Numerical simulation for anisotropic-diffusion convection reaction problems of inhomogeneous media

A R Jalil\textsuperscript{1}, M I Azis\textsuperscript{2,*}, S Amir\textsuperscript{2}, M Bahri\textsuperscript{2} and S Hamzah\textsuperscript{3}

\begin{itemize}
\item \textsuperscript{1}Department of Marine Science, Hasanuddin University, Makassar, Indonesia
\item \textsuperscript{2}Department of Mathematics, Hasanuddin University, Makassar, Indonesia
\item \textsuperscript{3}Department of Civil Engineering, Hasanuddin University, Makassar, Indonesia
\end{itemize}

E-mail: mohivanazis@yahoo.co.id (\textsuperscript{*}Corresponding author)

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

1. Introduction
By referring to the two-dimensional Cartesian coordinate system $Ox_1x_2$ this paper will concern with the diffusion-convection-reaction (DCR) equation of the form

$$\frac{\partial}{\partial x_1} \left[ d_{ij}(x) \frac{\partial \gamma(x)}{\partial x_1} \right] - \frac{\partial}{\partial x_i} [\nu_i(x)\gamma(x)] - \rho(x)\gamma(x) = 0 \quad (1)$$

where $i, j = 1, 2$, $x = (x_1, x_2)$, $d_{ij}$ is the anisotropic diffusion/conduction coefficient, $\nu_i$ is the velocity, $\rho$ is the reaction coefficient and $\gamma$ is the dependent variable. Within the domain in question $[d_{ij}]$ is a real symmetrical matrix satisfying $d_{11}d_{22} - d_{12}^2 > 0$. For the repeated indices in equation (1) summation convention applies so that equation (1) can be written explicitly

$$\frac{\partial}{\partial x_1} \left( d_{11} \frac{\partial \gamma}{\partial x_1} \right) + \frac{\partial}{\partial x_1} \left( d_{12} \frac{\partial \gamma}{\partial x_2} \right) + \frac{\partial}{\partial x_2} \left( d_{12} \frac{\partial \gamma}{\partial x_1} \right) + \frac{\partial}{\partial x_2} \left( d_{22} \frac{\partial \gamma}{\partial x_2} \right)$$

$$- \frac{\partial}{\partial x_1} (\nu_1 \gamma) - \frac{\partial}{\partial x_2} (\nu_2 \gamma) - \rho \gamma = 0$$

Also, in equation (1) the coefficients $d_{ij}$, $\nu_i$ and $\rho$ vary spatially and continuously which is applicable when the medium is inhomogeneous or is a functionally graded material.
DCR equation is usually used for modeling heat transfer and mass transport problems. According to Ravnik and Škerget [1], in mass transport which frequently occurs in environments, the convection process take places with a flow velocity which varies in the medium in question, and in the case of turbulence modelling with turbulent viscosity hypothesis, the diffusivity also change in the domain. These situations draw the relevancy of the DCR equation (1).

Functionally graded materials (FGMs) are materials possessing characteristics which vary (with time and position) according to a mathematical function. FGMs are mainly artificial materials which are produced to meet a preset practical performance (see for example [2, 3]). Heat transfer in FGMs, for which equation (1) is usually used as the governing equation, is among application that has been considerably studied by many people. This also constitutes relevancy of solving equation (1).

A number of authors had previously considered the DCR equation. For example, [4], [5], [6, 7] solved an isotropic-DCR equation with variable velocity, [8] considered a constant coefficients unsteady isotropic-DCR equation with a source term, and again [9] solved an isotropic-DCR equation with a source term.

Not so many works have been done on DCR equation of type (1) for anisotropic media with simultaneously variable diffusivity, velocity and reaction coefficients. For anisotropic materials some works on different governing equations have been done earlier. For example, [10, 11], [12] and [13] considered Helmholtz equation, [14] and [15, 16] concerned with DC equation, [17], [18], [19] and [20] discussed a vector elliptic equation for elasticity problems, [21] considered a scalar Laplace type equation, [22], [23], [24] and [25] focused on another scalar elliptic type equation, and papers [26, 27, 28] considered a modified Helmholtz type equation.

Numerical solutions \( \gamma \) and its derivatives \( \partial \gamma / \partial x_1, \partial \gamma / \partial x_2 \) to (1) in the domain \( \Omega \), subjected to the boundary condition that either \( \gamma \) or \( F = d_{ij} (\partial \gamma / \partial x_i) n_j \) is known on the boundary \( \partial \Omega \), are sought. The investigation of this paper is strictly mathematical. The purpose is mainly to develop a boundary element method for finding the numerical solutions.

2. A simplification to equation of constant coefficients

We limit the coefficients \( \nu_i, d_{ij} \) and \( \rho \) to be varying spatially according to a specific continuous function \( h(\mathbf{x}) \)

\[
d_{ij}(\mathbf{x}) = \hat{d}_{ij} h(\mathbf{x}) \\
\nu_i(\mathbf{x}) = \hat{\nu}_i h(\mathbf{x}) \\
\rho(\mathbf{x}) = \hat{\rho} h(\mathbf{x})
\]

where \( \hat{d}_{ij}, \hat{\nu}_i \) and \( \hat{\rho} \) are constant and the inhomogeneity function \( h(\mathbf{x}) \) is a differentiable function. Substitution of (3), (4) and (5) into (1) gives

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

Assume

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

therefore equation (6) can be written respectively as

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

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

(8)

Use of the identities

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

allows equation (8) to be written in the form

\[
h^{1/2} \left( \hat{d}_{ij} \frac{\partial^2 \varsigma}{\partial x_i \partial x_j} - \hat{\nu}_i \frac{\partial \varsigma}{\partial x_i} \right) - \varsigma \left( \hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + \hat{\nu}_i \frac{\partial h^{1/2}}{\partial x_i} \right) - \hat{\rho} h^{1/2} \varsigma = 0
\]

(9)

So that if \( h \) in (9) satisfies

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

(10)

where \( \lambda \) is a constant, then (7) transforms the equation of variable coefficients (1) to an equation of constant coefficients

\[
\hat{d}_{ij} \frac{\partial \varsigma}{\partial x_i \partial x_j} - \hat{\nu}_i \frac{\partial \varsigma}{\partial x_i} - (\hat{\rho} + \lambda) \varsigma = 0
\]

(11)

Or if \( h \) in (9) satisfies

\[
\hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + \hat{\nu}_i \frac{\partial h^{1/2}}{\partial x_i} + (\hat{\rho} - \lambda) h^{1/2} = 0
\]

(12)

then

\[
\hat{d}_{ij} \frac{\partial \varsigma}{\partial x_i \partial x_j} - \hat{\nu}_i \frac{\partial \varsigma}{\partial x_i} - \lambda \varsigma = 0
\]

(13)

Moreover, substitution of (3) and (7) into (2) gives

\[
F = -F_h \varsigma + F_i h^{1/2}
\]

(14)

where \( F_h (x) = \hat{d}_{ij} \left( \frac{\partial h^{1/2}}{\partial x_j} \right) n_i \) and \( F_i (x) = \hat{d}_{ij} \left( \frac{\partial \varsigma}{\partial x_j} \right) n_i \).

For incompressible flows, use of the zero velocity divergence

\[
\frac{\partial \nu_i (x)}{\partial x_i} = 0
\]

(15)

in (1) gives

\[
\frac{\partial}{\partial x_i} \left[ d_{ij} (x) \frac{\partial \gamma (x)}{\partial x_j} \right] - \nu_i (x) \frac{\partial \gamma (x)}{\partial x_i} - \rho (x) \gamma (x) = 0
\]

(16)
The equation (16) was considered in [1, 29] as the governing equations. Substitution of (4) into (15) gives
\[ \hat{\nu}_i \frac{\partial h^{1/2}}{\partial x_i} = 0 \]
so that (10) becomes
\[ \hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} - \lambda h^{1/2} = 0 \]
and (12) becomes
\[ \hat{d}_{ij} \frac{\partial^2 h^{1/2}}{\partial x_i \partial x_j} + (\hat{\rho} - \lambda) h^{1/2} = 0 \]
(17)
(18)
Feasible forms of function \( h(x) \) satisfying (10) and (12) for compressible flows are respectively
\[
\begin{align*}
 h(x) &= [A \exp (\alpha_i x_i)]^2, \quad \hat{d}_{ij} \alpha_i \alpha_j + \hat{\nu}_i \alpha_i - \lambda = 0 \\
 h(x) &= [A \exp (\alpha_i x_i)]^2, \quad \hat{d}_{ij} \alpha_i \alpha_j + (\hat{\rho} - \lambda) = 0
\end{align*}
\]
(19)
whereas for incompressible flows, given that \( \hat{\nu}_i \alpha_i = 0 \), feasible forms of function \( h(x) \) satisfying (17) are
\[
\begin{align*}
 h(x) &= [A (\alpha_0 + \alpha_1 x_1 + \alpha_2 x_2)]^2, \quad \lambda = 0 \\
 h(x) &= [A \cos (\alpha_i x_i) + B \sin (\alpha_i x_i)]^2, \quad \hat{d}_{ij} \alpha_i \alpha_j + \lambda = 0 \\
 h(x) &= [A \exp (\alpha_i x_i)]^2, \quad \hat{d}_{ij} \alpha_i \alpha_j - \lambda = 0
\end{align*}
\]
(20)
and those satisfying (18) are
\[
\begin{align*}
 h(x) &= [A (\alpha_0 + \alpha_1 x_1 + \alpha_2 x_2)]^2, \quad \lambda = \hat{\rho} \\
 h(x) &= [A \cos (\alpha_i x_i) + B \sin (\alpha_i x_i)]^2, \quad \hat{d}_{ij} \alpha_i \alpha_j - (\hat{\rho} - \lambda) = 0 \\
 h(x) &= [A \exp (\alpha_i x_i)]^2, \quad \hat{d}_{ij} \alpha_i \alpha_j + (\hat{\rho} - \lambda) = 0
\end{align*}
\]
(21)
where \( A, B \) and \( \alpha_i \) are constants.

3. The boundary integral equation

Equations (11) and (13) can be written in a form of boundary integral equation
\[
\eta(\chi) \zeta(\chi) = \int_{\partial \Omega} \{ F_\nu(x) \Lambda(x, \chi) - [F_\nu(x) \Lambda(x, \chi) + \Theta(x, \chi)] \zeta(x) \} ds(x)
\]
(22)
where \( F_\nu(x) = \hat{\nu}_i n_i(x) \) 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 \( (\chi_1, \chi_2) \). In (22) the fundamental solution \( \Lambda(x, \chi) \) for equations (11) and (13) respectively satisfies
\[
\begin{align*}
 \hat{d}_{ij} \frac{\partial^2 \Lambda(x, \chi)}{\partial x_i \partial x_j} + \hat{\nu}_i \frac{\partial \Lambda(x, \chi)}{\partial x_i} - (\hat{\rho} + \lambda) \Lambda(x, \chi) &= -\delta(x - \chi) \\
 \hat{d}_{ij} \frac{\partial^2 \Lambda(x, \chi)}{\partial x_i \partial x_j} + \hat{\nu}_i \frac{\partial \Lambda(x, \chi)}{\partial x_i} - \lambda \Lambda(x, \chi) &= -\delta(x - \chi)
\end{align*}
\]
and \( \Theta(x, \chi) \) satisfies
\[
\Theta(x, \chi) = \hat{d}_{ij} \frac{\partial \Lambda(x, \chi)}{\partial x_j} n_i
\]
where $\delta$ is the Dirac delta function. For 2-D problems $\Lambda$ for equations (11) and (13) is respectively given as (see for example [30])

$$
\Lambda(x, \chi) = \frac{\dot{\sigma}}{2\pi D} \exp \left( -\frac{\dot{\nu} \cdot \hat{R}}{2D} \right) K_0 \left( \mu_1 \hat{R} \right)
$$

$$
\Lambda(x, \chi) = \frac{\dot{\sigma}}{2\pi D} \exp \left( -\frac{\dot{\nu} \cdot \hat{R}}{2D} \right) K_0 \left( \mu_2 \hat{R} \right)
$$

where $\mu_1 = \sqrt{\left(\dot{\nu}/2D\right)^2 + \left[\ddot{\rho} + \lambda\right]/D}$, $\mu_2 = \sqrt{\left(\dot{\nu}/2D\right)^2 + \left(\lambda/D\right)}$, $D = [d_{11} + 2\dot{d}_{12} \dot{\sigma} + \dot{d}_{22} (\dot{\sigma}^2 + \ddot{\sigma}^2)/2]$, $\hat{R} = \hat{x} - \hat{x}' = (x_1 + \sigma x_2, \sigma x_2)$, $\chi = (\chi_1 + \sigma \chi_2, \sigma \chi_2)$, $\dot{\nu} = (\dot{\nu}_1 + \sigma \dot{\nu}_2, \sigma \dot{\nu}_2)$, $\hat{R} = \sqrt{x_1 + \sigma x_2 - \chi_1 - \sigma \chi_2)^2 + (\sigma x_2 - \sigma \chi_2)^2}$, and $\dot{\nu} = \sqrt{[\dot{\nu}_1 + \sigma \dot{\nu}_2]^2 + (\sigma \dot{\nu}_2)^2}$ where $\dot{\sigma}$ and $\ddot{\sigma}$ are respectively the real and the positive imaginary parts of the complex root $\sigma$ of the quadratic equation $d_{11} + 2\dot{d}_{12} \dot{\sigma} + \dot{d}_{22} \dot{\sigma}^2 = 0$ and $K_0$ is the modified Bessel function. Use of (7) and (14) in (22) yields

$$
\eta h^{1/2} = \int_{\partial \Omega} \left\{ \left( h^{-1/2} \Lambda \right) F + \left[ F_h - F_{\nu} h^{1/2} \right] \Lambda - h^{1/2} \Theta \right\} \gamma \right) ds \tag{23}
$$

The boundary integral equation (23) can be used to find the numerical solutions of $\gamma$, $\partial \gamma/\partial x_1$ and $\partial \gamma/\partial x_2$ at all points of $\Omega$.

**4. Discretisation**

We discretize the boundary $\partial \Omega$ into $L$ segments $\partial \Omega_l = [q_{l-1}, q_l]$ for $l = 1, 2, 3, \ldots, L$ where $q_{l-1}$ and $q_l$ are the endpoints of the segment $\partial \Omega_l$. It is assumed that $\gamma$ and $F$ are constant along each boundary segment $\partial \Omega_l$ taking on their values at the mid point $q_l = (q_{l-1} + q_l)/2$. then the discretised form of (23) may be written as

$$
\eta(\chi) h^{1/2}(\chi) \gamma(\chi) = \sum_{l=1}^{L} \left\{ F(q_l) \int_{q_{l-1}}^{q_l} \left[ h^{-1/2}(x) \Lambda(x, \chi) \right] ds(x) \right. \\
+ \gamma(q_l) \int_{q_{l-1}}^{q_l} \left\{ \left[ F_h(x) - F_{\nu}(x) h^{1/2}(x) \right] \Lambda(x, \chi) \\
- h^{1/2}(x) \Theta(\chi, x) \right\} ds(x) \right\} \tag{24}
$$

The integral equation (24) is used to find the unknowns $\gamma(x)$ or $F(x)$ on the boundary $\partial \Omega$. Then the complete boundary data $\gamma(x)$ and $F(x)$ on $\partial \Omega$ are used to evaluate the solutions $\gamma(x)$ and its derivatives in the domain $\Omega$.

If the source point $\chi \in \partial \Omega$ (thus $\eta(\chi) = 1/2$), say $\chi \in \partial \Omega_k$ ($k = 1, 2, \ldots, L$) so that $\chi = q_k$, then equation (24) can be written as

$$
\frac{1}{2} h^{1/2}(q_k) \gamma(q_k) = \sum_{l=1}^{L} \left\{ F(q_l) \int_{q_{l-1}}^{q_l} \left[ h^{-1/2}(x) \Lambda(x, q_k) \right] ds(x) \\
+ \gamma(q_l) \int_{q_{l-1}}^{q_l} \left\{ \left[ F_h(x) - F_{\nu}(x) h^{1/2}(x) \right] \Lambda(x, q_k) \\
- h^{1/2}(x) \Theta(x, q_k) \right\} ds(x) \right\}
$$
for \( k = 1, 2, \ldots, L \). In a matrix multiplication form, this equation can be written

\[
\frac{1}{2} h_k^{1/2} \gamma_k - \sum_{l=1}^L \hat{H}_{kl} \gamma_l = \sum_{l=1}^L G_{kl} F_l
\]

(25)

where \( h_k^{1/2} = h^{1/2}(\mathbf{q}_k) \), \( \gamma_k = \gamma(\mathbf{q}_k) \), \( F_l = F(\mathbf{q}_l) \), and

\[
\hat{H}_{kl} = \int_{\mathbf{q}_{l-1}}^{\mathbf{q}_l} \left\{ \left[ F_h(\mathbf{x}) - F_v(\mathbf{x}) h^{1/2}(\mathbf{x}) \right] \Lambda(\mathbf{x}, \mathbf{q}_k) - h^{1/2}(\mathbf{x}) \Theta(\mathbf{x}, \mathbf{q}_k) \right\} ds(\mathbf{x})
\]

(26)

\[
G_{kl} = \int_{\mathbf{q}_{l-1}}^{\mathbf{q}_l} h^{-1/2}(\mathbf{x}) \Lambda(\mathbf{x}, \mathbf{q}_k) ds(\mathbf{x})
\]

(27)

The line integrals in equations (26) and (27) can be calculated numerically. The values of the modified Bessel function \( K_0 \) which is involved in the fundamental solutions \( \Lambda \) can also be approximated using its polynomial approximations (see [31]). In a simpler way, (25) can be written as

\[
\sum_{l=1}^L H_{kl} \gamma_l = \sum_{l=1}^L G_{kl} F_l
\]

(28)

where

\[
H_{kl} = \begin{cases} 
-\hat{H}_{kl} & \text{when } k \neq l \\
\frac{1}{2} h_k^{1/2} - \hat{H}_{kl} & \text{when } k = l 
\end{cases}
\]

Rearranging equation (28) we obtain an \( L \times L \) linear system of algebraic equations

\[
\mathbf{AX} = \mathbf{B}
\]

(29)

which can be solved for the unknown matrix \( \mathbf{X} \).

Once the unknowns \( \gamma \) and \( F \) on the boundary \( \partial \Omega \) are obtained from the equation (29), we can calculate the value of \( \gamma, \partial \gamma/\partial \chi_1 \) and \( \partial \gamma/\partial \chi_2 \) at any point \( \chi \) inside the domain \( \Omega \) by using the equation (24). That is

\[
\gamma(\chi) = h^{-1/2}(\chi) \sum_{l=1}^L \left\{ \left. F(\mathbf{q}_l) \int_{\mathbf{q}_{l-1}}^{\mathbf{q}_l} \left[ h^{-1/2}(\mathbf{x}) \Lambda(\mathbf{x}, \chi) \right] ds(\mathbf{x}) \right\right.

+ \left. \gamma(\mathbf{q}_l) \int_{\mathbf{q}_{l-1}}^{\mathbf{q}_l} \left[ \left[ F_h(\mathbf{x}) - F_v(\mathbf{x}) h^{1/2}(\mathbf{x}) \right] \Lambda(\mathbf{x}, \chi) \right. \right.

- \left. h^{1/2}(\mathbf{x}) \Theta(\mathbf{x}, \chi) \right\} ds(\mathbf{x}) \right\}
\]

\[
\frac{\partial \gamma}{\partial \chi_1}(\chi) = h^{-1/2}(\chi) \left\{ \sum_{l=1}^L \left\{ \left. F(\mathbf{q}_l) \int_{\mathbf{q}_{l-1}}^{\mathbf{q}_l} \left[ h^{-1/2}(\mathbf{x}) \frac{\partial \Lambda(\mathbf{x}, \chi)}{\partial \chi_1} \right] ds(\mathbf{x}) \right\right. \right.

+ \left. \gamma(\mathbf{q}_l) \int_{\mathbf{q}_{l-1}}^{\mathbf{q}_l} \left[ \left[ F_h(\mathbf{x}) - F_v(\mathbf{x}) h^{1/2}(\mathbf{x}) \right] \frac{\partial \Lambda(\mathbf{x}, \chi)}{\partial \chi_1} \right. \right.

- \left. h^{1/2}(\mathbf{x}) \frac{\partial \Theta(\mathbf{x}, \chi)}{\partial \chi_1} \right\} ds(\mathbf{x}) \right\} - \gamma(\chi) \left. \frac{\partial h^{1/2}(\chi)}{\partial \chi_1} \right| \}
\]
\[
\frac{\partial \gamma}{\partial \chi_2}(\chi) = h^{-1/2}(\chi) \left\{ \sum_{l=1}^L \left\{ F(q_l) \int_{q_{l-1}}^{q_l} \left[ h^{-1/2}(x) \frac{\partial \Lambda(x, \chi)}{\partial \chi_2} \right] ds(x) \right. \right. \\
+ \gamma(q_l) \int_{q_{l-1}}^{q_l} \left[ \left[ F_h(x) - F_\nu(x) h^{1/2}(x) \right] \frac{\partial \Lambda(x, \chi)}{\partial \chi_2} \right. \\
- h^{1/2}(x) \frac{\partial \Theta(x, \chi)}{\partial \chi_2} \right) ds(x) \left. \right\} - \gamma(\chi) \frac{\partial h^{1/2}(\chi)}{\partial \chi_2} \right\}
\]

5. Numerical results

The aim of this section is to justify the analysis used to derive the boundary integral equation (23). Some problems will be solved using the BEM. Solutions to the problems are calculated using a FORTRAN script and a specific command is embedded inside the script to count the elapsed CPU computation time as to show the efficiency of the BEM. The other aspects that will be justified are the accuracy and consistency as to see whether or not the FORTRAN script works correctly. Moreover, we will also study the influence of the anisotropy and inhomogeneity of the material under consideration on the solutions.

5.1. Test problems

The domain and the boundary conditions are as depicted in Figure 1. A number of 320 segments of equal length, namely 80 segments on each side of the unit square, are used. The elapsed CPU time is counted for obtaining solutions \(\gamma(x)\) and its derivatives at \(19 \times 19\) interior points.

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

5.1.1. Compressible flows

The inhomogeneity function \(h(x)\) is assumed to satisfy (10) and (12), respectively taking one of the forms in (19). For problems considered in this section, the constant diffusion \(\hat{d}_{ij}\) and velocity \(\hat{\nu}_i\) coefficients, and the parameter \(\lambda\) are taken to be

\[
\hat{d}_{ij} = \begin{bmatrix} 1 & 1 \\ 1 & 1.5 \end{bmatrix}, \quad \hat{\nu}_i = (1.5, 1), \quad \lambda = 1
\]
Figure 2. The absolute errors of $\gamma$ (left), $\frac{\partial \gamma}{\partial x_1}$ (center), $\frac{\partial \gamma}{\partial x_2}$ (right) solutions of Problem 1

Figure 3. The BEM scattering $\gamma$ and flow vector $\left(\frac{\partial \gamma}{\partial x_1}, \frac{\partial \gamma}{\partial x_2}\right)$ solutions of Problem 1

**Problem 1:** $h(x)$ satisfies (10). The constant reaction coefficient is $\hat{\rho} = 1.25$. The inhomogeneity function $h$ is

$$h(x) = [2 \exp (0.25x_1 - 1.290569x_2)]^2$$

The exact solution is

$$\gamma(x) = 0.5 \exp (0.75x_1 - 0.437198x_2)$$

Figure 2 indicates that the BEM solutions are quite accurate. Meanwhile, Figure 3 shows a coherence between the scattering and the flow. The elapsed CPU time is 148.796875 seconds, so that the BEM is quite efficient.

**Problem 2:** $h(x)$ satisfies (12). The constant reaction coefficient is taken to be $\hat{\rho} = 0.25$. The inhomogeneity function $h$ is

$$h(x) = [2 \exp (0.5x_1 - 1.193713x_2)]^2$$

The exact solution is

$$\gamma(x) = 0.5 \exp (0.5x_1 - 0.193713x_2)$$

The accuracy of the BEM solution is shown by Figure 4 and its consistency is indicated by Figure 5. Meanwhile, the efficiency of the BEM is achieved by the fact that the elapsed CPU time is only 150.65625 seconds.
5.1.2. Incompressible flows  The inhomogeneity function \( h(x) \) is assumed to satisfy (17) or (18) taking one of the forms in equation (20) or (21). For problems considered in this section, the constant diffusion coefficients are as follows

\[
\hat{d}_{ij} = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 2 \end{bmatrix}
\]

**Problem 3:** \( h(x) \) satisfies (17). The constant velocity and reaction coefficients are respectively taken to be \( \hat{v}_i = (1, -0.5) \) and \( \hat{\rho} = 1 \). Taking the quadratical form in (20) the inhomogeneity function \( h \) is assumed to be

\[
h(x) = [2(1 + 0.25x_1 + 0.5x_2)]^2
\]

Satisfying (7) and (11), the exact solution is

\[
\gamma(x) = 0.5 \exp(0.5x_1 - 1.079156x_2) / (1 + 0.5x_1 + x_2)
\]

Figures 6 and 7 show again the accuracy and consistency of the numerical solutions. Efficiency of the BEM is indicated by a short elapsed CPU time which is only 150.828125 seconds.
Figure 7. The BEM scattering $\gamma$ and flow vector $\left(\frac{\partial \gamma}{\partial x_1}, \frac{\partial \gamma}{\partial x_2}\right)$ solutions of Problem 3

Figure 8. The absolute errors of $\gamma$ (left), $\frac{\partial \gamma}{\partial x_1}$ (center), $\frac{\partial \gamma}{\partial x_2}$ (right) solutions of Problem 4

Figure 9. The BEM scattering $\gamma$ and flow vector $\left(\frac{\partial \gamma}{\partial x_1}, \frac{\partial \gamma}{\partial x_2}\right)$ solutions of Problem 4

**Problem 4:** $h(x)$ satisfies (18). The constant velocity and reaction coefficients are respectively taken to be $\nu = (1, -2.8403)$ and $\rho = 0.25$. The inhomogeneity function $h$ is assumed to take the trigonometrical form in (21) with $\lambda = -0.15$, that is

$$h(x) = \left[\cos (0.5x_1 + 0.17604x_2) + 2\sin (0.5x_1 + 0.17604x_2)\right]^2$$

Satisfying (7) and (13), the exact solution is

$$\gamma(x) = \frac{\exp (0.25x_1 + 0.012041x_2)}{[\cos (0.5x_1 + 0.17604x_2) + 2\sin (0.5x_1 + 0.17604x_2)]}$$

The accuracy and consistency of the numerical solutions are shown by Figures 8 and 9. The elapsed CPU time is 197.609375 seconds.

5.2. A problem without exact solution

5.2.1. Problem 5: Incompressible flow in a layered material treated as a continuously varying material. A layered material consisting of eight layers of the same size as depicted in Figure
Table 1. Example of the diffusion $d_{ij}$, velocity $\nu_i$ and reaction $\rho$ coefficient data

| Layer | $d_{11}$ | $d_{12}$ | $d_{22}$ | $\nu_1$ | $\nu_2$ | $\rho$ |
|-------|----------|----------|----------|---------|---------|--------|
| 1     | 1.01254  | 0        | 2.02508  | 0.50627 | 0       | 0.75940|
| 2     | 1.03785  | 0        | 2.07570  | 0.51893 | 0       | 0.77839|
| 3     | 1.06348  | 0        | 2.12695  | 0.53174 | 0       | 0.79761|
| 4     | 1.08941  | 0        | 2.17883  | 0.54471 | 0       | 0.81706|
| 5     | 1.11566  | 0        | 2.23133  | 0.55783 | 0       | 0.83675|
| 6     | 1.14223  | 0        | 2.28445  | 0.57111 | 0       | 0.85667|
| 7     | 1.16910  | 0        | 2.33820  | 0.58455 | 0       | 0.87683|
| 8     | 1.19629  | 0        | 2.39258  | 0.59814 | 0       | 0.89722|

10 is under consideration. Each layer is supposed to be homogeneous, but from layer to layer the diffusion $d_{ij}$, velocity $\nu_i$ and reaction $\rho$ coefficients vary as smoothly as the variability can be fitted to a quadratical function $h(x) = (\alpha_0 + \alpha_2 x_2)^2$.

As an illustration, suppose that we have a set of data of the diffusion $d_{ij}$, velocity $\nu_i$ and reaction $\rho$ coefficient values at center point of each layer as shown in Table 1. And we also have reference values of constant coefficients

\[
\hat{d}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}, \quad \hat{\nu}_i = (0.1, 0), \quad \hat{\rho} = 0.15
\]

Fitting the data in Table 1 to the function $h(x) = (\alpha_0 + \alpha_2 x_2)^2$ we will get the values of the parameters $\alpha_0$ and $\alpha_2$

\[
\alpha_0 = 1, \quad \alpha_2 = 0.1
\]

Therefore we can then approximate the layered material as a sole material with continuously varying coefficients. So we may use the analysis in Sections 2 – 4 to solve the problem.

The boundary conditions are depicted in Figure 10. We take the parameter $\lambda = 0$ so that the inhomogeneity function $h(x)$ takes the quadratical form in equation (20). Again, a number of 320 segments of equal length, namely 80 segments on each side of the unit square, are used.

Figure 10. A layered material as the domain $\Omega$
Figure 11. The BEM scattering $\gamma$ and flow vector $\left( \frac{\partial \gamma}{\partial x_1}, \frac{\partial \gamma}{\partial x_2} \right)$ solutions for Problem 5 of the orthotropic inhomogeneous medium.

Figure 12. The BEM scattering $\gamma$ and flow vector $\left( \frac{\partial \gamma}{\partial x_1}, \frac{\partial \gamma}{\partial x_2} \right)$ solutions for Problem 5 of the anisotropic inhomogeneous medium.

As shown in Figure 11 for the given constant orthotropic diffusion coefficient $\hat{d}_{ij}$ above the solution $\gamma$ exhibits the nature of the considered medium as a layered material.

However, if we now 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

$$\hat{d}_{ij} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}$$

(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 $\gamma$ as shown in Figure 12. This means that the anisotropy of the medium gives an impact on the solution. Therefore in application it is necessary for the anisotropy to be taken into account.

Now if we assume that the medium is anisotropic homogeneous with

$$\hat{d}_{ij} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} \quad \alpha_0 = 1 \quad \alpha_2 = 0$$

then we will obtain a slightly different solution $\gamma$ as shown in Figure 13. This indicates that the inhomogeneity also gives an impact on the solution. Therefore one should put the inhomogeneity in consideration for any application.
Figure 13. The BEM scattering $\gamma$ and flow vector $\left(\frac{\partial \gamma}{\partial x_1}, \frac{\partial \gamma}{\partial x_2}\right)$ solutions for Problem 5 of the anisotropic homogeneous medium

6. Conclusion
A standard BEM has been used to find numerical solutions to boundary value problems governed by the anisotropic diffusion-convection-reaction equation (1) for inhomogeneous media. Some examples of problems have been solved for exponentially, quadratically and trigonometrically graded materials. The BEM gives accurate solutions and uses very efficient computation time for producing the results. In addition, the BEM solutions also present evidence for the impact of the anisotropy and inhomogeneity of the media on the solutions.

Acknowledgements
The authors acknowledge the research grants provided by The Ministry of Higher Education of Indonesia (KEMRISTEKDIKTI) under the contract numbered as 007/SP2H/PTNBH/DRPM/2019 and by The Hasanuddin University under the Hasanuddin University’s Rector decrees numbered as 2006/UN4.1/KEP/2019 and 641/UN4.1/KEP/2019.

References
[1] Ravnik J and Skerget L 2013 A gradient free integral equation for diffusion-convection equation with variable coefficient and velocity Engineering Analysis with Boundary Elements 37 683
[2] Abotula S, Kidane A, Chalivendra V B and Shukla A 2012 Dynamic curving cracks in functionally graded materials under thermo-mechanical loading International Journal of Solids and Structures 49 1637
[3] Abadikhah H and Folkow P D 2018 Dynamic equations for solid isotropic radially functionally graded circular cylinders Composite Structures 195 147
[4] Samec N and Skerget L 2004 Integral formulation of a diffusive–convective transport equation for reacting flows Engineering Analysis with Boundary Elements 28 1055
[5] Rocca A L, Rosales A H and Power H 2005 Radial basis function Hermite collocation approach for the solution of time dependent convection-diffusion problems Engineering Analysis with Boundary Elements 29 359
[6] AL-Bayati S A and Wrobel L C 2018 A novel dual reciprocity boundary element formulation for two-dimensional transient convection-diffusion-reaction problems with variable velocity Engineering Analysis with Boundary Elements 94 60
[7] AL-Bayati S A and Wrobel L C 2018 The dual reciprocity boundary element formulation for convection-diffusion-reaction problems with variable velocity field using different radial basis functions International Journal of Mechanical Sciences 145 367
[8] Fendoglu H, Bozkaya C and Tezer-Sezgin M 2018 DBEM and DRBEM solutions to 2D transient convection-diffusion-reaction type equations Engineering Analysis with Boundary Elements 93 124
[9] AL-Bayati S A and Wrobel L C 2019 Radial integration boundary element method for two-dimensional non-homogeneous convection-diffusion-reaction problems with variable source term Engineering Analysis with Boundary Elements 101 89
[10] Azis M I 2019 Numerical solutions for the Helmholtz boundary value problems of anisotropic homogeneous media Journal of Computational Physics 381 42
[11] Azis M I 2019 BEM solutions to exponentially variable coefficient Helmholtz equation of anisotropic media. *Journal of Physics: Conference Series* **1277** 012036

[12] Nurwahyu B, Abdullah B, Massinai A and Azis M I 2019 Numerical solutions for BVPs governed by a Helmholtz equation of anisotropic FGM. *IOP Conference Series: Earth and Environmental Science* **279** 012008

[13] Hamzah S, Azis M I and Amir A K 2019 Numerical solutions to anisotropic BVPs for quadratically graded media by a Helmholtz equation. *IOP Conference Series: Materials Science and Engineering* **619** 012060

[14] Haddade A, Salam N, Khaeruddin and Azis M I 2017 A boundary element method for 2D diffusion-convection problems in anisotropic media. *Far East Journal of Mathematical Sciences* **102**(8) 1593

[15] Azis M I, Asrul L, Khaeruddin and Paharuddin 2018 BEM solutions for unsteady transport problems in anisotropic media. *JP Journal of Heat and Mass Transfer* **15**(4) 915

[16] Azis M I, Kaswawati, Haddade A and Thamrin S A 2018 On some examples of pollutant transport problems solved numerically using the boundary element method. *Journal of Physics: Conference Series* **979** 012075

[17] Clements D L and Azis M I 2000 A note on a boundary element method for the numerical solution of boundary value problems in isotropic inhomogeneous elasticity. *Journal of the Chinese Institute of Engineers, Transactions of the Chinese Institute of Engineers, Series A/Chung-kuo Kung Ch'eng Hsuch K’an.* **23**(3) 261

[18] Azis M I and Clements D L 2014 On some problems concerning deformations of functionally graded anisotropic elastic materials. *Far East Journal of Mathematical Sciences* **87**(2) 173

[19] Azis M I, Toaha S, Bahri M and Ilyas N 2018 A boundary element method with analytical integration for deformation of inhomogeneous elastic materials. *Journal of Physics: Conference Series* **979** 012072

[20] Hamzah S, Azis M I and Syamsuddin E 2019 On some examples of BEM solution to elasticity problems of isotropic functionally graded materials. *IOP Conference Series: Materials Science and Engineering* **619** 012018

[21] Salam N, Haddade A, Clements D L and Azis M I 2017 A boundary element method for a class of elliptic boundary value problems of functionally graded media. *Engineering Analysis with Boundary Elements* **84**(3) 186

[22] Azis M I 2019 Numerical solutions to a class of scalar elliptic BVPs for anisotropic exponentially graded media. *Journal of Physics: Conference Series* **1218** 012001

[23] La Nafie N, Ilyas N, Azis M I and Amir A K 2019 A class of variable coefficient elliptic equations solved using BEM. *IOP Conference Series: Materials Science and Engineering* **619** 012025

[24] Haddade A, Azis M I, Djafar Z, Jabir St N and Nurwahyu B 2019 Numerical solutions to a class of scalar elliptic BVPs for anisotropic quadratically graded media. *IOP Conference Series: Earth and Environmental Science* **279** 012007

[25] Jabir St N, Azis M I, Djafar Z and Nurwahyu B 2019 BEM solutions to a class of elliptic BVPs for anisotropic trigonometrically graded media. *IOP Conference Series: Materials Science and Engineering* **619** 012059

[26] La Nafie N, Azis M I and Fähruddin 2019 Numerical solutions to BVPs governed by the anisotropic modified Helmholtz equation for trigonometrically graded media. *IOP Conference Series: Materials Science and Engineering* **619** 012058

[27] Syam R, Fähruddin, Azis M I and Hayat A 2019 Numerical solutions to anisotropic FGM BVPs governed by the modified Helmholtz type equation. *IOP Conference Series: Materials Science and Engineering* **619** 012061

[28] Azis M I, Syam R and Hamzah S 2019 BEM solutions to BVPs governed by the anisotropic modified Helmholtz equation for quadratically graded media. *IOP Conference Series: Earth and Environmental Science* **279** 012010

[29] Ravnik J and Skerget L 2014 Integral equation formulation of an unsteady diffusion-convection equation with variable coefficient and velocity. *Computers and Mathematics with Applications* **66** 2477

[30] Azis M I 2017 Fundamental solutions to two types of 2D boundary value problems of anisotropic materials. *Far East Journal of Mathematical Sciences* **101**(11) 2405

[31] Abramowitz M and Stegun I A 1972 *Handbook of mathematical functions: with formulas, graphs and mathematical tables*, Dover Publications, Washington