

# A Numerical Simulation for Transient Diffusion Convection Reaction Problems of Anisotropic Quadratically Graded Media with Incompressible Flow

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**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 transient problems of anisotropic functionally graded media governed by the diffusion convection equation.

**Keywords:** *anisotropic functionally graded materials, unsteady diffusion convection reaction equation, Laplace transform, boundary element method*

## 1 Introduction

The transient anisotropic diffusion convection reaction equation of variable coefficients and incompressible flow is written as

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

Referring to the two-dimensional Cartesian coordinate system  $Ox_1x_2$  this paper will concern with the transient anisotropic DCR equation (1) in which  $i, j = 1, 2$ ,

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$\mathbf{x} = (x_1, x_2)$ ,  $d_{ij}$  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 (1).

Functionally graded materials (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 [2, 3]). This constitutes relevancy of solving equation (1).

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, [4–7] 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 sev-

eral types of governing equations, for examples [11, 12] for the modified Helmholtz equation, [13–17] for the diffusion convection equation, [18–21] for the Laplace type equation, [22–26] for the Helmholtz equation.

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.

Not so many works have been done on DCR equation of type (1) for anisotropic media with simultaneously variable diffusivity, velocity and reaction coefficients. This paper is intended to extend the recently published works [27–33] on the steady DCR equation to the transient DCR equation for anisotropic functionally graded materials.

## 2 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 (1) 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

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

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

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

The method of solution will be to transform the variable coefficient equation (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). 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 (1) take the form  $d_{11} = d_{22}$  and  $d_{12} = 0$ .

## 3 The boundary integral equation

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

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

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

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

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

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 quadratically graded by taking  $g(\mathbf{x})$  as an quadratic function

$$g(\mathbf{x}) = [\beta_0 + \beta_i x_i]^2 \quad (8)$$

where  $\beta_0$  and  $\beta_i$  are constants. Therefore (8) satisfies

$$\hat{d}_{ij} \frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} = 0 \quad (9)$$

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

$$\hat{d}_{ij} \frac{\partial}{\partial x_i} \left( g \frac{\partial c}{\partial x_j} \right) - \hat{v}_i g \frac{\partial c}{\partial x_i} - \hat{k} g c = \hat{\alpha} g \frac{\partial c}{\partial t} \quad (10)$$

Assume

$$c(\mathbf{x}, t) = g^{-1/2}(\mathbf{x}) \psi(\mathbf{x}, t) \quad (11)$$

therefore substitution of (4) and (11) into (2) gives

$$P(\mathbf{x}, t) = -P_g(\mathbf{x}) \psi(\mathbf{x}, t) + g^{1/2}(\mathbf{x}) P_\psi(\mathbf{x}, t) \quad (12)$$

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 (10) can be written as

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

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

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

Rearranging and neglecting the zero terms give

$$\begin{aligned}
 &g^{1/2} \left( \hat{d}_{ij} \frac{\partial^2 \psi}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \psi}{\partial x_j} \right) \\
 &- \psi \left( \hat{d}_{ij} \frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial g^{1/2}}{\partial x_i} \right) \\
 &+ \left( \hat{d}_{ij} \frac{\partial \psi}{\partial x_j} \frac{\partial g^{1/2}}{\partial x_i} - \hat{d}_{ij} \frac{\partial \psi}{\partial x_j} \frac{\partial g^{1/2}}{\partial x_i} \right) \\
 &-\hat{k}g^{1/2}\psi = \hat{\alpha}g^{1/2} \frac{\partial \psi}{\partial t} \tag{13}
 \end{aligned}$$

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 (13) becomes

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

Equation (9) then implies

$$\hat{d}_{ij} \frac{\partial^2 \psi}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \psi}{\partial x_i} - \hat{k}\psi = \hat{\alpha} \frac{\partial \psi}{\partial t} \tag{14}$$

Taking a Laplace transform of (11), (12), (14) and applying the initial condition (3) we obtain

$$\psi^*(\mathbf{x}, s) = g^{1/2}(\mathbf{x}) c^*(\mathbf{x}, s) \tag{15}$$

$$P_{\psi^*}(\mathbf{x}, s) = [P^*(\mathbf{x}, s) + P_g(\mathbf{x}) \psi^*(\mathbf{x}, s)] g^{-1/2}(\mathbf{x}) \tag{16}$$

$$\hat{d}_{ij} \frac{\partial^2 \psi^*}{\partial x_i \partial x_j} - \hat{v}_i \frac{\partial \psi^*}{\partial x_i} - (\hat{k} + s\hat{\alpha}) \psi^* = 0 \tag{17}$$

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

By using Gauss divergence theorem, equation (17) can be transformed into a boundary integral equation

$$\begin{aligned}
 &\eta(\boldsymbol{\xi}) \psi^*(\boldsymbol{\xi}, s) = \int_{\partial\Omega} \{P_{\psi^*}(\mathbf{x}, s) \Phi(\mathbf{x}, \boldsymbol{\xi}) \\
 &- [P_v(\mathbf{x}) \Phi(\mathbf{x}, \boldsymbol{\xi}) + \Gamma(\mathbf{x}, \boldsymbol{\xi})] \psi^*(\mathbf{x}, s)\} dS(\mathbf{x}) \tag{18}
 \end{aligned}$$

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

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

where

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

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

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

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

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

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

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

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

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 (15) and (16) in (18) yields

$$\begin{aligned}
 \eta g^{1/2} c^* &= \int_{\partial\Omega} \left\{ \left( g^{-1/2} \Phi \right) P^* \right. \\
 &+ \left. \left[ \left( P_g - P_v g^{1/2} \right) \Phi - g^{1/2} \Gamma \right] c^* \right\} dS \tag{19}
 \end{aligned}$$

Equation (19) 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 (19), 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

$$\begin{aligned}
 c(\mathbf{x}, t) &\simeq \frac{\ln 2}{t} \sum_{m=1}^N V_m c^*(\mathbf{x}, s_m) \\
 \frac{\partial c(\mathbf{x}, t)}{\partial x_1} &\simeq \frac{\ln 2}{t} \sum_{m=1}^N V_m \frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_1} \\
 \frac{\partial c(\mathbf{x}, t)}{\partial x_2} &\simeq \frac{\ln 2}{t} \sum_{m=1}^N V_m \frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_2}
 \end{aligned} \tag{20}$$

where

$$s_m = \frac{\ln 2}{t} m$$

$$V_m = (-1)^{\frac{N}{2}+m} \times$$

$$\sum_{k=\lceil \frac{m+1}{2} \rceil}^{\min(m, \frac{N}{2})} \frac{k^{N/2} (2k)!}{(\frac{N}{2} - k)! (k-1)! (m-k)! (2k-m)!}$$

A simple script has been developed to calculate the values of the coefficients  $V_m, m = 1, 2, \dots, N$  for any number  $N$ .

## 4 Numerical results

In order to justify the analysis derived in the previous sections, we will consider two problems of an analytical solution and without a simple analytical solution. For both problems we take

$$g^{1/2}(\mathbf{x}) = 0.8 - 0.1x_1 + 0.2x_2$$

$$\hat{d}_{ij} = \begin{bmatrix} 0.65 & 0.15 \\ 0.15 & 1 \end{bmatrix}$$

$$\hat{v}_i = (0.2, 0.1)$$

For a simplicity, a unit square (depicted in Figure 1) will be taken as the geometrical domain.

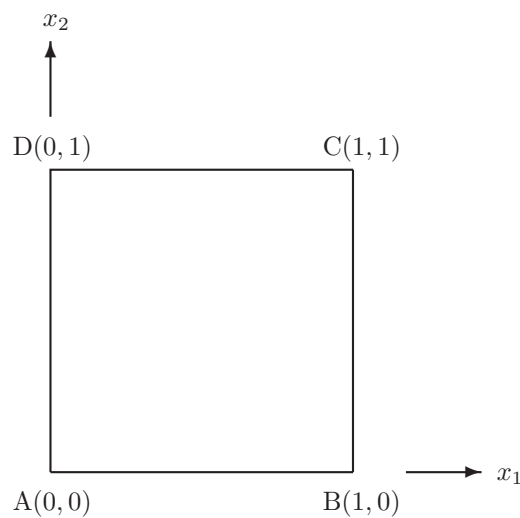


Figure 1: The domain  $\Omega$

### 4.1 Problem 1

Another aspect that will be justified is the accuracy of the numerical solutions. The analytical solution is assumed to be

$$c(\mathbf{x}, t) = \frac{[1 - \exp(-1.8t)] \exp(-0.5 + 0.2x_1 + 0.3x_2)}{0.8 - 0.1x_1 + 0.2x_2}$$

We choose

$$\hat{k} = 1 \quad \hat{\alpha} = -0.936/s$$

and a set of boundary conditions (see Figure 1)

Table 1: 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	0.0008	0.0008	0.0003	0.0003	0.0001	0.0001
0.5	0.5438	0.5437	0.1727	0.1727	0.0351	0.0352
1.0	0.7646	0.7648	0.2429	0.2429	0.0494	0.0495
1.5	0.8542	0.8547	0.2713	0.2715	0.0552	0.0553
2.0	0.8910	0.8912	0.2830	0.2831	0.0576	0.0577
2.5	0.9062	0.9061	0.2878	0.2878	0.0586	0.0586
3.0	0.9125	0.9121	0.2898	0.2897	0.0590	0.0590
3.5	0.9151	0.9146	0.2907	0.2905	0.0591	0.0592
4.0	0.9161	0.9156	0.2910	0.2908	0.0592	0.0592
4.5	0.9164	0.9160	0.2911	0.2910	0.0592	0.0593
5.0	0.9164	0.9161	0.2911	0.2910	0.0592	0.0593

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

Table 1 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. 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 7086.515625 seconds.

### 4.2 Problem 2

We choose

$$\hat{k} = 1 \quad \hat{\alpha} = 1$$

and boundary conditions (see Figure 1)

$P = 0$  on side AB  
 $c = 0$  on side BC  
 $P = 0$  on side CD  
 $P = P(t)$  on side AD

where  $P(t)$  takes four forms

$P(t) = 1$	constant
$P(t) = 1 - \exp(-1.8t)$	exponential
$P(t) = 0.2t$	linear
$P(t) = 0.12t(5-t)$	quadratic

The results in Figure 2 are expected. The trends of the solutions  $c$  mimics the trends of the exponential function  $P(t) = 1 - \exp(-1.8t)$ , the linear function  $P(t) = 0.2t$  and the quadratic function  $P(t) = 0.12t(5-t)$  of the boundary condition on side AD. Specifically, for the exponential function  $P(t) = 1 - \exp(-1.8t)$ , as time  $t$  goes

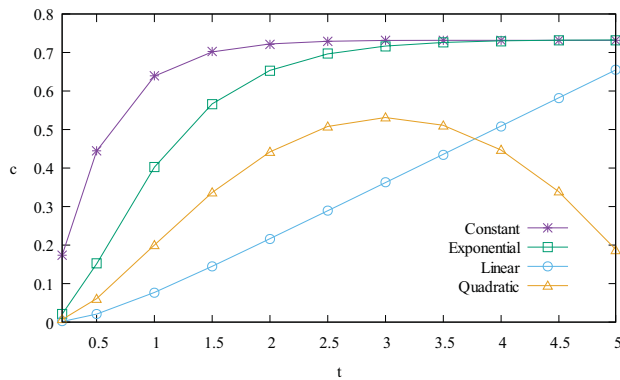


Figure 2: Solutions  $c$  at  $(x_1, x_2) = (0.5, 0.5)$  for Problem 2

to infinity, values of this function go to 1. So for big value of  $t$ , the case of  $P(t) = 1 - \exp(-1.8t)$  is similar to the case of  $P(t) = 1$ . And the two plots of solutions  $c$  for both cases in Figure 2 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-reaction 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-off error propagation as it solves the boundary integral equation (19) 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 may propagate.

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