Numerical simulation for steady anisotropic-diffusion convection problems of compressible flow in exponentially graded media

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Abstract. A boundary element method is utilized to find numerical solutions to boundary value problems of exponentially graded media governed by a spatially varying coefficients anisotropic-diffusion convection equation. The variable coefficients equation is firstly transformed into a constant coefficients equation for which a boundary integral equation can be formulated. A boundary element method (BEM) is then derived from the boundary integral equation. Some problems are considered. The numerical solutions justify the validity of the analysis used to derive the boundary element method with accurate and consistent solutions. A FORTRAN script is developed for the computation of the solutions. The computation shows that the BEM procedure elapses very efficient time in producing the solutions. In addition, results obtained from the considered examples show the effect of anisotropy of the media on the solutions. An example of a layered material is presented as an illustration of the application.

1. Introduction

The diffusion-convection equations with variable coefficient

\[
\frac{\partial}{\partial x_i} \left[ d_{ij}(x) \frac{\partial c(x)}{\partial x_j} \right] - \frac{\partial}{\partial x_i} \left[ v_i(x)c(x) \right] = 0
\] (1)

will be considered. It is assumed that the flow is compressible, so that in (1) it is strictly required that velocity divergence is not zero, that is \( \frac{\partial v_i(x)}{\partial x_i} \neq 0 \). Equation (1) was presented in [1] and [2] as the governing equation. For the case of incompressible flows, zero velocity divergence allows (1) to be written as

\[
\frac{\partial}{\partial x_i} \left[ d_{ij}(x) \frac{\partial c(x)}{\partial x_j} \right] - v_i(x) \frac{\partial c(x)}{\partial x_i} = 0
\] (2)

The equation (2) was considered in [3, 4] as the governing equations.

Equation (1) is usually used for modeling physical phenomena which involve anisotropic-diffusion or conduction and convection processes in functionally graded materials where both the conduction coefficient and the velocity change spatially and continuously. Among the physical phenomena of applications include pollutant transport and heat transfer.
A number of studies had been done on the initial/boundary value problems governed by the diffusion-convection equation to find either analytical or numerical solutions. The previous studies can be classified according to whether the material in question is homogeneous or inhomogeneous and isotropic or anisotropic, into those on isotropic homogeneous, anisotropic homogeneous and isotropic inhomogeneous media. In equation (1) the anisotropy and inhomogeneity of the media are indicated by the coefficients $d_{ij}$ and $v_i$. Specifically, the material is inhomogeneous if the coefficients are spatially variable, whereas it is homogeneous when the coefficients are constant. And it is anisotropic when the diffusion coefficient in one geometrical direction is different to diffusion coefficient in other directions, otherwise when $d_{11} = d_{22}, d_{12} = 0$ it is isotropic.

Papers [5], [6], [7] and [8] focused on the isotropic diffusion and homogeneous media. Papers [2], [9], [10, 11] and [12] (with Helmholtz type governing equation) considered the case of anisotropic diffusion but homogeneous media. Whereas for the case of isotropic diffusion and variable coefficients (inhomogeneous media), studies had been done in [1], [3, 4], [13] and [14].

Equation (1) covers the case of anisotropic and inhomogeneous media as well as isotropic and homogeneous media as special cases. Not so many studies have been done for the case of simultaneously anisotropic and inhomogeneous materials. Paper [15] focused 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 $d_{12} = 0$. Recently published works regarding the case of anisotropic and inhomogeneous media were done in [16] for Laplace type governing equation, [17] for diffusion-convection-reaction equation, [18, 19, 20] for Helmholtz equation, [21] for elasticity problems of vector elliptic type equation, [22, 23, 24, 25] for a class of scalar elliptic equations and [26, 27, 28] for the modified Helmholtz equation.

In (1) it is required that the coefficient $[d_{ij}]$ ($i,j = 1,2$) is a real positive definite symmetrical matrix and the summation convention for repeated indices holds. Therefore (1) can be written explicitly as

$$\frac{\partial}{\partial x_1} \left(d_{11} \frac{\partial c}{\partial x_1}\right) + \frac{\partial}{\partial x_1} \left(d_{12} \frac{\partial c}{\partial x_2}\right) + \frac{\partial}{\partial x_2} \left(d_{12} \frac{\partial c}{\partial x_1}\right) + \frac{\partial}{\partial x_2} \left(d_{22} \frac{\partial c}{\partial x_2}\right) - \frac{\partial}{\partial x_1} (v_1 c) - \frac{\partial}{\partial x_2} (v_2 c) = 0$$

Referred to the Cartesian frame $Ox_1x_2$ solutions $c$ and its derivatives to boundary value problems governed by (1) and defined in a region $\Omega$ in $\mathbb{R}^2$ with boundary $\partial \Omega$ which consists of a finite number of piecewise smooth curves are sought. On $\partial \Omega_1$ the dependent variable $c(x)$ is specified, and

$$P = d_{ij} (\partial c/\partial x_i) n_j$$

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 $\partial \Omega$.

A boundary integral equation which is relevant to the boundary value problem will be derived. A BEM is then formulated from the boundary integral equation. The BEM is used for finding numerical solutions $c$ and derivatives $\partial c/\partial x_i$ for any points in $\Omega$.

Through out the paper the analysis is purely mathematical. The main purpose is to construct a BEM for the numerical solution of the problem.
2. Reduction to constant coefficients equation

We assume the coefficients $d_{ij}$ and $v_i$ to vary according to a continuous function and to take the form

$$d_{ij}(x) = \hat{d}_{ij} h(x)$$
$$v_i(x) = \hat{v}_i h(x)$$

in which $h(x)$ is a differentiable function and $\hat{d}_{ij}$ and $\hat{v}_i$ are constant. The inhomogeneity function $h(x)$ is assumed to take the exponential form

$$h(x) = [A \exp(\alpha_i x_i)]^2$$

where $A$ and $\alpha_i$ are constants. So the material under consideration is an exponentially graded material.

Substitution of (4) and (5) into (1) gives

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

Assume

$$c(x) = h^{-1/2}(x) \phi(x)$$

therefore equation (7) can be written as

$$\hat{d}_{ij} \frac{\partial}{\partial x_i} \left[ h \frac{\partial (h^{-1/2} \phi)}{\partial x_j} \right] - \hat{v}_i \frac{\partial (h^{1/2} \phi)}{\partial x_i} = 0$$

which can be further written as

$$\hat{d}_{ij} \left[ \left( \frac{1}{4} h^{-3/2} \frac{\partial h}{\partial x_i} \frac{\partial h}{\partial x_j} - \frac{1}{2} h^{-1/2} \frac{\partial^2 h}{\partial x_i \partial x_j} \right) \phi + h^{1/2} \frac{\partial^2 \phi}{\partial x_i \partial x_j} \right] - \hat{v}_i \frac{\partial (h^{1/2} \phi)}{\partial x_i} = 0$$

Use of the identities

$$\frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} = -\left( \frac{1}{4} h^{-3/2} \frac{\partial h}{\partial x_i} \frac{\partial h}{\partial x_j} - \frac{1}{2} h^{-1/2} \frac{\partial^2 h}{\partial x_i \partial x_j} \right)$$
$$h \frac{\partial (h^{1/2} \phi)}{\partial x_i} = h^{1/2} \frac{\partial \phi}{\partial x_i} + \phi \frac{\partial h^{1/2}}{\partial x_i}$$

allows equation (9) to be written in the form

$$h^{1/2} \left( \hat{d}_{ij} \frac{\partial^2 \phi}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \phi}{\partial x_i} \right) - \phi \left( \hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + \hat{v}_i \frac{\partial h^{1/2}}{\partial x_i} \right) = 0$$

So that if $h$ satisfies

$$\hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + \hat{v}_i \frac{\partial h^{1/2}}{\partial x_i} - \lambda h^{1/2} = 0$$

where $\lambda$ is a constant, then (10) becomes

$$\hat{d}_{ij} \frac{\partial^2 \phi}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \phi}{\partial x_i} - \lambda \phi = 0$$
The exponential function \( h(x) \) in (6) will satisfy (11) when
\[
\dot{d}_{ij} \alpha_i \alpha_j + \dot{\nu}_i \alpha_i - \lambda = 0
\]  
(13)

Moreover, use of (4) and (8) in (3) gives
\[
P = -P_h \Phi + P_{\phi} h^{1/2}
\]  
(14)

where \( P_h(x) = \dot{d}_{ij} (\partial h^{1/2}/\partial x_j) n_i \) and \( P_{\phi}(x) = \dot{d}_{ij} (\partial \phi/\partial x_j) n_i \).

3. The boundary integral equation

By using Gauss divergence theorem a boundary integral equation can be derived from the constant coefficients equation (12) (see for example [29] for derivation) as follows
\[
\gamma(\varsigma) \phi(\varsigma) = \int_{\partial \Omega} \{ P_{\phi}(x) \Phi(x, \varsigma) - [P_{\nu}(x) \Phi(x, \varsigma) + \Gamma(x, \varsigma)] \phi(x) \} \, ds(x)
\]  
(15)

where \( P_{\nu}(x) = \dot{\nu}_i n_i(x) \) and \( \varsigma = (\varsigma_1, \varsigma_2) \), \( \gamma = 0 \) if \( \varsigma_1, \varsigma_2 \notin \Omega \cup \partial \Omega \), \( \gamma = 1 \) if \( \varsigma_1, \varsigma_2 \in \Omega \), \( \gamma = \frac{1}{2} \) if \( (\varsigma_1, \varsigma_2) \in \partial \Omega \) given that \( \partial \Omega \) has a continuously turning tangent at \( (\varsigma_1, \varsigma_2) \). In (15) the functions \( \Phi(x, \varsigma) \) and \( \Gamma(x, \varsigma) \) satisfy
\[
\dot{d}_{ij} \frac{\partial^2 \Phi(x, \varsigma)}{\partial x_i \partial x_j} + \dot{\nu}_i \frac{\partial \Phi(x, \varsigma)}{\partial x_i} - \lambda \Phi(x, \varsigma) = -\delta(x - \varsigma)
\]
\[
\Gamma(x, \varsigma) = \dot{d}_{ij} \frac{\partial \Phi(x, \varsigma)}{\partial x_j} n_i
\]

where \( \delta \) is the Dirac delta function. For 2-D problems \( \Phi \) is given as (see [29])
\[
\Phi(x, \varsigma) = \frac{F}{2\pi} \exp \left( -\frac{\mathbf{v} \cdot \mathbf{R}}{2E} \right) K_0 \left( \frac{\mu R}{2} \right)
\]  
(16)

where \( \mu = \sqrt{(\dot{\nu}/2E)^2 + (\lambda/E)} \), \( E = \left[ \dot{d}_{11} + 2\dot{d}_{12} \hat{\tau} + \dot{d}_{22} (\hat{\tau}^2 + \bar{\tau}^2) \right]/2 \), \( F = \bar{\tau}/E \), \( \mathbf{R} = \mathbf{x} - \mathbf{\varsigma} \), \( \dot{\mathbf{x}} = (x_1 + \hat{\tau} x_2, \hat{\tau} x_2) \), \( \mathbf{\varsigma} = (\varsigma_1 + \hat{\tau} \varsigma_2, \hat{\tau} \varsigma_2) \), \( \dot{\mathbf{v}} = (\dot{\nu}_1 + \hat{\tau} \dot{\nu}_2, \bar{\tau} \dot{\nu}_2) \), \( \hat{\mathbf{R}} = \sqrt{(x_1 + \hat{\tau} x_2 - \varsigma_1 - \hat{\tau} \varsigma_2)^2 + (\hat{\tau} x_2 - \bar{\tau} \varsigma_2)^2} \) and \( \dot{\mathbf{v}} = \sqrt{(\dot{\nu}_1 + \hat{\tau} \dot{\nu}_2)^2 + (\bar{\tau} \dot{\nu}_2)^2} \) where \( \hat{\tau} \) and \( \bar{\tau} \) are respectively the real and the positive imaginary parts of the complex root \( \tau \) of the quadratic equation \( \dot{d}_{11} + 2\dot{d}_{12} \tau + \dot{d}_{22} \tau^2 = 0 \) and \( K_0 \) is the modified Bessel function. Substituting (8) and (14) into (15)
\[
\gamma h^{1/2} c = \int_{\partial \Omega} \left\{ \left( h^{-1/2} \Phi \right) P + \left[ \left( P_h - P_{\phi} h^{1/2} \right) \Phi - h^{1/2} \Gamma \right] n \right\} \, ds
\]  
(17)

The boundary integral equation (17) is relevant to and may be used for determining the solution of equation (1).

4. Numerical results

Some problems will be considered for verification of the analysis derived in the previous sections. The domain of the problems is assumed to be a unit square. The boundary of the domain is divided into 320 elements of equal size. For the purpose of computation of the solution, a FORTRAN code is drawn. The elapsed computation time is measured by calling a specific built-in FORTRAN command.

Other aspects that will be verified are the accuracy, efficiency, and consistency of the scattering and flow BEM solutions. This is as to see whether or not the developed FORTRAN script works correctly. Moreover, we will also show the influence of the anisotropy of the material under consideration on the solutions.
4.1. Test problems
The boundary conditions are as shown in Figure 1. Solutions \( c(x) \) and its derivatives are calculated at 19\( \times \)19 interior points.

\[ \begin{array}{ccc}
D(0,1) & c \text{ known} & C(1,1) \\
P \text{ known} & & c \text{ known} \\
A(0,0) & c \text{ known} & B(1,0)
\end{array} \]

**Figure 1.** The domain \( \Omega \)

The inhomogeneity function \( h(x) \) is assumed to take exponential form (6) satisfying (13). The constant coefficients are assumed to be

\[
\hat{d}_{ij} = \begin{bmatrix} 1.5 & 1 \\ 1 & 2.5 \end{bmatrix} \quad \hat{v}_i = (1.5, 2.5)
\]

4.1.1. Example 1: \( \lambda = 0 \) The function \( h \) is taken to be

\[ h(x) = [\exp(0.35x_1 - 0.995106x_2)]^2 \]

The exact solution is

\[ c(x) = \exp(-0.85x_1 + 1.495106x_2) \]

The CPU time elapsed for obtaining the solutions is only 188.84375 seconds which is rather efficient. Quite accurate BEM solutions are shown in Figure 2. Whereas a consistency between the scattering solution \( c \) and the flow vector \( \partial c/\partial x_1, \partial c/\partial x_2 \) is indicated in Figure 3. This, after all, means the FORTRAN code works properly.

**Figure 2.** The errors of solutions \( c \) (left), \( \partial c/\partial x_1 \) (center), \( \partial c/\partial x_2 \) (right) for Example 1
Figure 3. Solutions \( c \) and \( (\partial c/\partial x_1, \partial c/\partial x_2) \) for Example 1

Figure 4. The errors of solutions \( c \) (left), \( \partial c/\partial x_1 \) (center), \( \partial c/\partial x_2 \) (right) for Example 2

Figure 5. Solutions \( c \) and \( (\partial c/\partial x_1, \partial c/\partial x_2) \) for Example 2

4.1.2. Example 2: \( \lambda = -0.25 \)  The inhomogeneity function \( h \) is

\[
h(x) = \exp(0.35x_1 - 0.801555x_2)^2
\]

The exact solution is

\[
c(x) = \exp(0.15x_1 + 0.727389x_2)
\]

The accuracy of the BEM solution is shown in Figure 4 and its consistency is indicated by Figure 5. The elapsed CPU time is 188.546875 seconds.

4.2. A problem without exact solution
4.2.1. Example 3: A layered material treated as a continuously varying material A layered material consisting of eight layers of the same size as depicted in Figure 6 is under consideration. Each layer is supposed to be homogeneous, but from layer to layer the diffusion \( d_{ij} \) and velocity \( v_i \) coefficients vary as smoothly as the variability can be fitted to the exponential function (6).

As an illustration, suppose that we have a set of data of the diffusion \( d_{ij} \) and velocity \( v_i \) values at the center point of each layer as shown in Table 1. And we also have reference values
Figure 6. A layered material as the domain $\Omega$

Table 1. Example of the diffusion $d_{ij}$ and velocity $v_i$ coefficients data

| Layer | $d_{11}$ | $d_{12}$ | $d_{22}$ | $v_1$  | $v_2$  |
|-------|----------|----------|----------|--------|--------|
| 1     | 0.15284  | 0        | 0.76420  | 0.25473| 0.35662|
| 2     | 0.15868  | 0        | 0.79339  | 0.26446| 0.37025|
| 3     | 0.16474  | 0        | 0.82371  | 0.27457| 0.38439|
| 4     | 0.17103  | 0        | 0.85518  | 0.28506| 0.39908|
| 5     | 0.17757  | 0        | 0.88786  | 0.29595| 0.41433|
| 6     | 0.18435  | 0        | 0.92179  | 0.30726| 0.43017|
| 7     | 0.19140  | 0        | 0.95701  | 0.31900| 0.44660|
| 8     | 0.19871  | 0        | 0.99358  | 0.33119| 0.46367|

of constant coefficients

$$\hat{d}_{ij} = \begin{bmatrix} 0.15 & 0 \\ 0 & 0.75 \end{bmatrix} \quad \hat{v}_i = (0.25, 0.35)$$

Fitting the data in Table 1 to the function $h(x) = [A \exp(\alpha_1 x_1 + \alpha_2 x_2)]^2$ we will get the values of the parameters

$$A = 1 \quad \alpha_1 = 0 \quad \alpha_2 = 0.15$$

Therefore we can then approximate the layered material as a sole material with continuously varying coefficients. So we may now use the analysis in sections 2 and (3) to solve the problem.

The boundary conditions are depicted in Figure 6. We take the parameter $\lambda = 0.069375$ so that the inhomogeneity function $h(x)$ takes the exponential form in equation (6) and satisfies (11) and (13).

As shown in Figure 7 for the given constant orthotropic diffusion coefficient $\hat{d}_{ij}$ above the solution $c$ exhibits the nature of the considered medium as a layered material.

However, if we assume that the material under consideration is a sole material varying continuously and we change the diffusion coefficient $\hat{d}_{ij}$ to an anisotropic diffusion coefficient

$$\hat{d}_{ij} = \begin{bmatrix} 0.15 & 0.15 \\ 0.15 & 0.75 \end{bmatrix}$$
Figure 7. Solutions $c$ and $(\partial c/\partial x_1, \partial c/\partial x_2)$ for Example 3 of the orthotropic inhomogeneous medium

Figure 8. Solutions $c$ and $(\partial c/\partial x_1, \partial c/\partial x_2)$ for Example 3 of the anisotropic inhomogeneous medium

(therefore the values of $d_{12}$ in Table 1 are not appropriate anymore) by keeping the other coefficients remain the same then we will obtain a significantly different solution $c$ as shown in Figure 8. This means that the anisotropy of the medium gives an impact on the solution. Therefore in the application, it is necessary for the anisotropy to be taken into account.

5. Conclusion
Problems governed by equation (1) for inhomogeneous media have been solved by using BEM. Some examples of problems have been solved for exponentially graded materials. 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 3 is valid.

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