{v}_i n_i(x) \) and \( \chi = (\chi_1, \chi_2) \), \( \eta = 0 \) if \( (\chi_1, \chi_2) \notin \Omega \cup \partial \Omega \), \( \eta = 1 \) if \( (\chi_1, \chi_2) \) lies inside the domain \( \Omega \), \( \eta = \frac{1}{2} \) if \( (\chi_1, \chi_2) \) is on the boundary \( \partial \Omega \) given that \( \partial \Omega \) has a continuously turning tangent at \( (\chi_1, \chi_2) \). The so called fundamental solution \( \Phi \) (see [30] for its derivation) is
\[
\Phi(x, \chi) = \frac{F}{2\pi} \exp \left( -\frac{\chi \cdot R}{2E} \right) K_0 \left( \frac{\chi \cdot R}{2E} \right) \quad (13)
\]
where $E = [\hat{d}_{11} + 2\hat{d}_{12}\hat{\sigma} + \hat{d}_{22}(\hat{\sigma}^2 + \hat{\sigma}^2)]/2$, $F = \hat{\sigma}/E$, $\hat{R} = \hat{x} - \hat{\chi}$, $\hat{x} = (x_1 + \hat{\sigma}x_2, \hat{\sigma}x_2)$, 
$\hat{\chi} = (\chi_1 + \hat{\sigma}\chi_2, \hat{\sigma}\chi_2)$, $\hat{v} = (\hat{v}_1 + \hat{\sigma}\hat{v}_2, \hat{\sigma}\hat{v}_2)$, $\hat{R} = \sqrt{(x_1 + \hat{\sigma}x_2 - \chi_1 - \hat{\sigma}\chi_2)^2 + (\hat{\sigma}x_2 - \hat{\sigma}\chi_2)^2}$, 
$\hat{v} = \sqrt{(\hat{v}_1 + \hat{\sigma}\hat{v}_2)^2 + (\hat{\sigma}\hat{v}_2)^2}$ where $\hat{\sigma}$ and $\hat{\sigma}$ are respectively the real and the positive imaginary parts of the complex root $\sigma$ of the quadratic equation $\hat{d}_{11} + 2\hat{d}_{12}\sigma + \hat{d}_{22}\sigma^2 = 0$ and $K_0$ is the modified Bessel function. Use of (6) and (11) in (12) yields

$$\eta h^{1/2}c = \int_{\partial\Omega} \left\{ \left( h^{-1/2}\Phi \right) P + \left[ \left( P_h - P \right) \frac{1}{h^{1/2}} \Phi - h^{1/2}\Gamma \right] c \right\} ds$$  

Equation (14) provides a boundary integral equation which is the starting point of BEM construction for determining the numerical solutions of $\phi$ and its derivatives at all points of $\Omega$.

3. Numerical results

In this section we will examine some problems. The aim is to justify the the analysis derived in the previous sections. For the problems, the domain is taken to a unit square as shown in Figure 1). The boundary of the square is divided into a number of elements of equal length on each side. To calculate the solutions, a FORTRAN code is constructed. A specific command for counting the elapsed CPU time is embedded in the code.

![Figure 1. The domain $\Omega$](image)

3.1. Problem 1: Test problem

The aim of test problems is to see the accuracy, convergence and consistency of the BEM solutions. The test problems are also aimed to see the efficiency of the BEM. The constant coefficients are taken to be

$$\hat{d}_{ij} = \begin{bmatrix} 1.5 & 1 \\ 1 & 1 \end{bmatrix} \quad \hat{v}_i = (1, 1.5)$$

and the boundary conditions are (see Figure 1)

- $P$ given on the side AB, BC, CD
- $c$ given on the side AD
The inhomogeneity function \( h(x) \) satisfying equation (9) is

\[
h(x) = [3 \exp (0.2x_1 - 0.1484x_2)]^2
\]

The analytical solution is

\[
c(x) = \frac{1}{3} \exp (0.3x_1 + 0.5346x_2)
\]

Figure 2 shows the errors for solutions \( c(x) \), which indicate that the BEM solutions obtained are quite accurate and convergent to the analytical solutions as the number of elements increases. Whereas, Figure 3 exhibits a consistency between the scattering and the flow. After all this is to say that the FORTRAN script has been working correctly. Moreover, Table 1 shows the CPU time elapsed for obtaining solutions \( c(x) \) and its derivatives at 19×19 interior points. It is observed that the standard BEM works quite efficiently, the elapsed CPU time is no longer than 3.5 minutes time.
Table 1. CPU computation time (in seconds) for Problem 1

| Elements  | 80 elements | 160 elements | 320 elements |
|-----------|-------------|--------------|--------------|
| Time      | 43.00       | 89.421875    | 192.375      |

3.2. Problems without simple analytical solutions

Now, the aim is to see the impacts of the change on the anisotropy and inhomogeneity of the medium, as well as the impact of the change on the velocity coefficient to the solutions. For problems considered in this section, the boundary conditions are

\[ P = 1 \text{ on the side AB} \]
\[ P = 0 \text{ on the side BC, CD} \]
\[ c = 1 \text{ on the side AD} \]

and the boundary is divided into 320 identical elements.

3.2.1. Problem 2

For the following both cases of anisotropy (anisotropic and isotropic) the constant velocity coefficient is assumed to be

\[ \hat{v}_i = (1, 2) \]

*Case of anisotropic medium*  The constant diffusion coefficients are taken to be

\[ \hat{d}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 0.75 \end{bmatrix} \]

the inhomogeneity function \( h \) satisfying equation (9) is assumed to be

\[ h(x) = [\exp (0.15x_1 - 0.0892x_2)]^2 \text{ for inhomogeneous medium} \]
\[ h(x) = 1 \text{ for homogeneous medium} \]

*Case of isotropic medium*  The constant diffusion coefficients are taken to be

\[ \hat{d}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \]

the inhomogeneity function \( h \) is

\[ h(x) = [\exp (0.15x_1 - 0.0903x_2)]^2 \text{ for inhomogeneous medium} \]
\[ h(x) = 1 \text{ for homogeneous medium} \]

Figure 4 shows a comparison of four cases of anisotropy and inhomogeneity of the medium, from which it is observed that the anisotropy and inhomogeneity of the medium give effects on the solutions, as expected.

3.2.2. Problem 3

Now, we will consider again the case of isotropic homogeneous medium, with

\[ \hat{d}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \]
\[ h(x) = 1 \]

but with constant velocity coefficient

\[ \hat{v}_i = (1, 1) \]

It is obvious from Figure 5 that the velocity also effects the solutions. These results are as expected.
Figure 4. Scattering of $c$ for the anisotropic inhomogeneous (top left), anisotropic homogeneous (top right), isotropic inhomogeneous (bottom left) and isotropic homogeneous (bottom right) medium of Problem 2

Figure 5. Scattering of $c$ of the isotropic homogeneous medium for Problem 2 (left) and Problem 3 (right)

4. Conclusion
Problems governed by equation (1) for inhomogeneous media have been solved by using the BEM. The BEM gives accurate and consistent solutions and elapses very efficient computation time. And this justifies the analysis for deriving the boundary integral equation in Section 2 is valid.

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