Numerical simulation for unsteady anisotropic-diffusion convection equation of spatially variable coefficients and incompressible flow

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Abstract. The anisotropic-diffusion convection equation of spatially variable co-
efficients which is relevant for functionally graded media is discussed in this paper
to find numerical solutions by using a combined Laplace transform and boundary
element method. The variable coefficients equation is transformed to a constant co-
efficients equation. The constant coefficients equation is then Laplace-transformed so
that the time variable vanishes. The Laplace-transformed equation is consequently
written in a pure boundary integral equation which involves a time-free fundamental
solution. The boundary integral equation is therefore employed to find numerical
solutions using a standard boundary element method. Finally the results obtained
are inversely transformed numerically using the Stehfest formula to get solutions in
the time variable. The combined Laplace transform and boundary element method
is easy to be implemented and accurate for solving unsteady problems of anisotropic
functionally graded media governed by the diffusion convection equation.

Keywords. Functionally graded materials, variable coefficients, anisotropic, unsteady,
diffusion-convection

1   Introduction

In the last decade investigations on the diffusion-convection equation had been done for finding
its numerical solutions. The investigations can be classified according to the anisotropy and in-
homogeneity of the media under consideration. For example, Wu et al. [34], Hernandez-Martinez
et al. [12], Wang et al. [33] and Fendoğlu et al. [7] had been working on problems of *isotropic
diffusion and homogeneous media*, Yoshida and Nagaoka [35], Meenal and Eldho [19], Azis [3] (for
Helmholtz type governing equation) studied problems of *anisotropic diffusion but homogeneous
media*. Rap et al. [23], Ravnik and Škerget [25, 26], Li et al. [18] and Pettres and Lacerda
[22] considered the case of *isotropic diffusion and variable coefficients (inhomogeneous media)*.
Recently Azis and co-workers had been working on steady state problems of *anisotropic inho-
mogeneous* media for several types of governing equations, for examples [5, 32] for the modified
Helmholtz equation, [4, 14, 24, 30, 27, 11, 17] for the diffusion convection reaction equation,
[29, 8, 13, 16] for the Laplace type equation, [10, 2, 20, 21, 15] for the Helmholtz equation.

Referred to the Cartesian frame Ox_1x_2 we will consider initial boundary value problems governed by an unsteady anisotropic-diffusion convection equation with incompressible flow and variable coefficients of the form

$$\frac{\partial}{\partial x_i}\left[d_{ij}\left(\mathbf{x}\right)\frac{\partial c\left(\mathbf{x},t\right)}{\partial x_j}\right] - \frac{\partial}{\partial x_i}\left[v_i\left(\mathbf{x}\right)c\left(\mathbf{x},t\right)\right] = \alpha\left(\mathbf{x}\right)\frac{\partial c\left(\mathbf{x},t\right)}{\partial t} \tag{1.1}$$

The coefficient $[d_{ij}]$ $(i,j=1,2)$ is a real positive definite symmetrical matrix. Also, in (1.1) the summation convention for repeated indices holds, so that explicitly (1.1) can be respectively written as

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

Equation (1.1) is used to model unsteady diffusion convection process in anisotropic and inhomogeneous (functionally graded) materials. Among the physical phenomena of applications include pollutant transport and heat transfer.

Nowadays functionally graded materials (FGMs) have become an important issue, and numerous studies on this issue for a variety of applications have been reported. Authors commonly define an FGM as an inhomogeneous material having a specific property such as thermal conductivity, hardness, toughness, ductility, corrosion resistance, etc. that changes spatially in a continuous fashion. Therefore equation (1.1) is relevant for FGMs.

Equation (1.1) applies for unsteady problems of *anisotropic and inhomogeneous* therefore provides a wider class of problems. It covers problems of isotropic and homogeneous media as special cases which occur respectively when $d_{11}=d_{22}, d_{12}=0$ and the coefficients d_{ij}, v_i and α are constant.

Zoppou and Knight [36] 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 (1.1) but with limitation $d_{11} \neq d_{22}, d_{12}=0$. This paper is intended to extend the recently published works on anisotropic diffusion convection equation with variable coefficients [31, 6, 9, 28, 1] from the steady state to unsteady state equation.

2 The initial boundary value problem

Given the coefficients $d_{ij}\left(\mathbf{x}\right), v_i\left(\mathbf{x}\right), \alpha\left(\mathbf{x}\right)$ solutions $c\left(\mathbf{x},t\right)$ and its derivatives to (1.1) are sought which are valid for time interval $t \geq 0$ and in a region Ω in R^2 with boundary $\partial\Omega$ which consists of a finite number of piecewise smooth curves. On $\partial\Omega_1$ the dependent variable $c\left(\mathbf{x},t\right)$ is specified, and

$$P\left(\mathbf{x},t\right) = d_{ij}\left(\mathbf{x}\right)\frac{\partial c\left(\mathbf{x},t\right)}{\partial x_i}n_j \tag{2.1}$$

is specified on $\partial\Omega_2$ where $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$ and $\mathbf{n} = (n_1, n_2)$ denotes the outward pointing normal to $\partial\Omega$. The initial condition is taken to be

$$c\left(\mathbf{x},0\right) = 0 \tag{2.2}$$

The method of solution will be to transform the variable coefficient equation (1.1) to a constant coefficient equation, and then taking a Laplace transform of the constant coefficient equation, and

to obtain a boundary integral equation in the Laplace transform variable s. The boundary integral equation is then solved using a standard boundary element method (BEM). An inverse Laplace transform is applied to get the solution c and its derivatives for all $(\mathbf{x}, t)$ in the domains. The inverse Laplace transform is implemented numerically using the Stehfest formula. The analysis is specially relevant to an anisotropic medium but it equally applies to isotropic media. For isotropy, the coefficients in (1.1) take the form $d_{11} = d_{22}$ and $d_{12} = 0$ and use of these equations in the following analysis immediately yields the corresponding results for an isotropic medium.

The analysis in this paper is purely mathematical, the main aim is to derive a BEM for finding the numerical solutions to problems governed by equation (1.1).

3   The boundary integral equation

We restrict the coefficients d_{ij}, v_i, α to be of the form

$$d_{ij}(\mathbf{x}) = \hat{d}_{ij}\, g(\mathbf{x}) \tag{3.1}$$

$$v_i(\mathbf{x}) = \hat{v}_i\, g(\mathbf{x}) \tag{3.2}$$

$$\alpha(\mathbf{x}) = \hat{\alpha}\, g(\mathbf{x}) \tag{3.3}$$

where $g(\mathbf{x})$ is a differentiable function and $\hat{d}_{ij}, \hat{v}_i, \hat{\alpha}$ are constants. Further we assume that the coefficients $d_{ij}(\mathbf{x})$, $v_i(\mathbf{x})$ and $\alpha(\mathbf{x})$ are exponentially graded by taking $g(\mathbf{x})$ as an exponential function

$$g(\mathbf{x}) = \left[\exp(\beta_0 + \beta_i x_i)\right]^2 \tag{3.4}$$

where β_0 and β_i are constants. Therefore if

$$\hat{d}_{ij}\beta_i\beta_j - \lambda = 0 \tag{3.5}$$

then (3.4) satisfies

$$\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} - \lambda g^{1/2} = 0 \tag{3.6}$$

Substitution of (3.1)-(3.3) into (1.1) gives

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left(g\frac{\partial c}{\partial x_j}\right) - \hat{v}_i g\frac{\partial c}{\partial x_i} = \hat{\alpha}g\frac{\partial c}{\partial t} \tag{3.7}$$

Assume

$$c(\mathbf{x}, t) = g^{-1/2}(\mathbf{x})\,\psi(\mathbf{x}, t) \tag{3.8}$$

therefore substitution of (3.1) and (3.8) into (2.1) gives

$$P(\mathbf{x}, t) = -P_g(\mathbf{x})\,\psi(\mathbf{x}, t) + g^{1/2}(\mathbf{x})\,P_\psi(\mathbf{x}, t) \tag{3.9}$$

where

$$P_g(\mathbf{x}, t) = \hat{d}_{ij}\frac{\partial g^{1/2}(\mathbf{x})}{\partial x_j}n_i \quad P_\psi(\mathbf{x}, t) = \hat{d}_{ij}\frac{\partial \psi(\mathbf{x}, t)}{\partial x_j}n_i$$

And equation (3.7) can be written as

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left[g\frac{\partial\left(g^{-1/2}\psi\right)}{\partial x_j}\right] - \hat{v}_i g\frac{\partial\left(g^{-1/2}\psi\right)}{\partial x_i} = \hat{\alpha}g\frac{\partial\left(g^{-1/2}\psi\right)}{\partial t}$$

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left[g\left(g^{-1/2}\frac{\partial\psi}{\partial x_j} + \psi\frac{\partial g^{-1/2}}{\partial x_j}\right)\right] - \hat{v}_i g\left(g^{-1/2}\frac{\partial\psi}{\partial x_i} + \psi\frac{\partial g^{-1/2}}{\partial x_i}\right) = \hat{\alpha}g\left(g^{-1/2}\frac{\partial\psi}{\partial t}\right)$$

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left(g^{1/2}\frac{\partial\psi}{\partial x_j} + g\psi\frac{\partial g^{-1/2}}{\partial x_j}\right) - \hat{v}_i\left(g^{1/2}\frac{\partial\psi}{\partial x_i} + g\psi\frac{\partial g^{-1/2}}{\partial x_i}\right) = \hat{\alpha}g^{1/2}\frac{\partial\psi}{\partial t}$$

Use of the identity

$$\frac{\partial g^{-1/2}}{\partial x_i} = -g^{-1}\frac{\partial g^{1/2}}{\partial x_i}$$

implies

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left(g^{1/2}\frac{\partial\psi}{\partial x_j} - \psi\frac{\partial g^{1/2}}{\partial x_j}\right) - \hat{v}_i\left(g^{1/2}\frac{\partial\psi}{\partial x_i} - \psi\frac{\partial g^{1/2}}{\partial x_i}\right) = \hat{\alpha}g^{1/2}\frac{\partial\psi}{\partial t}$$

$$\begin{aligned} g^{1/2}\left(\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_j}\right) - \psi\left(\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial g^{1/2}}{\partial x_i}\right) \\ + \left(\hat{d}_{ij}\frac{\partial\psi}{\partial x_j}\frac{\partial g^{1/2}}{\partial x_i} - \hat{d}_{ij}\frac{\partial\psi}{\partial x_j}\frac{\partial g^{1/2}}{\partial x_i}\right) = \hat{\alpha}g^{1/2}\frac{\partial\psi}{\partial t} \end{aligned} \qquad (3.10)$$

For incompressible flow

$$\frac{\partial v_i\left(\mathbf{x}\right)}{\partial x_i} = 2g^{1/2}(\mathbf{x})\hat{v}_i\frac{\partial g^{1/2}(\mathbf{x})}{\partial x_i} = 0$$

that is

$$\hat{v}_i\frac{\partial g^{1/2}(\mathbf{x})}{\partial x_i} = 0$$

Thus (3.10) becomes

$$g^{1/2}\left(\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_i}\right) - \psi\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i\partial x_j} = \hat{\alpha}g^{1/2}\frac{\partial\psi}{\partial t}$$

Equation (3.6) then implies

$$\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_i} - \lambda\psi = \hat{\alpha}\frac{\partial\psi}{\partial t} \qquad (3.11)$$

Taking a Laplace transform of (3.8), (3.9), (3.11) and applying the initial condition (2.2) we obtain

$$\psi^*\left(\mathbf{x}, s\right) = g^{1/2}\left(\mathbf{x}\right)c^*\left(\mathbf{x}, s\right) \qquad (3.12)$$

$$P_{\psi^*}\left(\mathbf{x}, s\right) = \left[P^*\left(\mathbf{x}, s\right) + P_g\left(\mathbf{x}\right)\psi^*\left(\mathbf{x}, s\right)\right] g^{-1/2}\left(\mathbf{x}\right) \tag{3.13}$$

$$\hat{d}_{ij}\frac{\partial^2\psi^*}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial\psi^*}{\partial x_i} - \left(\lambda + s\hat{\alpha}\right)\psi^* = 0 \tag{3.14}$$

where s is the variable of the Laplace-transformed domain.

By using Gauss divergence theorem, equation (3.14) can be transformed into a boundary integral equation

$$
\begin{aligned}
\eta\left(\boldsymbol{\xi}\right)\psi^*\left(\boldsymbol{\xi}, s\right) &= \int_{\partial\Omega}\left\{P_{\psi^*}\left(\mathbf{x}, s\right)\Phi\left(\mathbf{x}, \boldsymbol{\xi}\right) - \left[P_v\left(\mathbf{x}\right)\Phi\left(\mathbf{x}, \boldsymbol{\xi}\right)\right.\right. \\
&\quad \left.\left. + \Gamma\left(\mathbf{x}, \boldsymbol{\xi}\right)\right]\psi^*\left(\mathbf{x}, s\right)\right\} dS\left(\mathbf{x}\right)
\end{aligned}
\tag{3.15}
$$

where

$$P_v\left(\mathbf{x}\right) = \hat{v}_i\, n_i\left(\mathbf{x}\right)$$

For 2-D problems the fundamental solutions $\Phi(\mathbf{x}, \boldsymbol{\xi})$ and $\Gamma(\mathbf{x}, \boldsymbol{\xi})$ are given as

$$\Phi\left(\mathbf{x}, \boldsymbol{\xi}\right) = \frac{\rho_i}{2\pi D}\exp\left(-\frac{\dot{\mathbf{v}}.\dot{\mathbf{R}}}{2D}\right) K_0\left(\dot{\mu}\dot{R}\right) \tag{3.16}$$

$$\Gamma\left(\mathbf{x}, \boldsymbol{\xi}\right) = \hat{d}_{ij}\frac{\partial\Phi\left(\mathbf{x}, \boldsymbol{\xi}\right)}{\partial x_j}n_i \tag{3.17}$$

where

$$\dot{\mu} = \sqrt{\left(\dot{v}/2D\right)^2 + \left[\left(\lambda + s\hat{\alpha}\right)/D\right]}$$

$$D = \left[\hat{d}_{11} + 2\hat{d}_{12}\rho_r + \hat{d}_{22}\left(\rho_r^2 + \rho_i^2\right)\right]/2$$

$$\dot{\mathbf{R}} = \dot{\mathbf{x}} - \dot{\boldsymbol{\xi}}$$

$$\dot{\mathbf{x}} = \left(x_1 + \rho_r x_2, \rho_i x_2\right)$$

$$\dot{\boldsymbol{\xi}} = \left(\xi_1 + \rho_r \xi_2, \rho_i \xi_2\right)$$

$$\dot{\mathbf{v}} = \left(\hat{v}_1 + \rho_r \hat{v}_2, \rho_i \hat{v}_2\right)$$

$$\dot{R} = \sqrt{\left(x_1 + \rho_r x_2 - \xi_1 - \rho_r \xi_2\right)^2 + \left(\rho_i x_2 - \rho_i \xi_2\right)^2}$$

$$\dot{v} = \sqrt{\left(\hat{v}_1 + \rho_r \hat{v}_2\right)^2 + \left(\rho_i \hat{v}_2\right)^2}$$

where ρ_r and ρ_i are respectively the real and the positive imaginary parts of the complex root ρ of the quadratic equation

$$\hat{d}_{11} + 2\hat{d}_{12}\rho + \hat{d}_{22}\rho^2 = 0$$

and K_0 is the modified Bessel function. Use of (3.12) and (3.13) in (3.15) yields

$$\eta g^{1/2}c^* = \int_{\partial\Omega}\left\{\left(g^{-1/2}\Phi\right)P^* + \left[\left(P_g - P_v g^{1/2}\right)\Phi - g^{1/2}\Gamma\right]c^*\right\} dS \tag{3.18}$$

Equation (3.18) provides a boundary integral equation for determining the numerical solutions of c^* and its derivatives $\partial c^*/\partial x_1$ and $\partial c^*/\partial x_2$ at all points of Ω.

Knowing the solutions $c^*\left(\mathbf{x}, s\right)$ and its derivatives $\partial c^*/\partial x_1$ and $\partial c^*/\partial x_2$ which are obtained from (3.18), the numerical Laplace transform inversion technique using the Stehfest formula is

Table 1: Values of V_m of the Stehfest formula for $N = 4, 6, 8, 10$

V_m	$N = 4$	$N = 6$	$N = 8$	$N = 10$
V_1	-2	1	$-1/3$	0.083333333333333
V_2	26	-49	$145/3$	-32.083333333333336
V_3	-48	366	-906	1279
V_4	24	-858	$16394/3$	-15623.666666666666
V_5		810	$-43130/3$	84244.1666666666
V_6		-270	18730	-236957.5
V_7			$-35840/3$	375911.6666666666
V_8			$8960/3$	-340071.6666666666
V_9				164062.5
V_{10}				-32812.5

then employed to find the values of $c(\mathbf{x}, t)$ and its derivatives $\partial c / \partial x_1$ and $\partial c / \partial x_2$. The Stehfest formula is

$$
\begin{aligned}
c(\mathbf{x}, t) &\simeq \frac{\ln 2}{t} \sum_{m=1}^{N} V_m c^*(\mathbf{x}, s_m) \\
\frac{\partial c(\mathbf{x}, t)}{\partial x_1} &\simeq \frac{\ln 2}{t} \sum_{m=1}^{N} V_m \frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_1} \\
\frac{\partial c(\mathbf{x}, t)}{\partial x_2} &\simeq \frac{\ln 2}{t} \sum_{m=1}^{N} V_m \frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_2}
\end{aligned}
\tag{3.19}
$$

where

$$
\begin{aligned}
s_m &= \frac{\ln 2}{t} m \\
V_m &= (-1)^{\frac{N}{2}+m} \sum_{k=\left[\frac{m+1}{2}\right]}^{\min\left(m, \frac{N}{2}\right)} \frac{k^{N/2}(2k)!}{\left(\frac{N}{2} - k\right)! k! (k-1)! (m-k)! (2k-m)!}
\end{aligned}
$$

A simple script has been developed to calculate the values of the coefficients $V_m, m = 1, 2, \ldots, N$ for any number N. Table (1) shows the values of V_m for $N = 4, 6, 8, 10$.

4   Numerical results

In order to justify the analysis derived in the previous sections, we will consider several problems either as test examples of analytical solutions or problems without simple analytical solutions. We assume each problem belongs to a system which is valid in given spatial and time domains and governed by equation (1.1) and satisfying the initial condition (2.2) and some boundary conditions as defined in Section 2. The characteristics of the system which are represented by the coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), \alpha(\mathbf{x})$ in equation (1.1) are assumed to be of the form (3.1), (3.2) and (3.3) in which $g(\mathbf{x})$ is an exponential function of the form (3.4). The coefficients

$d_{ij}(\mathbf{x}), v_i(\mathbf{x}), \alpha(\mathbf{x})$ represents respectively the diffusivity or conductivity, the velocity of flow existing in the system and the change rate of the unknown or dependent variable $c(\mathbf{x}, t)$. As the flow is assumed to be incompressible, the velocity $v_i(\mathbf{x})$ must satisfy $\partial v_i(\mathbf{x})/\partial x_i = 0$.

A standard BEM is derived by discretizing the boundary integral equation (3.18). The boundary is discretized into a number of elements and the dependent variables c and P are assumed to be constant on each element (constant element), taking their values on the mid-point of each element. For the contour integrals, we use the 10-nodal-point Bode quadrature of error of order $O(h^{11})$ where $9h$ is equal to the length of the element. To some extent, this quadrature provides avoidance of the computation of the values of the fundamental solutions (3.16) and (3.17) on their singularities (if available), as the sink points never coincide with the source points (mid-point of elements). It also will guarantee the convergence of the solution as the number of boundary elements is increased.

The value of N in (3.19) for the Stehfest formula is chosen to be $N = 10$. For each time t, a number of $N = 10$ solutions of Laplace transform frame c^* and its derivatives are calculated. Then, we use the values of these solutions to find the solutions of the original frame c and its derivatives by utilizing the Stehfest formula (3.19).

For a simplicity, a unit square (depicted in Figure 1) will be taken as the geometrical domain for all problems. A number of 320 elements of equal length, namely 80 elements on each side of the unit square, are used. A FORTRAN script is developed to compute the solutions.
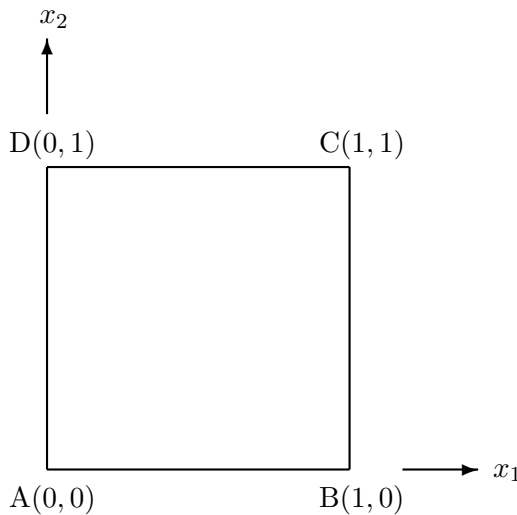

Figure 1: The domain Ω

4.1 Test problems

Other aspects that will be justified are the accuracy and consistency (between the scattering and flow) of the numerical solutions. The errors of the numerical solutions are computed using the formula $\sqrt{(\mu_a^2 - \mu_n^2)}$ where μ_a, μ_n are the analytical and numerical solutions, respectively. The analytical solutions are assumed to take a separable variables form

$$c(\mathbf{x}, t) = g^{-1/2}(\mathbf{x}) h(\mathbf{x}) f(t)$$
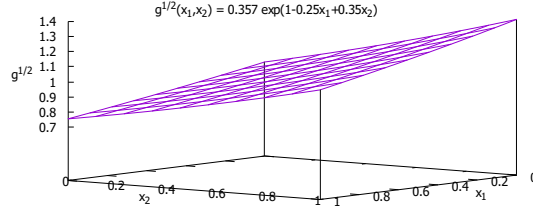
Figure 2: Function $g\left(\mathbf{x}\right)$

where

$$h\left(\mathbf{x}\right) \quad = \quad 2.7\exp\left[-\left(1 + 0.1x_1 + 0.15x_2\right)\right]$$

The function $g^{1/2}\left(\mathbf{x}\right)$ is

$$g^{1/2}\left(\mathbf{x}\right) \quad = \quad 0.357\exp\left(1 - 0.25x_1 + 0.35x_2\right)$$

and depicted in Figure 2.

We will consider three forms of time variation functions $f\left(t\right)$ of time domain $t = \left[0 : 5\right]$ which are

$$
\begin{aligned}
f\left(t\right) &= 1 - \exp\left(-1.5t\right) \\
f\left(t\right) &= 0.2t \\
f\left(t\right) &= t\left(5 - t\right)/6.25
\end{aligned}
$$

We take mutual coefficients $\hat{d}_{ij}$ and $\hat{v}_i$ for the problems

$$\hat{d}_{ij} = \begin{bmatrix} 1 & 0.15 \\ 0.15 & 0.45 \end{bmatrix} \quad \hat{v}_i = (0.7, 0.5)$$

so that from (3.5) we have

$$\lambda = 0.091375$$

For $h\left(\mathbf{x}\right)$ to be a solution to (3.14), the value of $\hat{\alpha}$ has to be

$$\hat{\alpha} = 0.07825/s$$

We also take a set of boundary conditions (see Figure 1)

$$
\begin{aligned}
&P \text{ is given on side AB, BC, CD} \\
&c \text{ is given on side AD}
\end{aligned}
$$
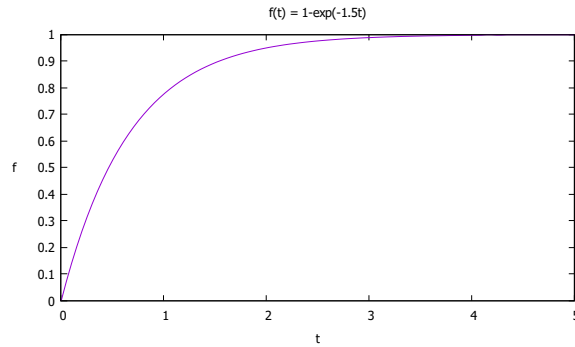
Figure 3: Function $f(t)$ for Problem 1
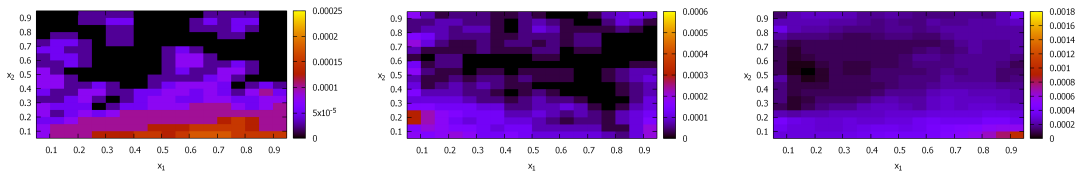
Figure 4: The errors of solutions c (left), $\partial c/\partial x_1$ (middle), $\partial c/\partial x_2$ (right) at $t = 2.5$ for Problem 1

Problem 1:   First, we suppose that the time variation function is

$$f(t) = 1 - \exp(-1.5t)$$

Function $f(t)$ is depicted in Figure 3.

Figure 4 and Table 2 show the accuracy of the BEM solutions. The errors occur in the fourth decimal place for the c and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ solutions. Figure 5 shows the consistency between the scattering and the flow solutions which verifies that the solutions for the derivatives had also been computed correctly. Figure 6 shows that the solution c changes with time t in a similar way the function $f(t) = 1 - \exp(-1.5t)$ does (see Figure 3) and tends to approach a steady state solution as the time goes to infinity, as expected.
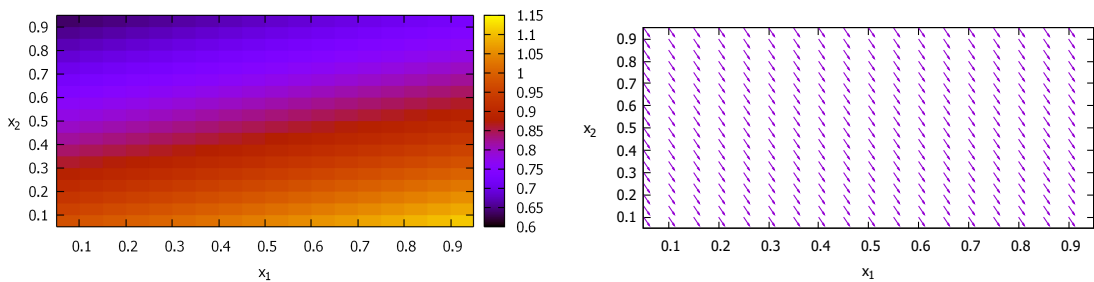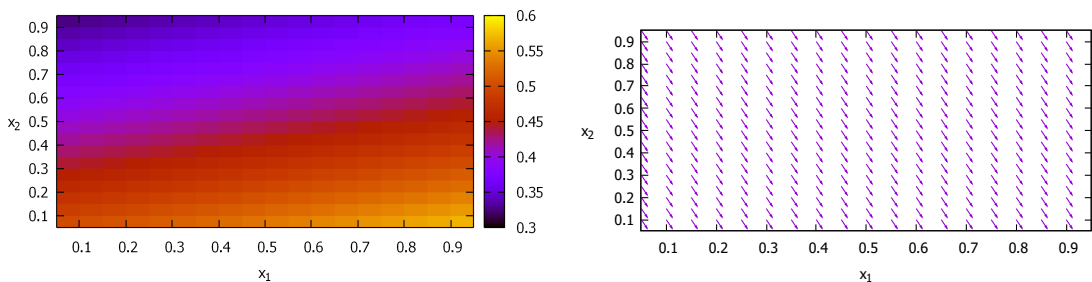

Figure 5: Solutions c and $(\partial c/\partial x_1, \partial c/\partial x_2)$ at $t = 2.5$ for Problem 1

Table 2: A comparison between numerical and analytical solutions at the centre point $(0.5, 0.5)$ for Problem 1

t	Numerical solution			Analytical solution		
	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$
0.0005	0.0006	0.0001	-0.0003	0.0006	0.0001	-0.0003
0.5	0.4535	0.0680	-0.2267	0.4534	0.0680	-0.2267
1.0	0.6676	0.1001	-0.3337	0.6675	0.1001	-0.3338
1.5	0.7685	0.1153	-0.3841	0.7687	0.1153	-0.3843
2.0	0.8162	0.1224	-0.4080	0.8164	0.1225	-0.4082
2.5	0.8390	0.1258	-0.4194	0.8390	0.1259	-0.4195
3.0	0.8499	0.1275	-0.4248	0.8497	0.1275	-0.4248
3.5	0.8552	0.1283	-0.4275	0.8547	0.1282	-0.4274
4.0	0.8577	0.1286	-0.4287	0.8571	0.1286	-0.4285
4.5	0.8588	0.1288	-0.4293	0.8582	0.1287	-0.4291
5.0	0.8593	0.1289	-0.4295	0.8587	0.1288	-0.4294
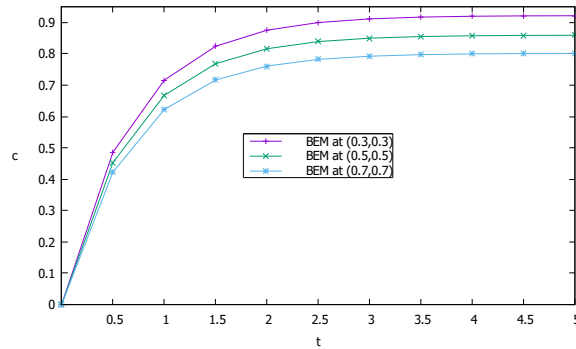
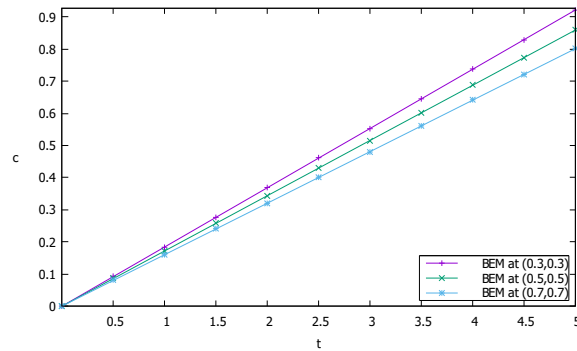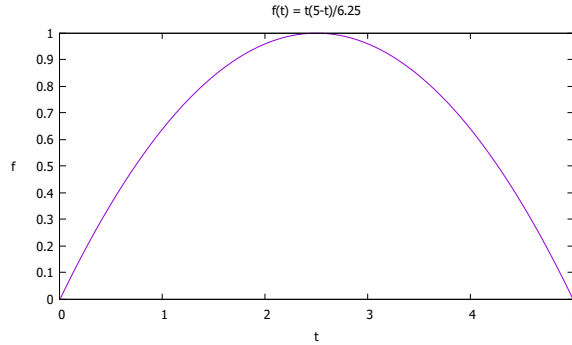Figure 6: Solutions c for Problem 1
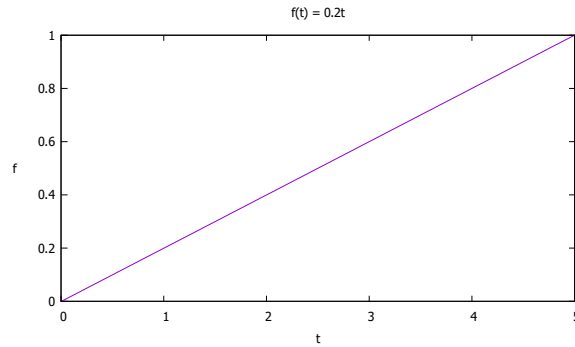
Figure 7: Function $f(t)$ for Problem 2
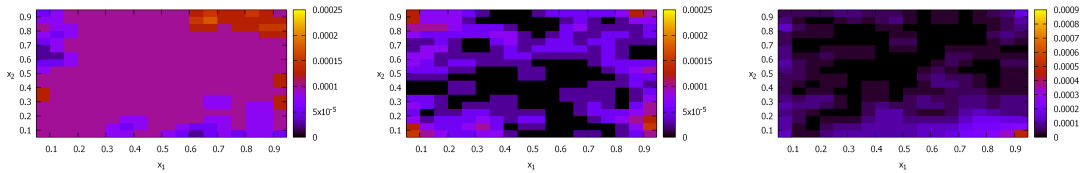
Figure 8: The errors of solutions c (left), $\partial c/\partial x_1$ (middle), $\partial c/\partial x_2$ (right) at $t = 2.5$ for Problem 2

Problem 2: Next, we suppose that the time variation function is (see Figure 7)

$$f(t) = 0.2t$$

Figure 8 and Table 3 show the accuracy of the BEM solutions. The errors occur in the fourth decimal place for the c and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ solutions. Figure 9 shows the consistency between the scattering and the flow solutions. Figure 10 shows that the solution c changes with time t in a manner which is almost similar to as the function $f(t) = 0.2t$ does (see Figure 7), as expected.

Problem 3: Now, we suppose that the time variation function is (see Figure 11)

Figure 9: Solutions c and $(\partial c/\partial x_1, \partial c/\partial x_2)$ at $t = 2.5$ for Problem 2

Table 3: A comparison between numerical and analytical solutions at the centre point $(0.5, 0.5)$ for Problem 2

t	Numerical solution			Analytical solution		
	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$
0.0005	0.0001	0.0000	-0.0000	0.0001	0.0000	-0.0000
0.5	0.0859	0.0129	-0.0430	0.0859	0.0129	-0.0430
1.0	0.1719	0.0258	-0.0859	0.1718	0.0258	-0.0859
1.5	0.2578	0.0387	-0.1289	0.2578	0.0387	-0.1289
2.0	0.3438	0.0516	-0.1718	0.3437	0.0516	-0.1718
2.5	0.4297	0.0645	-0.2148	0.4296	0.0644	-0.2148
3.0	0.5157	0.0773	-0.2578	0.5155	0.0773	-0.2578
3.5	0.6016	0.0902	-0.3007	0.6015	0.0902	-0.3007
4.0	0.6875	0.1031	-0.3437	0.6874	0.1031	-0.3437
4.5	0.7735	0.1160	-0.3866	0.7733	0.1160	-0.3866
5.0	0.8594	0.1289	-0.4296	0.8592	0.1289	-0.4296

Figure 10: Solutions c for Problem 2
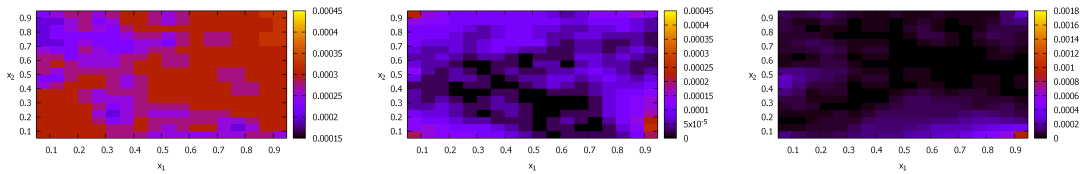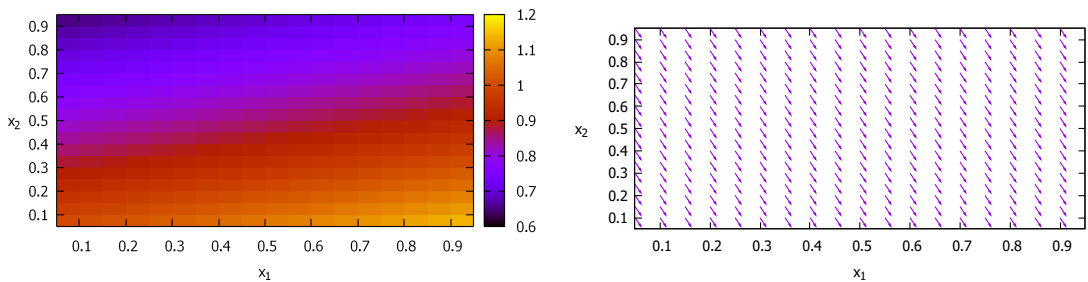
Figure 11: Function $f(t)$ for Problem 3

Figure 12: The errors of solutions c (left), $\partial c/\partial x_1$ (middle), $\partial c/\partial x_2$ (right) at $t = 2.5$ for Problem 3

$$f(t) = t(5 - t)/6.25$$

Figure 12 and Table 4 show the accuracy of the BEM solutions. Again, the errors occur in the fourth decimal place for the c and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ solutions. Figure 13 shows the consistency between the scattering and the flow solutions which again verifies that the solutions for the derivatives had also been computed correctly. Figure 14 shows that the solution c changes with time t in a similar way the function $f(t) = t(5 - t)/6.25$ does.

Figure 13: Solutions c and $(\partial c/\partial x_1, \partial c/\partial x_2)$ at $t = 2.5$ for Problem 3
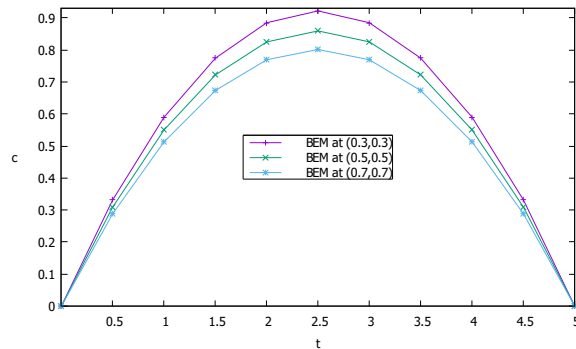

4.2   Examples without analytical solutions

Furthermore, we will show the impact of the anisotropy and the inhomogeneity of the material under consideration on the solutions. We choose

$$\hat{v}_i = (0.7, 0.5) \quad \hat{\alpha} = 1$$

Problem 4:   For this problem the medium is supposed to be inhomogeneous or homogeneous, anisotropic or isotropic with grading function $g(\mathbf{x})$, constant coefficients $\hat{d}_{ij}$ and corresponding λ satisfying (3.5) and (3.6) as respectively follows:

- inhomogeneous and anisotropic case

$$
\begin{aligned}
g^{1/2}(\mathbf{x}) &= 0.357 \exp\left(1 - 0.25x_1 + 0.35x_2\right) \\
\hat{d}_{ij} &= \begin{bmatrix} 1 & 0.15 \\ 0.15 & 0.45 \end{bmatrix} \\
\lambda &= 0.091375
\end{aligned}
$$

- inhomogeneous and isotropic case

$$
\begin{aligned}
g^{1/2}(\mathbf{x}) &= 0.357 \exp\left(1 - 0.25x_1 + 0.35x_2\right) \\
\hat{d}_{ij} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\
\lambda &= 0.185
\end{aligned}
$$

- homogeneous and isotropic case

$$
\begin{aligned}
g^{1/2}(\mathbf{x}) &= 1 \\
\hat{d}_{ij} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\
\lambda &= 0
\end{aligned}
$$

- homogeneous and anisotropic case

$$
\begin{aligned}
g^{1/2}(\mathbf{x}) &= 1 \\
\hat{d}_{ij} &= \begin{bmatrix} 1 & 0.15 \\ 0.15 & 0.45 \end{bmatrix} \\
\lambda &= 0
\end{aligned}
$$

The boundary conditions are that (see Figure 1)

$$
\begin{aligned}
P &= 0 \text{ on side AB} \\
c &= 0 \text{ on side BC} \\
P &= 0 \text{ on side CD} \\
P &= 1 \text{ on side AD}
\end{aligned}
$$

There is no simple analytical solution for the problem. The results in Figure 15 show that the solutions c at point $(0.5, 0.1)$ coincide with the solutions at $(0.5, 0.9)$ only when the material is isotropic homogeneous. This is to be expected as the system is in fact geometrically symmetric
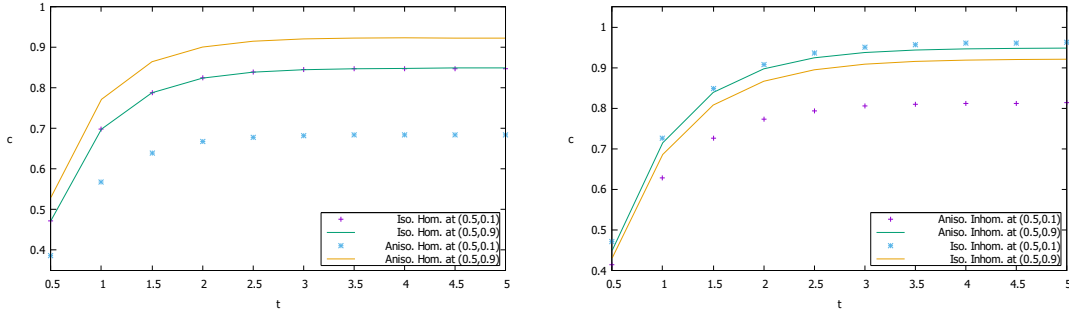
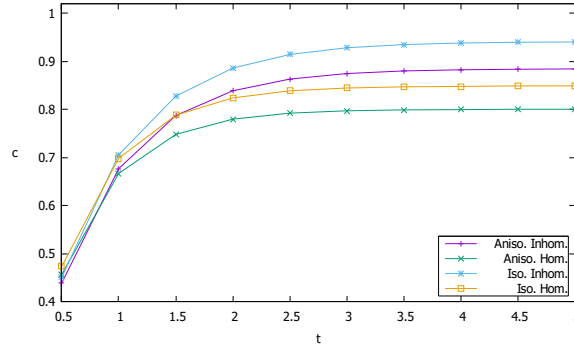Figure 15: Symmetry of solutions c about $x_2 = 0.5$ for Problem 4

Figure 16: Solutions c at $(x_1, x_2) = (0.5, 0.5)$ for Problem 4

about the axis $x_2 = 0.5$ if the material is isotropic homogeneous. Otherwise, if the material is anisotropic or inhomogeneous, the solutions c at point $(0.5, 0.1)$ do not coincide with the solutions at $(0.5, 0.9)$. This indicates that anisotropy and inhomogeneity give impact to the values of solution c for being asymmetric about $x_2 = 0.5$. Furthermore, the results in Figure 16 also indicate the impact of the anisotropy and inhomogeneity of the material. The values of c differ for each type of anisotropy and inhomogeneity.

Problem 5: We consider the inhomogeneous and anisotropic case of Problem 4 again. But we change slightly the set of the boundary conditions of Problem 4 especially on the side AD. Now we use three cases of the boundary condition on the side AD, namely

$$P = 1 - \exp(-1.5t) \text{ on side AD}$$
$$P = 0.2t \text{ on side AD}$$
$$P = t(5 - t)/6.25 \text{ on side AD}$$

The results in Figure 17 are expected. The trends of the solutions c mimics the trends of the exponential function $1 - \exp(-1.5t)$, the linear function $0.2t$ and the quadratic function $t(5 - t)/6.25$ of the boundary condition on side AD. Specifically, for the exponential function $1 - \exp(-1.5t)$, as time t goes to infinity, values of this function go to 1. So for big value of t,
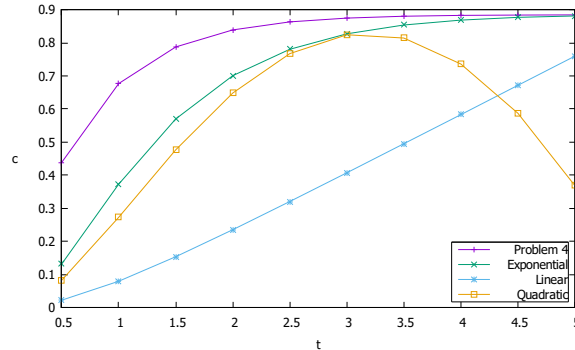
Figure 17: Solutions c at $(x_1, x_2) = (0.5, 0.5)$ for Problem 5

Problem 5 is similar to Problem 4 of the anisotropic inhomogeneous case. And the two plots of solutions c for Problem 4 and Problem 5 in Figure 17 verifies this, they approach a same steady state solution as t gets bigger.

5   Conclusion

A mixed Laplace transform and standard BEM has been used to find numerical solutions to initial boundary value problems for anisotropic functionally graded materials which are governed by the diffusion-convection equation (1.1) of incompressible flow. The method is easy to be implemented and involves a time variable free fundamental solution therefore it gives more accurate solutions. It does not generate round errors as it solves the boundary integral equation (3.18) independently for each specific value of t at which the solution is computed. Unlikely, the methods with time variable fundamental solution may produce less accurate solutions as the fundamental solution sometimes contain time singular points and also solution for the next time step is based on the solution of the previous time step so that the round error may propagate.

The numerical method has been applied to exponentially graded materials. As the coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), \alpha(\mathbf{x})$ do depend on the spatial variable $\mathbf{x}$ only and on the same inhomogeneity or grading function $g(\mathbf{x})$, it will be good to extend the study in the future to the case when the coefficients depend on different grading functions varying also with the time variable t.

In order to use the boundary integral equation (3.18), the values $c(\mathbf{x}, t)$ or $P(\mathbf{x}, t)$ of the boundary conditions as stated in Section (2) of the original system in time variable t have to be Laplace transformed first. This means that from the beginning when we set up a problem, we actually put a set of approximating boundary conditions. Therefore it is really important to find a very accurate technique of numerical Laplace transform inversion.

Acknowledgments

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