# Numerical Solution for Unsteady Anisotropic Diffusion-Convection-Reaction Equation of Exponentially Varying Coefficients and Compressible Flow

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***Abstract*—The unsteady diffusion-convection-reaction equation with exponentially varying coefficients and for anisotropic inhomogeneous media is discussed in this paper. Numerical solutions to problems which are governed by the equation are sought by using a combined Laplace transform and boundary element method. The variable coefficients equation is transformed to a constant coefficients equation. The constant coefficients equation after being Laplace transformed is then written in a boundary integral equation involving a time-free fundamental solution. The boundary-only integral equation is therefore employed to find the 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. Some problems of anisotropic exponentially graded media are considered. The results show that the combined Laplace transform and boundary element method is easy to implement and accurate.**

***Index Terms*—variable coefficients, anisotropic exponentially graded materials, unsteady diffusion-convection-reaction equation, Laplace transform, boundary element method**

## I. Introduction

Referred to the two-dimensional Cartesian coordinate system $Ox_1x_2$ this paper will concern with the unsteady anisotropic diffusion-convection-reaction (DCR) equation of variable coefficients of the form

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

where $i,j=1,2$, $\mathbf{x}=(x_1,x_2)$, $d_{ij}$ is the anisotropic diffusion/conduction coefficient, $v_i$ is the flow 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 $d_{11}d_{22}-d_{12}^2>0$. We assume that the flow is compressible so that

$$\frac{\partial v_i\left(\mathbf{x}\right)}{\partial x_i}\neq 0$$

For the repeated indices in equation (1) summation convention applies so that equation (1) can be written explicitly as

$$\frac{\partial}{\partial x_1}\left(d_{11}\frac{\partial c}{\partial x_1}\right)+\frac{\partial}{\partial x_1}\left(d_{12}\frac{\partial c}{\partial x_2}\right)+\frac{\partial}{\partial x_2}\left(d_{12}\frac{\partial c}{\partial x_1}\right)$$
$$+\frac{\partial}{\partial x_2}\left(d_{22}\frac{\partial c}{\partial x_2}\right)-\frac{\partial\left(v_1c\right)}{\partial x_1}-\frac{\partial\left(v_2c\right)}{\partial x_2}-kc=\alpha\frac{\partial c}{\partial t}$$

Also, in equation (1) the coefficients $d_{ij}$, $v_i$, $k$ and $\alpha$ vary exponentially with the spatial variable, therefore equation (1) may be applied for problems of exponentially graded materials.

Recently, functionally graded materials (FGMs) have become an important topic, and numerous studies on them for a variety of applications have been reported. FGMs are materials possessing characteristics which vary (with time and position) according to a mathematical function. Therefore equation (1) is relevant for FGMs. FGMs are mainly artificial materials which are produced to meet a preset practical performance (see for example [1], [2]). This constitutes relevancy of solving equation (1).

Heat transfer and mass transport problems are among applications for which DCR equation is usually taken to be the governing equation. According to Ravnik and Škerget [3], 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 modeling with turbulent viscosity hypothesis, the diffusivity also change in the domain. This situation draws a relevancy of the DCR equation (1).

A number of studies on the DC or DCR equation had been done for finding its numerical solutions. The studies can be classified according to the anisotropy of the media and the variability of coefficients (inhomogeneity of the media). For examples, [4]–[7] considered a *constant coefficients* (homogeneous media) isotropic equation, [3], [8]–[12] solved an isotropic equation with *variable coefficients* (inhomogeneous media). In general the works on the variable coefficient equation considered the case where the coefficients take the form of constant-plus-variable terms.

Recently Azis and co-workers had been working on *steady state* problems of *inhomogeneous* media for several types of *anisotropic* equations such as the modified Helmholtz equation (see for example [13], [14]), the diffusion convection equation (see for example [15]–[19]), the Laplace type equation (see for example [20]–[23]), the Helmholtz equation (see for example [24]–[28]) and the DCR equation (see for example [29]–[35]). The works considered the case of other classes of coefficients which are different from the class of

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the constant-plus-variable coefficients. Some other classes of inhomogeneity functions for FGMs that differ from the class of constant-plus-variable coefficients are reported from these papers. Azis et al. also had been working on *unsteady state* problems of *anisotropic inhomogeneous* media for several types of governing equations (see for example [36]–[40]).

The present work is intended to extend the recently published papers [29]–[35] on the steady DCR equation to the unsteady DCR equation for anisotropic exponentially graded materials. Equation (1) 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 media which occurs when the coefficients $d_{ij}(\mathbf{x})$, $v_i(\mathbf{x})$, $k(\mathbf{x})$ and $\alpha(\mathbf{x})$ are constant.

## II. Statement of the 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 to (1) are sought. The solutions are assumed to be valid for the 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 the flux

$$P(\mathbf{x}, t) = d_{ij}(\mathbf{x}) \frac{\partial c(\mathbf{x}, t)}{\partial x_i} n_j \tag{2}$$

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

$$c(\mathbf{x}, 0) = 0 \tag{3}$$

## III. The boundary integral equation

The method of solution will be to transform the variable coefficient equation (1) to a constant coefficient equation. A Laplace transform is then applied to the constant coefficient equation, followed by deriving 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 taken to obtain the solution $c$ and its derivatives for all $(\mathbf{x}, t)$ in the domain. 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) 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.

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

$$d_{ij}(\mathbf{x}) = \hat{d}_{ij}\, g(\mathbf{x}) \tag{4}$$

$$v_i(\mathbf{x}) = \hat{v}_i\, g(\mathbf{x}) \tag{5}$$

$$k(\mathbf{x}) = \hat{k}\, g(\mathbf{x}) \tag{6}$$

$$\alpha(\mathbf{x}) = \hat{\alpha}\, g(\mathbf{x}) \tag{7}$$

where $\hat{d}_{ij}, \hat{v}_i, \hat{k}, \hat{\alpha}$ 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

$$g(\mathbf{x}) = \left[\exp(\beta_0 + \beta_i x_i)\right]^2 \tag{8}$$

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

$$\hat{d}_{ij}\beta_i\beta_j + \hat{v}_i\beta_i - \lambda = 0 \tag{9}$$

then (8) satisfies

$$\hat{d}_{ij} \frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} + \hat{v}_i \frac{\partial g^{1/2}}{\partial x_i} - \lambda g^{1/2} = 0 \tag{10}$$

Substitution of (4)-(7) into (1) gives

$$\hat{d}_{ij} \frac{\partial}{\partial x_i}\left(g \frac{\partial c}{\partial x_j}\right) - \hat{v}_i \frac{\partial (gc)}{\partial x_i} - \hat{k} g c = \hat{\alpha} g \frac{\partial c}{\partial t} \tag{11}$$

Assume

$$c(\mathbf{x}, t) = g^{-1/2}(\mathbf{x})\, \psi(\mathbf{x}, t) \tag{12}$$

therefore substitution of (4) and (12) into (2) gives

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

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 (11) can be written as

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

which can be simplified

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

Use of the identity

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

implies

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

Rearranging and neglecting the zero terms yield

$$g^{1/2}\left(\hat{d}_{ij} \frac{\partial^2 \psi}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \psi}{\partial x_j}\right)$$
$$-\psi\left(\hat{d}_{ij} \frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} + \hat{v}_i \frac{\partial g^{1/2}}{\partial x_i}\right)$$
$$+\left(\hat{d}_{ij} \frac{\partial \psi}{\partial x_j} \frac{\partial g^{1/2}}{\partial x_i} - \hat{d}_{ij} \frac{\partial \psi}{\partial x_j} \frac{\partial g^{1/2}}{\partial x_i}\right)$$
$$-\hat{k} g^{1/2}\psi = \hat{\alpha} g^{1/2} \frac{\partial \psi}{\partial t} \tag{14}$$

Equation (10) then implies

$$\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_i} - \left(\lambda + \hat{k}\right)\psi = \hat{\alpha}\frac{\partial\psi}{\partial t} \quad (15)$$

Taking a Laplace transform of (12), (13), (15) and applying the initial condition (3) we obtain

$$\psi^*(\mathbf{x}, s) = g^{1/2}(\mathbf{x})\, c^*(\mathbf{x}, s) \quad (16)$$

$$P_{\psi^*}(\mathbf{x}, s) = \left[P^*(\mathbf{x}, s) + P_g(\mathbf{x})\,\psi^*(\mathbf{x}, s)\right] g^{-1/2}(\mathbf{x}) \quad (17)$$

$$\hat{d}_{ij}\frac{\partial^2\psi^*}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi^*}{\partial x_i} - \left(\lambda + \hat{k} + s\hat{\alpha}\right)\psi^* = 0 \quad (18)$$

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

By using Gauss divergence theorem, equation (18) can be transformed into a boundary integral equation

$$\begin{aligned}\eta(\boldsymbol{\xi})\,\psi^*(\boldsymbol{\xi}, s) = &\int_{\partial\Omega}\{P_{\psi^*}(\mathbf{x}, s)\,\Phi(\mathbf{x}, \boldsymbol{\xi}) \\ &- [P_v(\mathbf{x})\,\Phi(\mathbf{x}, \boldsymbol{\xi}) \\ &+\Gamma(\mathbf{x}, \boldsymbol{\xi})]\,\psi^*(\mathbf{x}, s)\}\, dS(\mathbf{x})\end{aligned} \quad (19)$$

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

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

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 (16) and (17) in (19) yields

$$\begin{aligned}\eta g^{1/2} c^* = &\int_{\partial\Omega}\left\{\left(g^{-1/2}\Phi\right) P^*\right. \\ &+\left.\left[\left(P_g - P_v g^{1/2}\right)\Phi - g^{1/2}\Gamma\right] c^*\right\} dS\end{aligned} \quad (20)$$

Equation (20) 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 $\Omega$.

TABLE I
VALUES OF $V_m$ OF THE STEHFEST FORMULA

| $V_m$ | $N=6$ | $N=8$ | $N=10$ | $N=12$ |
|---|---|---|---|---|
| $V_1$ | 1 | −1/3 | 1/12 | −1/60 |
| $V_2$ | −49 | 145/3 | −385/12 | 961/60 |
| $V_3$ | 366 | −906 | 1279 | −1247 |
| $V_4$ | −858 | 16394/3 | −46871/3 | 82663/3 |
| $V_5$ | 810 | −43130/3 | 505465/6 | −1579685/6 |
| $V_6$ | −270 | 18730 | −236957.5 | 1324138.7 |
| $V_7$ | | −35840/3 | 1127735/3 | −58375583/15 |
| $V_8$ | | 8960/3 | −1020215/3 | 21159859/3 |
| $V_9$ | | | 164062.5 | −8005336.5 |
| $V_{10}$ | | | −32812.5 | 5552830.5 |
| $V_{11}$ | | | | −2155507.2 |
| $V_{12}$ | | | | 359251.2 |

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 (20), 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

$$\begin{aligned}c(\mathbf{x}, t) &\simeq \frac{\ln 2}{t}\sum_{m=1}^{N} V_m c^*(\mathbf{x}, s_m) \\ \frac{\partial c(\mathbf{x}, t)}{\partial x_1} &\simeq \frac{\ln 2}{t}\sum_{m=1}^{N} V_m\frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_1} \\ \frac{\partial c(\mathbf{x}, t)}{\partial x_2} &\simeq \frac{\ln 2}{t}\sum_{m=1}^{N} V_m\frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_2}\end{aligned} \quad (21)$$

where

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

A simple script is developed to calculate the values of the coefficients $V_m, m = 1, 2, \ldots, N$ for any even number $N$. Table (I) shows the values of $V_m$ for several values of $N$.

## IV. NUMERICAL RESULTS

In order to verify 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) and satisfying the initial condition (3) 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 (1) are assumed to be of the form (4), (5), (6) and (7) in which $g(\mathbf{x})$ is an exponential function of the form (8). The coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), k(\mathbf{x}), \alpha(\mathbf{x})$ represents 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. 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.

We try to use $N = 6, 8, 10, 12$ for the Stehfest formula and find out the convergence of the error when $N$ changes from $N = 6$ to $N = 10$ and $N = 10$ is the best value of $N$ that makes the error stable and optimized. Increasing $N$ from $N = 10$ to $N = 12$ gives worse results. According to Hassanzadeh and Pooladi-Darvish [41] these worse results are induced by round-off errors. This justifies to choose $N = 10$ in (20) for the Stehfest formula.

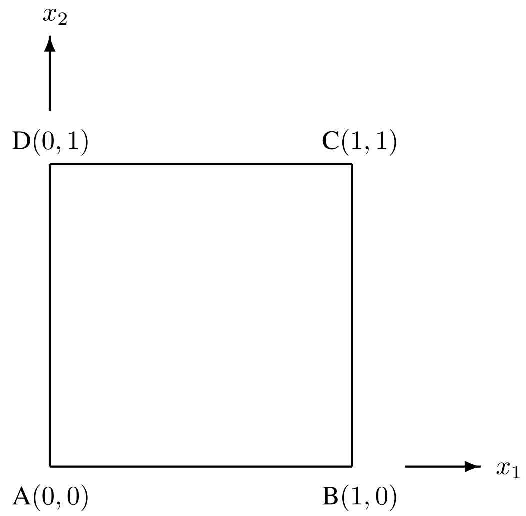


Fig. 1. The domain Ω

### A. *Test problems*

Other aspects that will be verified are the accuracy and consistency (between the scattering and flow) 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

$$h(\mathbf{x}) = \exp\left[-0.75 + 0.25x_1 + 0.5x_2\right]$$

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

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

and depicted in Figure 2.
We will consider three forms of time variation functions $f(t)$ of time domain $t = [0 : 5]$ which are

$$\begin{aligned} f(t) &= 1 - \exp(-1.8t) \\ f(t) &= 0.2t \\ f(t) &= 0.12t(5 - t) \end{aligned}$$

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

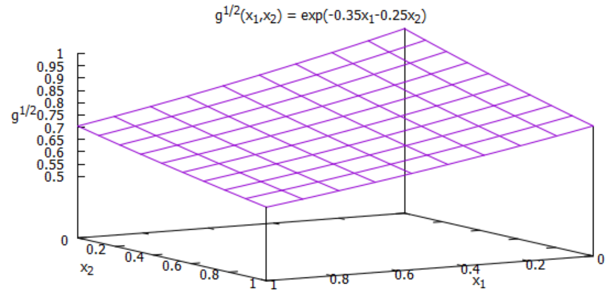


Fig. 2. Function $g(\mathbf{x})$

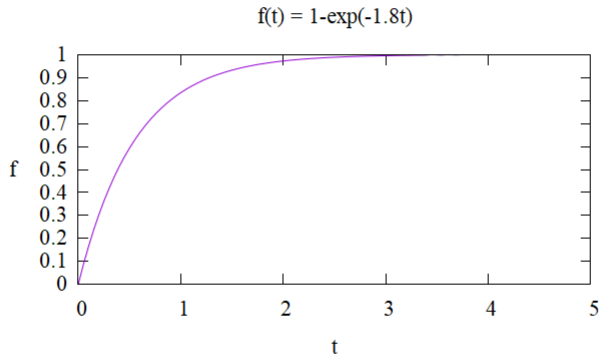


Fig. 3. Function $f(t)$ for Problem 1

$$\hat{d}_{ij} = \begin{bmatrix} 0.75 & 0.35 \\ 0.35 & 1 \end{bmatrix} \quad \hat{v}_i = (0.15, 0.25)$$

so that from (9) we have

$$\lambda = 0.100625$$

We choose

$$\hat{k} = 1 \quad \hat{\alpha} = -0.87875/s$$

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

$$f(t) = 1 - \exp(-1.8t)$$

Function $f(t)$ is depicted in Figure 3. Figure 4 shows 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 $f(t) = 1 - \exp(-1.8t)$ 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.

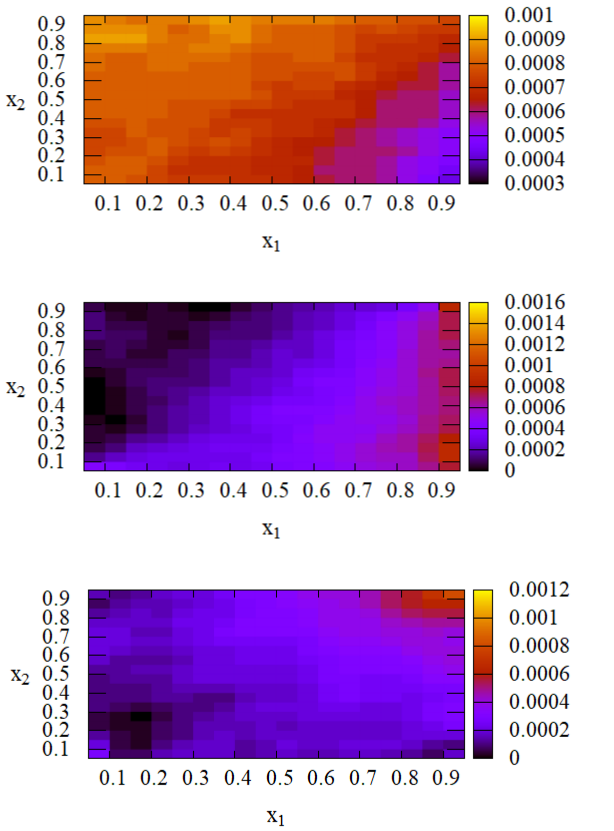


Fig. 4. The errors of solutions $c$ (top), $\partial c/\partial x_1$ (center), $\partial c/\partial x_2$ (bottom) at $t = 5$ for Problem 1

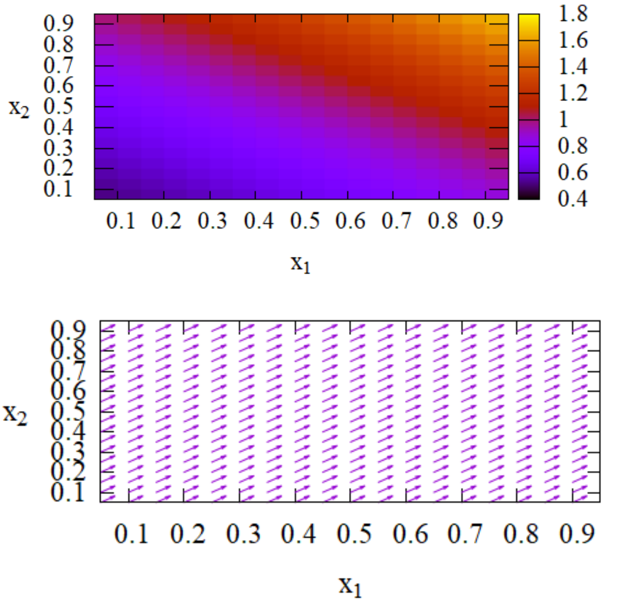


Fig. 5. Solutions $c$ and $(\partial c/\partial x_1, \partial c/\partial x_2)$ at $t = 5$ for Problem 1

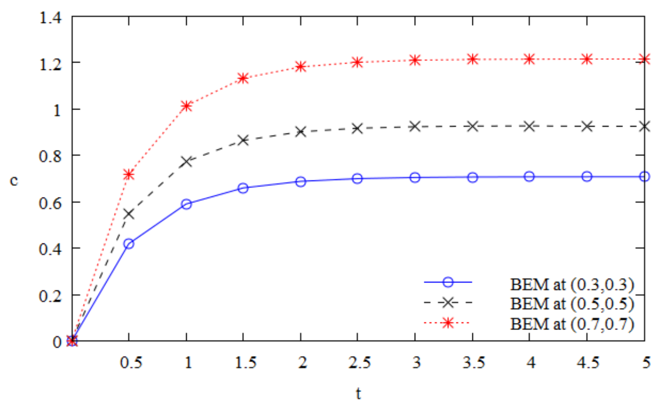


Fig. 6. Solutions $c$ for Problem 1

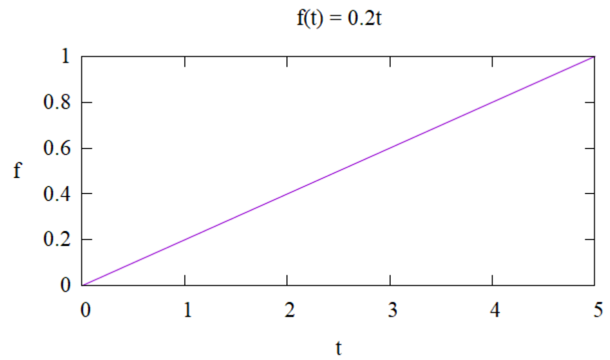


Fig. 7. Function $f(t)$ for Problem 2

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

$$f(t) = 0.2t$$

Figure 8 shows 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. 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 11)

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

Figure 12 shows 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 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 $f(t) = 0.12t(5 - t)$ 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.

### B. *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

$$\hat{v}_i = (0.15, 0.25) \quad \hat{k} = 1 \quad \hat{\alpha} = 1$$

*Problem 4:* For this problem the medium is supposed to be inhomogeneous or homogeneous, anisotropic or isotropic with a gradation function $g(\mathbf{x})$, constant coefficients $\hat{d}_{ij}$ and corresponding $\lambda$ satisfying (9) and (10) as respectively follows:

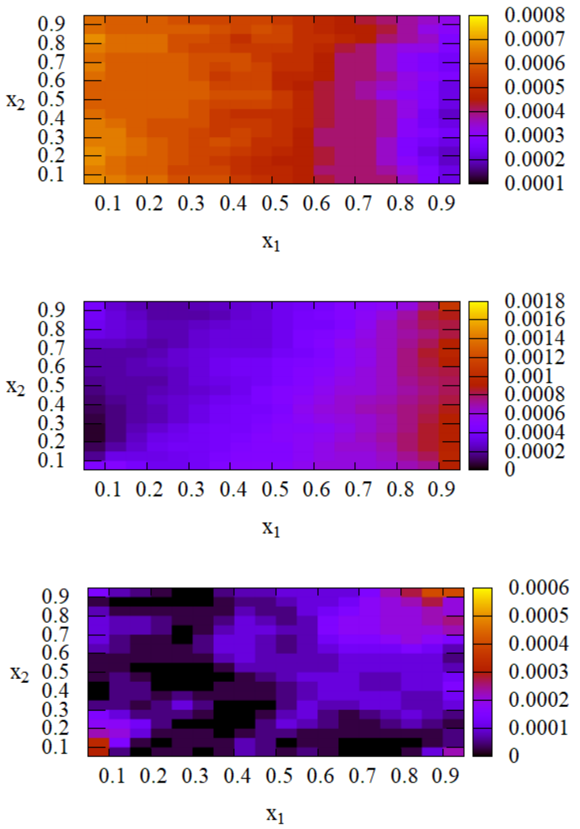

Fig. 8. The errors of solutions $c$ (top), $\partial c/\partial x_1$ (center), $\partial c/\partial x_2$ (bottom) at $t = 5$ for Problem 2

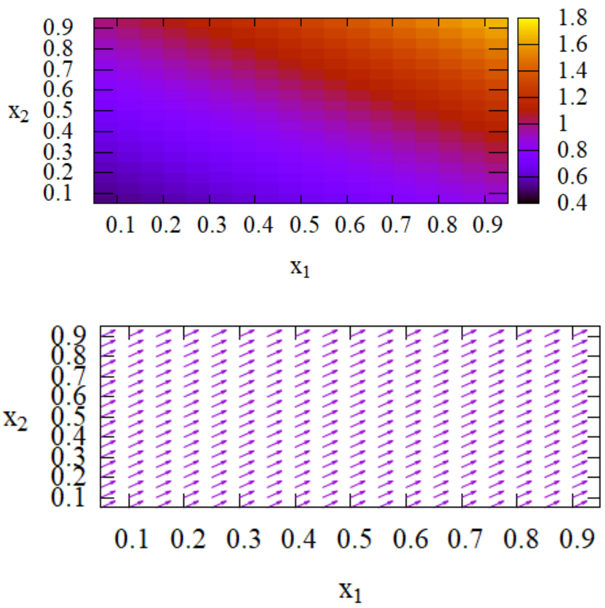

Fig. 9. Solutions $c$ and $(\partial c/\partial x_1, \partial c/\partial x_2)$ at $t = 5$ for Problem 2

- inhomogeneous and anisotropic case

$$
\begin{aligned}
g^{1/2}(\mathbf{x}) &= \exp\left(-0.35x_1 - 0.25x_2\right) \\
\hat{d}_{ij} &= \begin{bmatrix} 0.75 & 0.35 \\ 0.35 & 1 \end{bmatrix} \\
\lambda &= 0.100625
\end{aligned}
$$

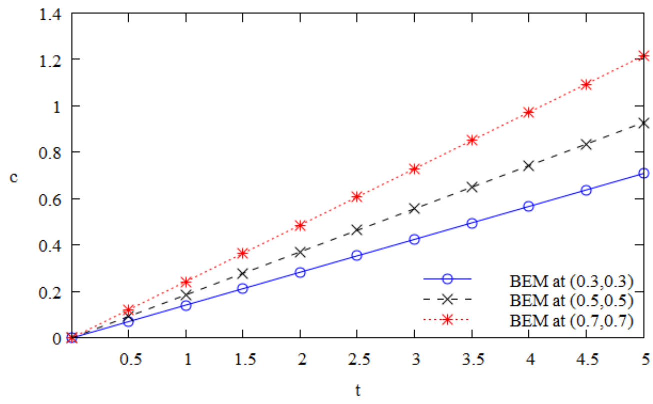


Fig. 10. Solutions $c$ for Problem 2

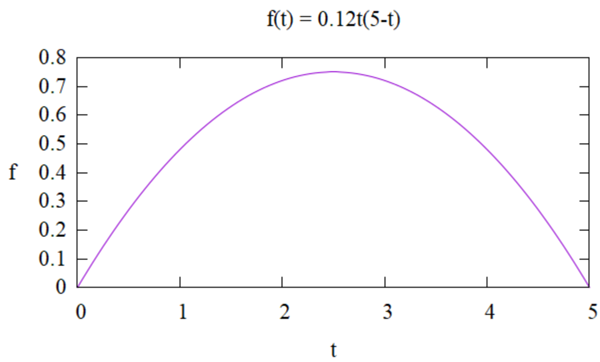


Fig. 11. Function $f(t)$ for Problem 3

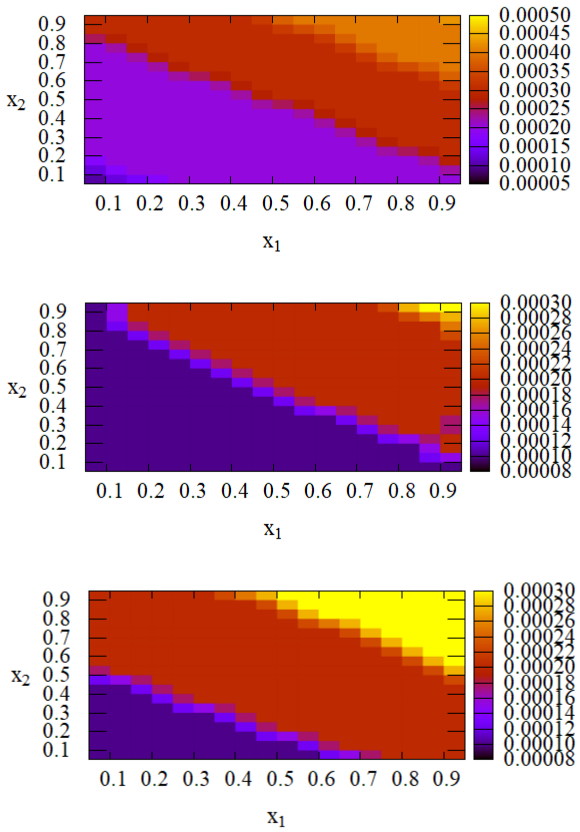

Fig. 12. The errors of solutions $c$ (top), $\partial c/\partial x_1$ (center), $\partial c/\partial x_2$ (bottom) at $t = 5$ for Problem 3

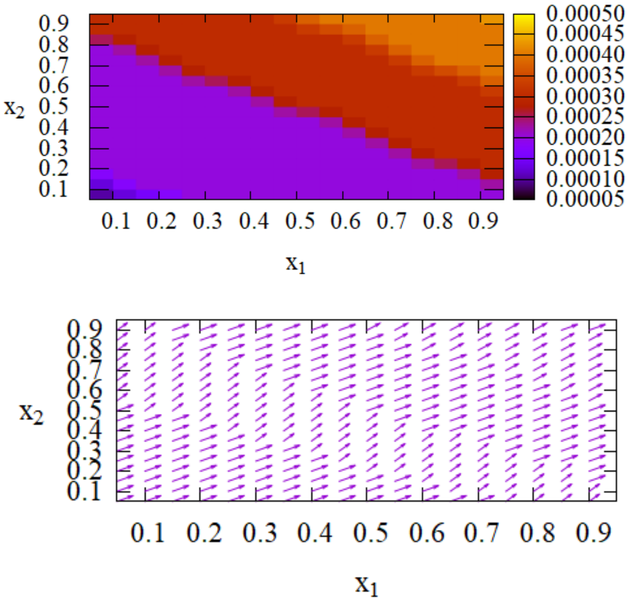


Fig. 13. Solutions $c$ and $(\partial c/\partial x_1, \partial c/\partial x_2)$ at $t = 5$ for Problem 3

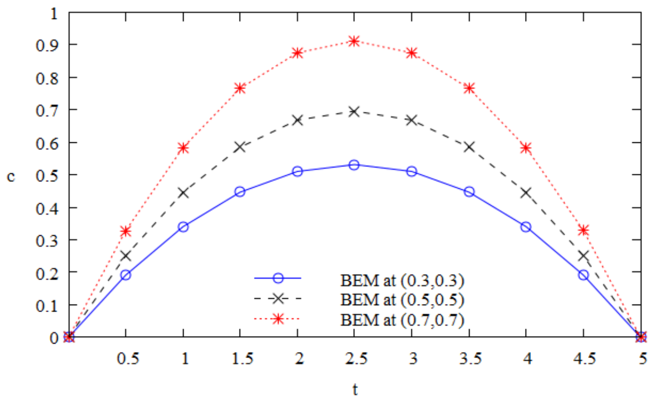


Fig. 14. Solutions $c$ for Problem 3

- inhomogeneous and isotropic case

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

- 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

$$\begin{aligned} g^{1/2}(\mathbf{x}) &= 1 \\ \hat{d}_{ij} &= \begin{bmatrix} 0.75 & 0.35 \\ 0.35 & 1 \end{bmatrix} \\ \lambda &= 0 \end{aligned}$$

The boundary conditions are that (see Figure 1)

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

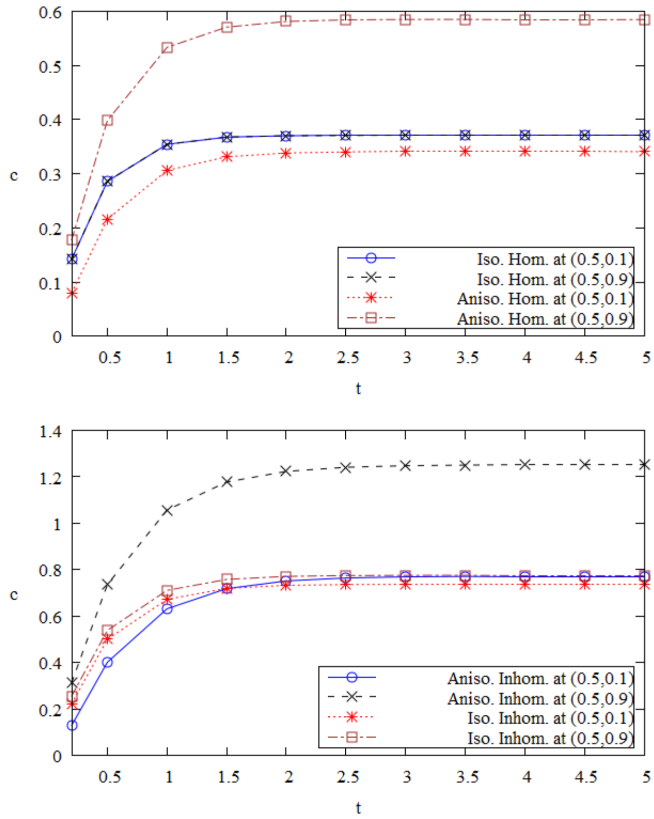


Fig. 15. Symmetry of solutions $c$ about $x_2 = 0.5$ for Problem 4

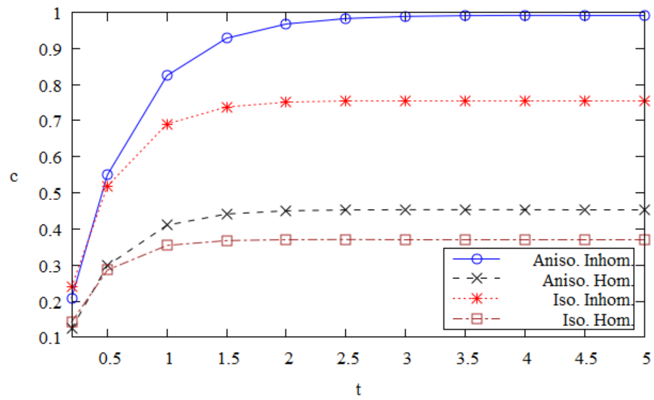


Fig. 16. Solutions $c$ at $(x_1, x_2) = (0.5, 0.5)$ for Problem 4

There is no simple analytical solution for the problem. In fact the system is geometrically symmetric about the axis $x_2 = 0.5$.The results in Figure 15 verify 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. Moreover, for all cases the results in Figure 16 indicate that the system has a steady state solution. After all, the results suggest that it is important 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

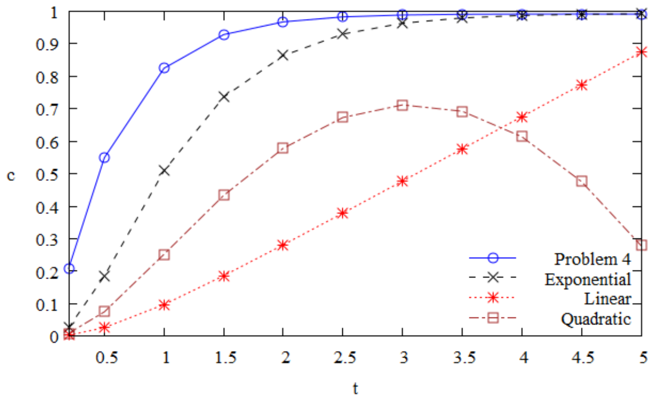


Fig. 17. Solutions $c$ at $(x_1, x_2) = (0.5, 0.5)$ for Problem 5

condition on the side AD, namely

$$P = 1 - \exp(-1.8t) \text{ on side AD}$$
$$P = 0.2t \text{ on side AD}$$
$$P = 0.12t(5-t) \text{ on side AD}$$

The results in Figure 17 are expected. The trends of the solutions $c$ mimics the trends of the exponential function $1-\exp(-1.8t)$, 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 $1-\exp(-1.8t)$, 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 17 verify 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 exponentially graded materials which are governed by the diffusion-convection-reaction equation (1) of compressible flow. The method is easy to implement and involves a time variable free fundamental solution therefore it gives quite accurate solutions. It does not produce round-off error propagation as it solves the boundary integral equation (20) 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-off error will propagate.

The numerical method has been applied to a class of exponentially graded materials where 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, taking the forms (4), (5), (6) and (7) and on the same inhomogeneity or gradation function $g(\mathbf{x})$ of exponential form (8). Therefore, it will be of interest 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 (20), 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. The results of the problems in Section IV-A show that the Stehfest formula 21 is quite accurate.

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