# An Integral Equation Method for Unsteady Anisotropic Diffusion Convection Reaction Problems of Exponentially Graded Materials and Incompressible Flow

Moh. Ivan Azis

***Abstract*—The diffusion convection reaction equation with variable coefficients and for anisotropic inhomogeneous media is discussed in this paper to find numerical solutions by using a combined Laplace transform and boundary element method. In this study, the coefficients only depend on the spatial variable. First the variable coefficients equation is transformed to a constant coefficients equation. The constant coefficients equation is then Laplace-transformed so that the time variable vanishes. The Laplace-transformed equation is consequently written in a purely 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, efficient and accurate for solving unsteady problems of anisotropic functionally graded media governed by the diffusion convection equation.**

***Index Terms*—anisotropic functionally graded materials, unsteady diffusion convection reaction equation, Laplace transform, boundary element method.**

## I. Introduction

The unsteady anisotropic diffusion convection reaction (DCR) equation of variable coefficients is written as

$$\frac{\partial}{\partial x_i}\left[d_{ij}(\mathbf{x})\frac{\partial c(\mathbf{x},t)}{\partial x_j}\right]-\frac{\partial}{\partial x_i}\left[v_i(\mathbf{x})\,c(\mathbf{x},t)\right] -k(\mathbf{x})\,c(\mathbf{x},t)=\alpha(\mathbf{x})\frac{\partial c(\mathbf{x},t)}{\partial t} \quad (1)$$

We will consider the case of incompressible flow for which the divergence of the velocity is zero, that is

$$\frac{\partial v_i(\mathbf{x})}{\partial x_i}=0$$

so that equation (1) becomes

$$\frac{\partial}{\partial x_i}\left[d_{ij}(\mathbf{x})\frac{\partial c(\mathbf{x},t)}{\partial x_j}\right]-v_i(\mathbf{x})\frac{\partial c(\mathbf{x},t)}{\partial x_i} -k(\mathbf{x})\,c(\mathbf{x},t)=\alpha(\mathbf{x})\frac{\partial c(\mathbf{x},t)}{\partial t} \quad (2)$$

Referring to the two-dimensional Cartesian coordinate system $Ox_1x_2$ this paper will concern with the unsteady anisotropic DCR equation (2) in which $i,j=1,2$, $\mathbf{x}=(x_1,x_2)$, $d_{ij}$ is the anisotropic diffusion/conduction coefficient, $v_i$ is the velocity, $k$ is the reaction coefficient, $\alpha$ is the rate of change and $c$ 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

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

Heat transfer and mass transport problems are among applications for which DCR equation is taken to be the governing equation. 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 (2).

Functionally graded materials (FGMs) are materials possessing characteristics which vary (with time and position) according to a mathematical function. Therefore equation (2) is relevant for FGMs. FGMs are mainly artificial materials which are produced to meet a preset practical performance (see for example [2], [3]). This constitutes relevancy of solving equation (2).

In the last decade studies on the DCR equation had been done for finding its numerical solutions. The studies can be classified according to the anisotropy and inhomogeneity of the media under consideration. For examples, [4], [5], [6], [7] solved an isotropic-DCR equation with variable velocity, [8], [9] considered a constant coefficients unsteady isotropic-DCR equation with a source term, and again [10] solved an isotropic-DCR equation with a source term. Recently Azis and co-workers had been working on steady state problems of *anisotropic inhomogeneous* media for several types of governing equations, for examples [11]–[13] for the modified Helmholtz equation, [14]–[18] for the diffusion convection equation, [19]–[22] for the Laplace type equation, [23]–[27] for the Helmholtz equation, [28] for elasticity problems.

Equation (2) provides a wider class of problems since it applies for *anisotropic and inhomogeneous* media but nonetheless cover the case of isotropic diffusion that happens when $d_{11}=d_{22}, d_{12}=0$ and also the case of homogeneous

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M. I. Azis is a lecturer at the Department of Mathematics, Hasanuddin University, Makassar, Indonesia. e-mail: ivan@unhas.ac.id

media which occurs when the coefficients $d_{ij}(\mathbf{x})$, $v_i(\mathbf{x})$, $k(\mathbf{x})$ and $\alpha(\mathbf{x})$ are constant.

Not so many works have been done on DCR equation of type (2) for anisotropic media with simultaneously variable diffusivity, velocity and reaction coefficients. This paper is intended to extend the recently published works [29]–[35] on the steady DCR equation to the unsteady DCR equation for anisotropic functionally graded materials.

## II. The initial boundary value problem

Given the coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), k(\mathbf{x}), \alpha(\mathbf{x})$ solutions $c(\mathbf{x},t)$ and its derivatives of (2) are sought which are valid for time interval $t \geq 0$ and 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 $c(\mathbf{x},t)$ is specified, and

$$P(\mathbf{x},t) = d_{ij}(\mathbf{x}) \frac{\partial c(\mathbf{x},t)}{\partial x_i} n_j \tag{3}$$

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

$$c(\mathbf{x},0) = 0 \tag{4}$$

The method of solution will be to transform the variable coefficient equation (2) 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). A Laplace transform inversion is taken to get the solution $c$ and its derivatives for all $(\mathbf{x},t)$ in the domain. The Laplace transform inversion 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 (2) take the form $d_{11} = d_{22}$ and $d_{12} = 0$.

## III. The boundary integral equation

We restrict the coefficients $d_{ij}, v_i, k, \alpha$ to be of the form

$$d_{ij}(\mathbf{x}) = \hat{d}_{ij}\, g(\mathbf{x}) \tag{5}$$
$$v_i(\mathbf{x}) = \hat{v}_i\, g(\mathbf{x}) \tag{6}$$
$$k(\mathbf{x}) = \hat{k}\, g(\mathbf{x}) \tag{7}$$
$$\alpha(\mathbf{x}) = \hat{\alpha}\, g(\mathbf{x}) \tag{8}$$

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

$$g(\mathbf{x}) = [\exp(\beta_0 + \beta_i x_i)]^2 \tag{9}$$

where $\beta_0$ and $\beta_i$ are constants. Therefore if

$$\hat{d}_{ij}\beta_i\beta_j - \lambda = 0 \tag{10}$$

then (9) satisfies

$$\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} - \lambda g^{1/2} = 0 \tag{11}$$

Substitution of (5)-(8) into (2) gives

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left(g\frac{\partial c}{\partial x_j}\right) - \hat{v}_i g\frac{\partial c}{\partial x_i} - \hat{k}gc = \hat{\alpha}g\frac{\partial c}{\partial t} \tag{12}$$

Assume

$$c(\mathbf{x},t) = g^{-1/2}(\mathbf{x})\,\psi(\mathbf{x},t) \tag{13}$$

therefore substitution of (5) and (13) into (3) gives

$$P(\mathbf{x},t) = -P_g(\mathbf{x})\,\psi(\mathbf{x},t) + g^{1/2}(\mathbf{x})\,P_\psi(\mathbf{x},t) \tag{14}$$

where

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

Equation (12) can be written as

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

which can be simplified

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

Use of the identity

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

implies

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

Rearrranging and neglecting the zero terms gives

$$\begin{aligned}&g^{1/2}\left(\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_j}\right)\\ &-\psi\left(\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial g^{1/2}}{\partial x_i}\right)\\ &+\left(\hat{d}_{ij}\frac{\partial\psi}{\partial x_j}\frac{\partial g^{1/2}}{\partial x_i} - \hat{d}_{ij}\frac{\partial\psi}{\partial x_j}\frac{\partial g^{1/2}}{\partial x_i}\right)\\ &-\hat{k}g^{1/2}\psi = \hat{\alpha}g^{1/2}\frac{\partial\psi}{\partial t}\end{aligned} \tag{15}$$

For incompressible flow

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

that is

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

Thus (15) becomes

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

Equation (11) then implies

$$\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j}-\hat{v}_i\frac{\partial\psi}{\partial x_i}-\left(\lambda+\hat{k}\right)\psi=\hat{\alpha}\frac{\partial\psi}{\partial t} \quad (16)$$

Taking a Laplace transform of (13), (14), (16) and applying the initial condition (4) we obtain

$$\psi^*(\mathbf{x},s)=g^{1/2}(\mathbf{x})\,c^*(\mathbf{x},s) \quad (17)$$

$$P_{\psi^*}(\mathbf{x},s)=\left[P^*(\mathbf{x},s)+P_g(\mathbf{x})\,\psi^*(\mathbf{x},s)\right]g^{-1/2}(\mathbf{x}) \quad (18)$$

$$\hat{d}_{ij}\frac{\partial^2\psi^*}{\partial x_i\partial x_j}-\hat{v}_i\frac{\partial\psi^*}{\partial x_i}-\left(\lambda+\hat{k}+s\hat{\alpha}\right)\psi^*=0 \quad (19)$$

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

By using Gauss divergence theorem, equation (19) can be transformed into a boundary integral equation

$$\eta(\boldsymbol{\xi})\ \psi^*(\boldsymbol{\xi},s)=\int_{\partial\Omega}\{P_{\psi^*}(\mathbf{x},s)\ \Phi(\mathbf{x},\boldsymbol{\xi})$$
$$-\left[P_v(\mathbf{x})\ \Phi(\mathbf{x},\boldsymbol{\xi})+\Gamma(\mathbf{x},\boldsymbol{\xi})\right]\psi^*(\mathbf{x},s)\}\,dS(\mathbf{x}) \quad (20)$$

where

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

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

$$\Phi(\mathbf{x},\boldsymbol{\xi}) = \frac{\rho_i}{2\pi D}\exp\left(-\frac{\dot{\mathbf{v}}.\dot{\mathbf{R}}}{2D}\right)K_0\left(\dot{\mu}\dot{R}\right)$$
$$\Gamma(\mathbf{x},\boldsymbol{\xi}) = \hat{d}_{ij}\frac{\partial\Phi(\mathbf{x},\boldsymbol{\xi})}{\partial x_j}n_i$$

where

$$\dot{\mu}=\sqrt{(\dot{v}/2D)^2+\left[\left(\lambda+\hat{k}+s\hat{\alpha}\right)/D\right]}$$
$$D=\left[\hat{d}_{11}+2\hat{d}_{12}\rho_r+\hat{d}_{22}\left(\rho_r^2+\rho_i^2\right)\right]/2$$
$$\dot{\mathbf{R}}=\dot{\mathbf{x}}-\dot{\boldsymbol{\xi}}$$
$$\dot{\mathbf{x}}=(x_1+\rho_r x_2,\rho_i x_2)$$
$$\dot{\boldsymbol{\xi}}=(\xi_1+\rho_r\xi_2,\rho_i\xi_2)$$
$$\dot{\mathbf{v}}=(\hat{v}_1+\rho_r\hat{v}_2,\rho_i\hat{v}_2)$$
$$\dot{R}=\sqrt{(x_1+\rho_r x_2-\xi_1-\rho_r\xi_2)^2+(\rho_i x_2-\rho_i\xi_2)^2}$$
$$\dot{v}=\sqrt{(\hat{v}_1+\rho_r\hat{v}_2)^2+(\rho_i\hat{v}_2)^2}$$

where $\rho_r$ and $\rho_i$ are respectively the real and the positive imaginary parts of the complex root $\rho$ 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 (17) and (18) in (20) yields

$$\eta g^{1/2}c^*=\int_{\partial\Omega}\left\{\left(g^{-1/2}\Phi\right)P^*\right.$$
$$\left.+\left[\left(P_g-P_v g^{1/2}\right)\Phi-g^{1/2}\Gamma\right]c^*\right\}dS \quad (21)$$

TABLE I
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 |

Equation (21) 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 $\Omega$.

Knowing the solutions $c^*(\mathbf{x},s)$ and its derivatives $\partial c^*/\partial x_1$ and $\partial c^*/\partial x_2$ which are obtained from (21), the numerical Laplace transform inversion technique using the Stehfest formula is 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

$$\begin{aligned} c(\mathbf{x},t) &\simeq \frac{\ln 2}{t}\sum_{m=1}^{N}V_m c^*(\mathbf{x},s_m)\\ \frac{\partial c(\mathbf{x},t)}{\partial x_1} &\simeq \frac{\ln 2}{t}\sum_{m=1}^{N}V_m\frac{\partial c^*(\mathbf{x},s_m)}{\partial x_1}\\ \frac{\partial c(\mathbf{x},t)}{\partial x_2} &\simeq \frac{\ln 2}{t}\sum_{m=1}^{N}V_m\frac{\partial c^*(\mathbf{x},s_m)}{\partial x_2}\end{aligned} \quad (22)$$

where

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

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 (I) shows the values of $V_m$ for $N=4,6,8,10$.

## IV. 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 (2) and satisfying the initial condition (4) and some boundary conditions as mentioned in Section II. The characteristics of the system which are represented by the coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), k(\mathbf{x}), \alpha(\mathbf{x})$ in equation (2) are assumed to be of the form (5), (6), (7) and (8) in which $g(\mathbf{x})$ is an exponential function of the form (9). The coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), k(\mathbf{x}), \alpha(\mathbf{x})$ represent respectively the diffusivity or conductivity, the velocity of flow existing in the system, the reaction coefficient and the change rate of the unknown variable $c(\mathbf{x},t)$.

Standard BEM with constant elements is employed to obtain numerical results. And the value of $N$ in (22) for the Stehfest formula is chosen to be $N = 10$. 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 and a specific FORTRAN command is imposed to calculate the elapsed CPU time for obtaining the results as to measure the efficiency of the numerical procedure.

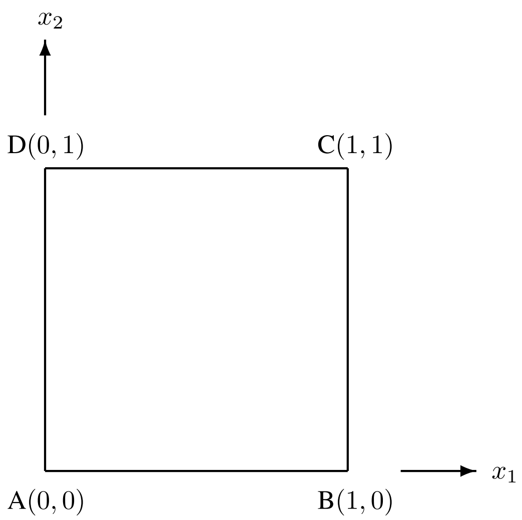


Fig. 1. The domain $\Omega$

### A. Test problems

Another aspect that will be justified os the accuracy of the numerical solutions. The analytical solutions are assumed to take a separable variables form

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

where

$$h(\mathbf{x}) = \exp[-0.4 + 0.1x_1 + 0.3x_2]$$

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

$$g^{1/2}(\mathbf{x}) = \exp(0.1 - 0.2x_1 + 0.1x_2)$$

and depicted in Figure 2.

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

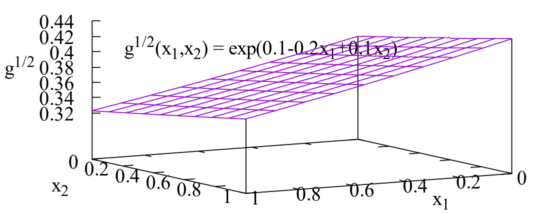


Fig. 2. Function $g(\mathbf{x})$

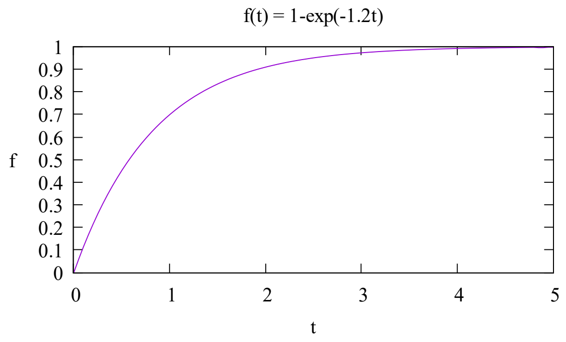


Fig. 3. Function $f(t)$ for Problem 1

$$\begin{aligned} f(t) &= 1 - \exp(-1.2t) \\ f(t) &= 0.2t \\ f(t) &= 0.12t(5 - t) \end{aligned}$$

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

$$\hat{d}_{ij} = \begin{bmatrix} 0.75 & 0.15 \\ 0.15 & 0.25 \end{bmatrix} \quad \hat{v}_i = (0.1, 0.2)$$

so that from (10) we have

$$\lambda = 0.0265$$

We choose

$$\hat{k} = 1 \quad \hat{\alpha} = -1.0575/s$$

and a mutual set of boundary conditions (see Figure 1)

$P$ is given on side AB
$c$ is given on side BC
$P$ is given on side CD
$P$ is given on side AD

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

$$f(t) = 1 - \exp(-1.2t)$$

Function $f(t)$ is depicted in Figure 3. Table II shows the accuracy of the numerical solutions $c$ and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ solutions in the domain for Problem 1. The errors mainly occur in the fourth decimal place for the $c, \partial c/\partial x_1, \partial c/\partial x_2$ solutions. Figure 4 shows that the solution $c$ changes with time $t$ in a similar way the function $f(t) = 1 - \exp(-1.2t)$ does (see Figure 3) and tends to approach a steady state solution as the time goes to infinity, as expected. The elapsed CPU time for the computation of the numerical solutions at $19 \times 19$ spatial positions and 11 time steps from $t = 0.0005$ to $t = 5$ is 7777.546875 seconds.

*Problem 2::* Next, we suppose that the time variation function is (see Figure 5)

$$f(t) = 0.2t$$

Table III shows the accuracy of the numerical solutions $c$ and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ solutions in the domain for Problem 2. The errors mainly occur in the fourth decimal place for the $c, \partial c/\partial x_1, \partial c/\partial x_2$ solutions. Figure 6 shows that the solution $c$ changes with time $t$ in a manner

TABLE II
COMPARISON OF THE NUMERICAL (NUM) AND THE ANALYTICAL (ANAL) SOLUTIONS AT $(x_1, x_2) = (0.5, 0.5)$ FOR PROBLEM 1

| $t$ | $c$ | | $\frac{\partial c}{\partial x_1}$ | | $\frac{\partial c}{\partial x_2}$ | |
|---|---|---|---|---|---|---|
| | Num | Anal | Num | Anal | Num | Anal |
| 0.0005 | 0.0005 | 0.0005 | 0.0001 | 0.0001 | 0.0001 | 0.0001 |
| 0.5 | 0.3514 | 0.3514 | 0.1054 | 0.1054 | 0.0703 | 0.0703 |
| 1.0 | 0.5443 | 0.5442 | 0.1632 | 0.1633 | 0.1089 | 0.1088 |
| 1.5 | 0.6500 | 0.6501 | 0.1949 | 0.1950 | 0.1300 | 0.1300 |
| 2.0 | 0.7079 | 0.7081 | 0.2123 | 0.2124 | 0.1416 | 0.1416 |
| 2.5 | 0.7397 | 0.7400 | 0.2218 | 0.2220 | 0.1480 | 0.1480 |
| 3.0 | 0.7574 | 0.7575 | 0.2271 | 0.2273 | 0.1515 | 0.1515 |
| 3.5 | 0.7672 | 0.7671 | 0.2301 | 0.2301 | 0.1534 | 0.1534 |
| 4.0 | 0.7726 | 0.7724 | 0.2317 | 0.2317 | 0.1545 | 0.1545 |
| 4.5 | 0.7757 | 0.7753 | 0.2326 | 0.2326 | 0.1551 | 0.1551 |
| 5.0 | 0.7773 | 0.7769 | 0.2331 | 0.2331 | 0.1555 | 0.1554 |

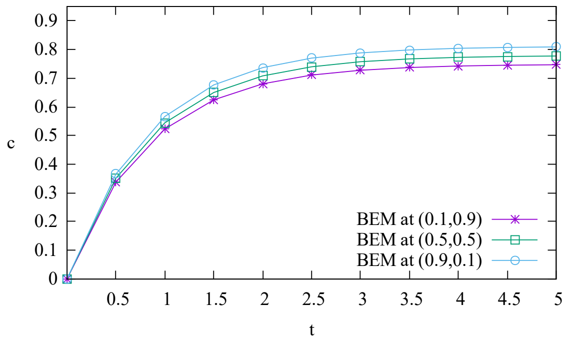


Fig. 4. Solutions $c$ for Problem 1

which is almost similar to as the function $f(t) = 0.2t$ does (see Figure 5), as expected. The elapsed CPU time for the computation of the numerical solutions at $19 \times 19$ spatial positions and 11 time steps from $t = 0.0005$ to $t = 5$ is 7777.21875 seconds.

*Problem 3::* Now, we suppose that the time variation function is (see Figure 7)

$$f(t) = 0.12t(5 - t)$$

Table IV shows the accuracy of the numerical solutions $c$ and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ solutions in the domain for Problem 3. The errors mainly occur in the fourth decimal place for the $c, \partial c/\partial x_1, \partial c/\partial x_2$ solutions. Figure 8 shows that the solution $c$ changes with time $t$ in a similar way the function $f(t) = 0.12t(5 - t)$ does. The elapsed CPU time for the computation of the numerical solutions at $19 \times 19$ spatial positions and 11 time steps from $t = 0.0005$ to $t = 5$ is 7779.53125 seconds.

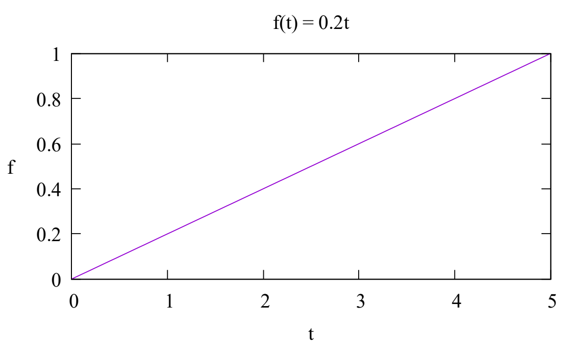


Fig. 5. Function $f(t)$ for Problem 2

TABLE III
COMPARISON OF THE NUMERICAL (NUM) AND THE ANALYTICAL (ANAL) SOLUTIONS AT $(x_1, x_2) = (0.5, 0.5)$ FOR PROBLEM 2

| $t$ | $c$ | | $\frac{\partial c}{\partial x_1}$ | | $\frac{\partial c}{\partial x_2}$ | |
|---|---|---|---|---|---|---|
| | Num | Anal | Num | Anal | Num | Anal |
| 0.0005 | 0.0001 | 0.0001 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 0.5 | 0.0779 | 0.0779 | 0.0234 | 0.0234 | 0.0156 | 0.0156 |
| 1.0 | 0.1558 | 0.1558 | 0.0467 | 0.0467 | 0.0312 | 0.0312 |
| 1.5 | 0.2337 | 0.2336 | 0.0701 | 0.0701 | 0.0467 | 0.0467 |
| 2.0 | 0.3116 | 0.3115 | 0.0934 | 0.0935 | 0.0623 | 0.0623 |
| 2.5 | 0.3895 | 0.3894 | 0.1168 | 0.1168 | 0.0779 | 0.0779 |
| 3.0 | 0.4673 | 0.4673 | 0.1402 | 0.1402 | 0.0935 | 0.0935 |
| 3.5 | 0.5452 | 0.5452 | 0.1635 | 0.1635 | 0.1091 | 0.1090 |
| 4.0 | 0.6231 | 0.6230 | 0.1869 | 0.1869 | 0.1246 | 0.1246 |
| 4.5 | 0.7010 | 0.7009 | 0.2102 | 0.2103 | 0.1402 | 0.1402 |
| 5.0 | 0.7789 | 0.7788 | 0.2336 | 0.2336 | 0.1558 | 0.1558 |

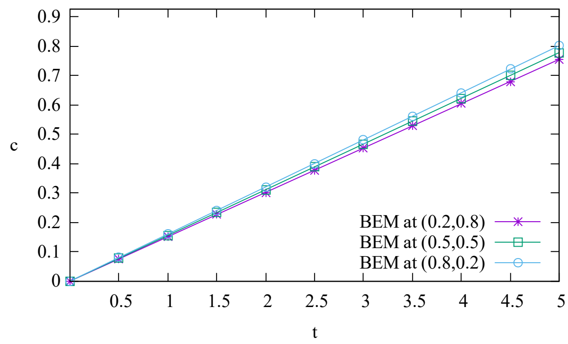


Fig. 6. Solutions $c$ for Problem 2

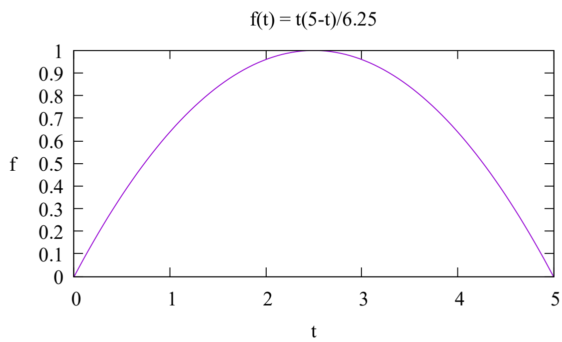


Fig. 7. Function $f(t)$ for Problem 3

TABLE IV
COMPARISON OF THE NUMERICAL (NUM) AND THE ANALYTICAL (ANAL) SOLUTIONS AT $(x_1, x_2) = (0.5, 0.5)$ FOR PROBLEM 3

| $t$ | $c$ | | $\frac{\partial c}{\partial x_1}$ | | $\frac{\partial c}{\partial x_2}$ | |
|---|---|---|---|---|---|---|
| | Num | Anal | Num | Anal | Num | Anal |
| 0.0005 | 0.0002 | 0.0002 | 0.0001 | 0.0001 | 0.0000 | 0.0000 |
| 0.5 | 0.2103 | 0.2103 | 0.0631 | 0.0631 | 0.0421 | 0.0421 |
| 1.0 | 0.3739 | 0.3738 | 0.1121 | 0.1121 | 0.0748 | 0.0748 |
| 1.5 | 0.4907 | 0.4906 | 0.1472 | 0.1472 | 0.0981 | 0.0981 |
| 2.0 | 0.5608 | 0.5607 | 0.1682 | 0.1682 | 0.1122 | 0.1121 |
| 2.5 | 0.5842 | 0.5841 | 0.1752 | 0.1752 | 0.1169 | 0.1168 |
| 3.0 | 0.5609 | 0.5607 | 0.1682 | 0.1682 | 0.1122 | 0.1121 |
| 3.5 | 0.4908 | 0.4906 | 0.1472 | 0.1472 | 0.0982 | 0.0981 |
| 4.0 | 0.3740 | 0.3738 | 0.1122 | 0.1121 | 0.0748 | 0.0748 |
| 4.5 | 0.2105 | 0.2103 | 0.0631 | 0.0631 | 0.0421 | 0.0421 |
| 5.0 | 0.0002 | 0.0000 | 0.0001 | 0.0000 | 0.0000 | 0.0000 |

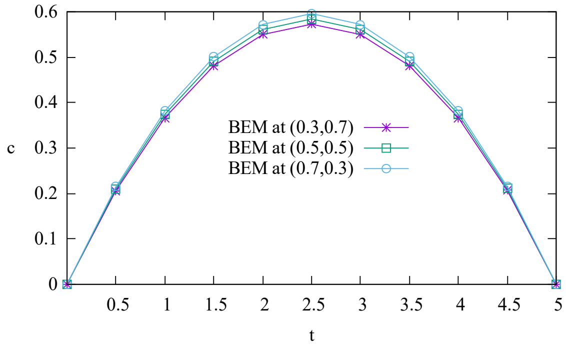


Fig. 8. Solutions $c$ for Problem 3

### B. Examples without analytical solutions

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

$$\hat{v}_i = (0.1, 0.2) \quad \hat{k} = 1 \quad \hat{\alpha} = 1$$

*Problem 4::* For this problem the medium is supposed to be inhomogeneous or homogeneous, anisotropic or isotropic with gradation function $g(\mathbf{x})$, constant coefficients $\hat{d}_{ij}$ and corresponding $\lambda$ satisfying (10) and (11) as respectively follows:

- inhomogeneous and anisotropic case

$$\begin{aligned} g^{1/2}(\mathbf{x}) &= \exp(0.1 - 0.2x_1 + 0.1x_2) \\ \hat{d}_{ij} &= \begin{bmatrix} 0.75 & 0.15 \\ 0.15 & 0.25 \end{bmatrix} \\ \lambda &= 0.0265 \end{aligned}$$

- inhomogeneous and isotropic case

$$\begin{aligned} g^{1/2}(\mathbf{x}) &= \exp(0.1 - 0.2x_1 + 0.1x_2) \\ \hat{d}_{ij} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ \lambda &= 0.05 \end{aligned}$$

- 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

$$\begin{aligned} g^{1/2}(\mathbf{x}) &= 1 \\ \hat{d}_{ij} &= \begin{bmatrix} 0.75 & 0.15 \\ 0.15 & 0.25 \end{bmatrix} \\ \lambda &= 0 \end{aligned}$$

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. In fact the system is geometrically symmetric about the axis $x_2 = 0.5$. And this had been justified by the results in Figure 9 in which it is observed that anisotropy and inhomogeneity give impact to the values of solution $c$ for being asymmetric about $x_2 = 0.5$. Solutions are symmetric only for homogeneous isotropic case, as expected. As also expected, the results (see Figure 10) show that inhomogeneity and anisotropy effects the values of solution $c$. Moreover, for all cases the results in Figure 10 indicate that the system has a steady state solution.

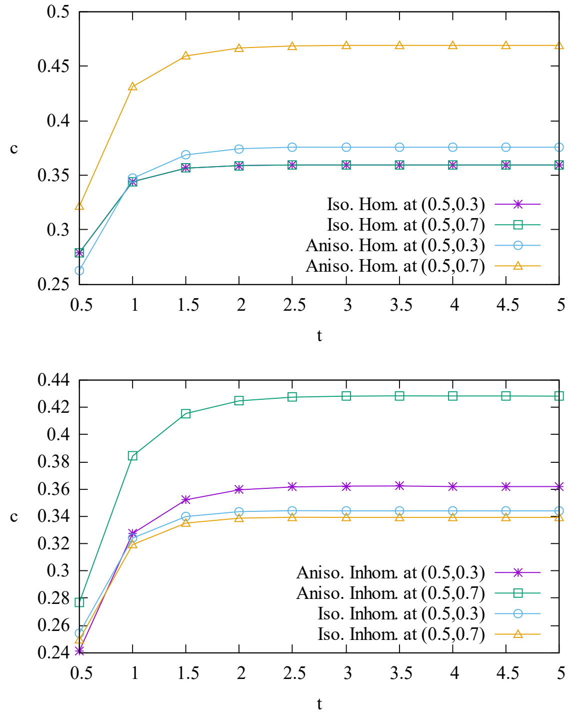


Fig. 9. Symmetry of solutions $c$ about $x_2 = 0.5$ for Problem 4

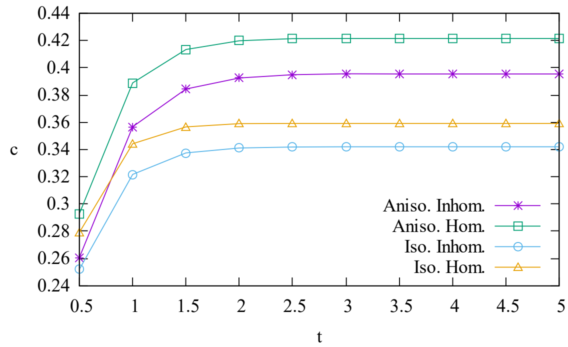


Fig. 10. Solutions $c$ at $(x_1, x_2) = (0.5, 0.5)$ for Problem 4

After all, the results suggest to take both aspects of inhomogeneity and anisotropy into account when doing an experimental study.

*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

$$\begin{aligned} &P = 1 - \exp(-1.2t) \text{ on side AD} \\ &P = 0.2t \text{ on side AD} \\ &P = 0.12t\,(5 - t) \text{ on side AD} \end{aligned}$$

The results in Figure 11 are expected. The trends of the solutions $c$ mimics the trends of the exponential function

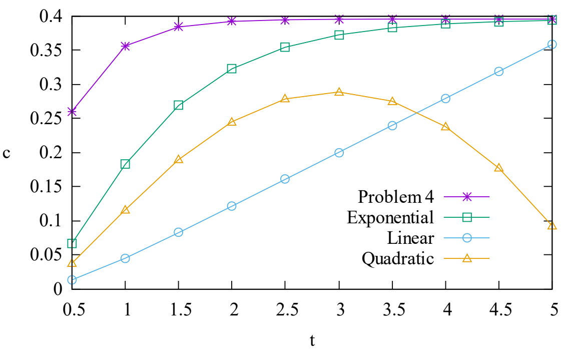


Fig. 11. Solutions $c$ at $(x_1, x_2) = (0.5, 0.5)$ for Problem 5

$1 - \exp(-1.2t)$, the linear function $0.2t$ and the quadratic function $0.12t\,(5 - t)$ of the boundary condition on side AD. Specifically, for the exponential function $1 - \exp(-1.2t)$, as time $t$ goes to infinity, values of this function go to 1. So for big value of $t$, 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 11 verifies this, they approach a same steady state solution as $t$ gets bigger.

## V. 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). It involves a time variable free fundamental solution and therefore that is why it would be more accurate. It is easy and accurate and does not involve round error propagation as it solves the boundary integral equation (21) 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 $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), k(\mathbf{x}), \alpha(\mathbf{x})$ do depend on the spatial variable $\mathbf{x}$ only and on the same inhomogeneity or gradation function $g(\mathbf{x})$, it will be good to extend the study in the future to the case when the coefficients depend on different gradation functions varying also with the time variable $t$.

In order to use the boundary integral equation (21), the values $c(\mathbf{x}, t)$ or $P(\mathbf{x}, t)$ of the boundary conditions as stated in Section (II) 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.

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