Numerical Simulation for Unsteady Diffusion-Convection Problems of Quadratically Graded Anisotropic Materials

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***Abstract*—The unsteady problems of anisotropic quadratically graded materials are discussed in this paper. Numerical solutions to a diffusion-convection equation of quadratically varying coefficients are sought by using a combined Laplace transform and boundary element method. 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 can consequently be 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. Some examples are considered to verify the analysis and also to show the accuracy, efficiency and consistency of the numerical procedure. The combined Laplace transform and boundary element method is easy to implement for solving unsteady diffusion-convection problems of anisotropic quadratically graded media.**

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

I. Introduction

The unsteady anisotropic diffusion convection equation of incompressible flow with variable coefficient of the form

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

will be considered. In equation (1) summation convention applies for the repeated indices so that equation (1) can be written explicitly

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

Equation (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 where 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 concentration $c(\mathbf{x},t)$. As the flow is assumed to be incompressible, the velocity $v_i(\mathbf{x})$ must satisfy $\partial v_i(\mathbf{x})/\partial x_i = 0$.

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) is relevant for FGMs.

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 inhomogeneity of the media under consideration. For example, Wu et al. [1], Hernandez-Martinez et al. [2], Wang et al. [3] and Fendoğlu et al. [4] had been working on problems of *isotropic diffusion and homogeneous media*, Yoshida and Nagaoka [5], Meenal and Eldho [6], Azis [7] (for Helmholtz type governing equation) studied problems of *anisotropic diffusion but homogeneous media*. Rap et al. [8], Ravnik and Škerget [9], [10], Li et al. [11] and Pettres and Lacerda [12] considered the case of *isotropic diffusion and variable coefficients (inhomogeneous media)*. Zoppou and Knight [13] had been working on finding the analytical solution to the unsteady *orthotropic diffusion-convection* equation with spatially variable coefficients. The equation considered by Zoppou and Knight [13] is almost similar to equation (1) but with limitation $d_{11} \neq d_{22}, d_{12} = 0$ and the components of the velocity vector $v_i(\mathbf{x})$ is a linear with one independent variable function and the diffusivity matrix $d_{ij}(\mathbf{x})$ is a quadratic with one independent variable function. Recently author (Azis) and co-workers had been working on steady state problems of several other classes of *anisotropic inhomogeneous* media for several types of governing equations, for examples [14], [15] for the modified Helmholtz equation, [16], [17] for the diffusion convection reaction equation, [18]–[20] for the Laplace type equation, [21], [22] for the Helmholtz equation, [23], [24] for the diffusion convection equation and [25] for elasticity problems. Azis et al. had also been working on *unsteady state* problems of *anisotropic inhomogeneous* media for some types of governing equations (see [26]–[30]).

This paper is intended to extend the recently published works [23], [24] from the steady state to unsteady state equation (1).

II. The initial boundary value problem

Given the coefficients $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), \alpha(\mathbf{x})$ solutions $c(\mathbf{x},t)$ and its derivatives to (1) are sought which are valid

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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 $c(\mathbf{x},t)$ 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 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. The analysis also applies for homogeneous media that is the case when the coefficients d_{ij}, v_i and α are constant.

III. The boundary integral equation

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

$$d_{ij}(\mathbf{x}) = \hat{d}_{ij}\, g(\mathbf{x}) \quad (4)$$
$$v_i(\mathbf{x}) = \hat{v}_i\, g(\mathbf{x}) \quad (5)$$
$$\alpha(\mathbf{x}) = \hat{\alpha}\, g(\mathbf{x}) \quad (6)$$

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

$$g(\mathbf{x}) = (\beta_0 + \beta_i x_i)^2 \quad (7)$$

where β_0 and β_i are constants. Therefore (7) satisfies

$$\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i \partial x_j} = 0 \quad (8)$$

Substitution of (4)-(6) into (1) gives

$$\hat{d}_{ij}\frac{\partial}{\partial x_i}\left(g\frac{\partial c}{\partial x_j}\right) - \hat{v}_i g\frac{\partial c}{\partial x_i} = \hat{\alpha} g\frac{\partial c}{\partial t} \quad (9)$$

Assume

$$c(\mathbf{x},t) = g^{-1/2}(\mathbf{x})\,\psi(\mathbf{x},t) \quad (10)$$

therefore substitution of (4) and (10) into (2) gives

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

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 (9) can be written as

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

which can be simplified

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

Use of the identity

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

implies

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

Rearranging and neglecting the zero terms yield

$$g^{1/2}\left(\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_j}\right) - \psi\left(\hat{d}_{ij}\frac{\partial^2 g^{1/2}}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial g^{1/2}}{\partial x_i}\right) + \left(\hat{d}_{ij}\frac{\partial\psi}{\partial x_j}\frac{\partial g^{1/2}}{\partial x_i} - \hat{d}_{ij}\frac{\partial\psi}{\partial x_j}\frac{\partial g^{1/2}}{\partial x_i}\right) = \hat{\alpha} g^{1/2}\frac{\partial\psi}{\partial t} \quad (12)$$

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 (12) 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 (8) then implies

$$\hat{d}_{ij}\frac{\partial^2\psi}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi}{\partial x_i} = \hat{\alpha}\frac{\partial\psi}{\partial t} \quad (13)$$

Taking a Laplace transform of (10), (11), (13) and applying the initial condition (3) we obtain

$$\psi^*(\mathbf{x},s) = g^{1/2}(\mathbf{x})\,c^*(\mathbf{x},s) \quad (14)$$

$$P_{\psi^*}(\mathbf{x},s) = \left[P^*(\mathbf{x},s) + P_g(\mathbf{x})\,\psi^*(\mathbf{x},s)\right]g^{-1/2}(\mathbf{x}) \quad (15)$$

$$\hat{d}_{ij}\frac{\partial^2\psi^*}{\partial x_i\partial x_j} - \hat{v}_i\frac{\partial\psi^*}{\partial x_i} - s\hat{\alpha}\psi^* = 0 \quad (16)$$

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

By using Gauss divergence theorem, equation (16) can be transformed into a boundary integral equation

$$\eta(\boldsymbol{\xi})\,\psi^*(\boldsymbol{\xi},s) = \int_{\partial\Omega}\{P_{\psi^*}(\mathbf{x},s)\,\Phi(\mathbf{x},\boldsymbol{\xi}) - [P_v(\mathbf{x})\,\Phi(\mathbf{x},\boldsymbol{\xi}) + \Gamma(\mathbf{x},\boldsymbol{\xi})]\,\psi^*(\mathbf{x},s)\}\,dS(\mathbf{x}) \quad (17)$$

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

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

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

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

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

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

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

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

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

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 (14) and (15) in (17) yields

$$\begin{aligned}\eta g^{1/2} c^* = &\int_{\partial\Omega} \left\{ \left(g^{-1/2}\Phi\right) P^* \right. \\ &\left. + \left[\left(P_g - P_v g^{1/2}\right)\Phi - g^{1/2}\Gamma\right] c^* \right\} dS \qquad (18)\end{aligned}$$

Equation (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.

After having the solutions $c^*(\mathbf{x}, s)$ and its derivatives $\partial c^*/\partial x_1$ and $\partial c^*/\partial x_2$ from (18), the Stehfest formula is then utilized 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

$$\begin{aligned} c(\mathbf{x}, t) &\simeq \frac{\ln 2}{t} \sum_{m=1}^{N} V_m c^*(\mathbf{x}, s_m) \\ \frac{\partial c(\mathbf{x}, t)}{\partial x_1} &\simeq \frac{\ln 2}{t} \sum_{m=1}^{N} V_m \frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_1} \qquad (19) \\ \frac{\partial c(\mathbf{x}, t)}{\partial x_2} &\simeq \frac{\ln 2}{t} \sum_{m=1}^{N} V_m \frac{\partial c^*(\mathbf{x}, s_m)}{\partial x_2} \end{aligned}$$

where

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

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

IV. NUMERICAL RESULTS

In order to verify the analysis derived in the previous sections, we will consider several problems either of analytical solutions or without simple analytical solutions. From the test problems we will also show the convergence and the time efficiency. The convergence will be evaluated by examining the errors and the time efficiency will be investigated by studying the CPU time elapsed for obtaining the numerical solutions of corresponding error or accuracy.

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 $d_{ij}(\mathbf{x}), v_i(\mathbf{x}), \alpha(\mathbf{x})$ in equation (1) are assumed to be of the form (4), (5) and (6) in which $g(\mathbf{x})$ is a quadratic function of the form (7).

Standard BEM with constant elements is employed to obtain numerical results. For a simplicity, a unit square 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 code is developed to compute the numerical solutions. The code contains some commands to calculate the elapsed CPU time for the computation of the numerical solutions. A simple script is also embedded 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.

A. Problems with analytical solutions

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

$$h(\mathbf{x}) = \exp\left[-\left(1 + 0.15x_1 + 0.35x_2\right)\right]$$

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

$$g^{1/2}(\mathbf{x}) = \left(1 - 0.15x_1 + 0.25x_2\right)$$

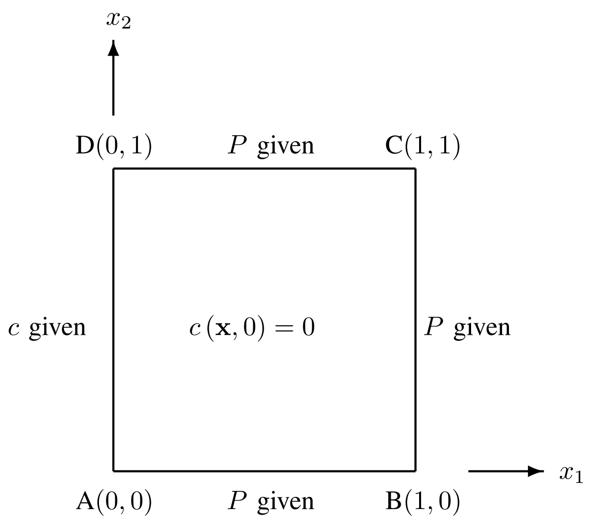

Fig. 1. The boundary conditions for the problems in Section IV-A

We will consider several forms of time variation functions $f(t)$ of time domain $t = [0 : 10]$. For the problems we take a mutual coefficient $\hat{d}_{ij}$

$$\hat{d}_{ij} = \begin{bmatrix} 1 & 0.45 \\ 0.45 & 0.75 \end{bmatrix}$$

velocity $\hat{v}_i$ and rate of change $\hat{\alpha}$

$$\hat{v}_i = (0.5, 0.3), \hat{\alpha} = 0.341625/s$$

and a set of boundary conditions (see Figure 1)

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

For each problem, numerical solutions for c and the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$ at 19×19 points inside the space domain which are

$$(x_1, x_2) = \{.05, .1, .15, \ldots, .9, .95\} \times \{.05, .1, .15, \ldots, .9, .95\}$$

and 11 time-steps which are

$$t = 0.1, 1.0, 2.0, \ldots, 8.0, 9.0, 9.9$$

are sought.

For each time-step t the elapsed CPU time τ_t (in seconds), the relative error E_t and the CPU time efficiency number ε_t for obtaining the numerical solutions at 19×19 interior points are calculated using the formula

$$E_t = \left[\frac{\sum_{i=1}^{19\times19} (\mu_{n,i} - \mu_{a,i})^2}{\sum_{i=1}^{19\times19} \mu_{a,i}^2} \right]^{\frac{1}{2}}$$
$$\varepsilon_t = \tau_t E_t$$

where μ_n and μ_a are respectively the numerical and analytical solutions c or the derivatives $\partial c/\partial x_1$ and $\partial c/\partial x_2$. The aggregate values of relative error E and efficiency number ε, namely

$$E = \left[\frac{\sum_t \sum_{i=1}^{19\times19} (\mu_{n,i} - \mu_{a,i})^2}{\sum_t \sum_{i=1}^{19\times19} \mu_{a,i}^2} \right]^{\frac{1}{2}}$$
$$\varepsilon = \tau E$$

are also computed for each N where τ is the total elapsed CPU time.

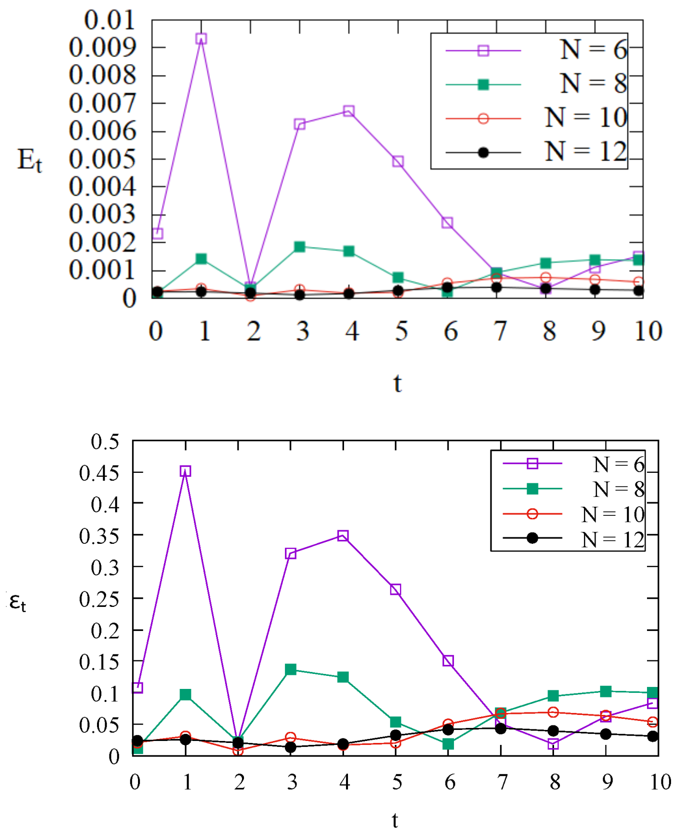

Fig. 2. The average error E_t and the CPU time efficiency ε_t of the numerical solution c for Problem 1.

Therefore the CPU time efficiency ε_t or ε is calculated using the time τ_t or τ elapsed for obtaining the numerical solutions of error E_t or E. Accordingly, the smaller time τ_t or τ with smaller error E_t or E, the more efficient the procedure (smaller ε_t or ε). Based on the values of the parameters τ, E, ε it will be decided the optimized N that gives solutions of the best CPU-time efficiency of corresponding accuracy.

Problem 1:: We suppose that the time variation function is

$$f(t) = 1 - \exp(-0.85t)$$

The convergence and the efficiency may be seen from Figures 2 – 5, Tables II, III. In general the numerical solutions c and $\partial c/\partial x_2$ converge to the analytical solutions, and their time efficiency also become better (smaller) as N increases from $N = 6$ to $N = 12$ (see Figures 2, 4, 5 or Table II). As shown in Figures 3 and 5 or Table II, the numerical solution $\partial c/\partial x_1$ on the other hand, converges slowly when $N = 6$ to $N = 10$ but it gets divergent when $N = 12$. The decrease of its error when N changes form $N = 6$ to $N = 10$ is not significant, whereas the elapsed CPU time gets bigger significantly. This gives inefficiency as N moves from $N = 6$ to $N = 12$. The optimized value of N for obtaining the numerical solutions $c, \partial c/\partial x_1, \partial c/\partial x_2$ of best error E and efficiency number ε can be seen in Table III. In addition, Table IV shows solutions c, $\partial c/\partial x_1$ and $\partial c/\partial x_2$ at $(x_1, x_2) = (0.5, 0.5)$.

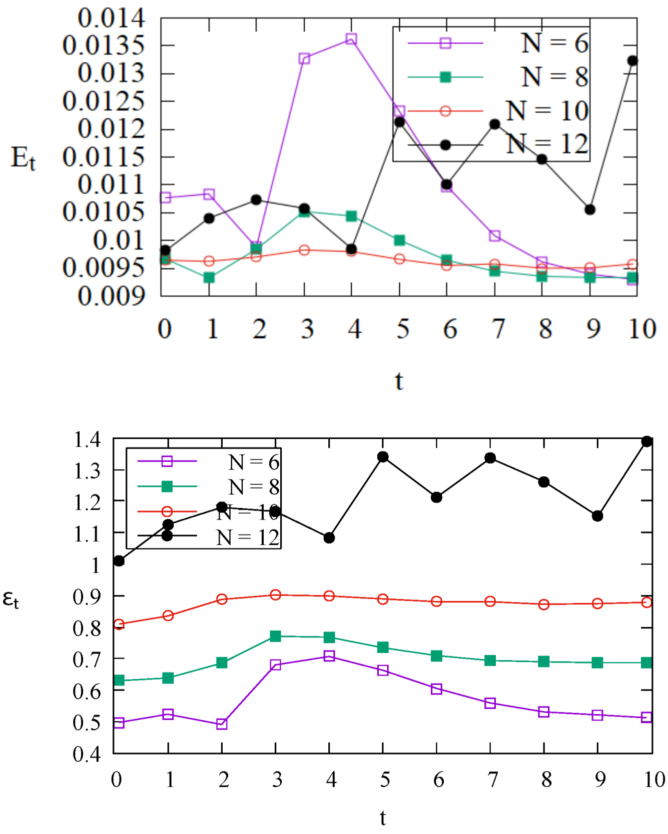

Fig. 3. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_1$ for Problem 1.

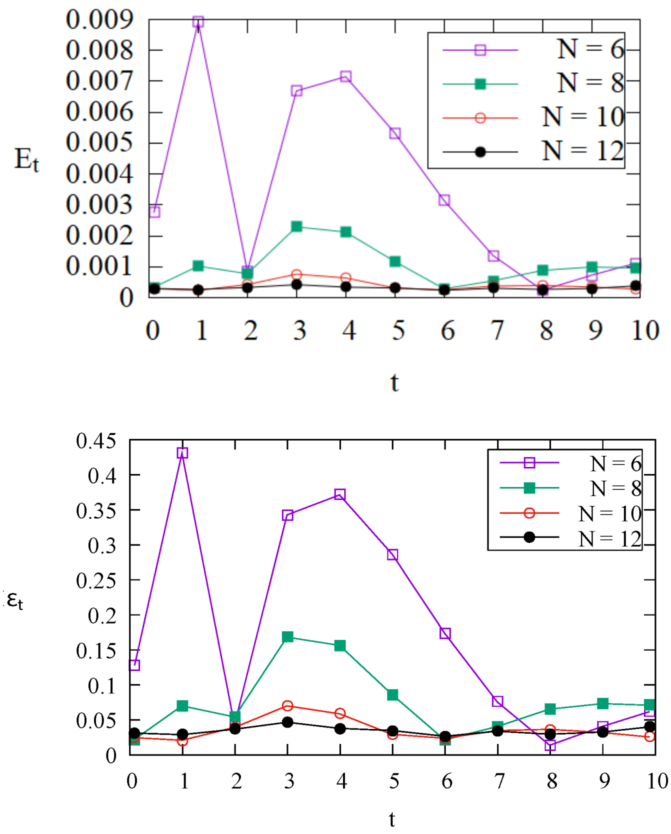

Fig. 4. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_2$ for Problem 1.

TABLE II
THE TOTAL ELAPSED CPU TIME τ, THE GLOBAL AVERAGE ERROR E, THE EFFICIENCY NUMBER $\varepsilon = \tau E$ FOR PROBLEM 1

N		6	8	10	12
τ		577.500	791.516	997.641	1197.172
c	E	0.00399585	0.00122654	0.00052155	0.00029665
	ε	0.22014620	0.09024660	0.04785226	0.03118099
$\frac{\partial c}{\partial x_1}$	E	0.01102688	0.00974164	0.00962781	0.01134571
	ε	0.60751216	0.71677178	0.88335146	1.19254064
$\frac{\partial c}{\partial x_2}$	E	0.00418966	0.00125583	0.00043486	0.00031991
	ε	0.23082399	0.09240191	0.03989865	0.03362539

TABLE III
THE OPTIMIZED VALUE OF N FOR OBTAINING THE NUMERICAL SOLUTIONS $c, \partial c/\partial x_1, \partial c/\partial x_2$ OF BEST ERROR E AND EFFICIENCY NUMBER ε FOR PROBLEM 1

	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$
E	$N = 12$	$N = 10$	$N = 12$
ε	$N = 12$	$N = 6$	$N = 12$

TABLE IV
THE SOLUTIONS c, $\partial c/\partial x_1$ AND $\partial c/\partial x_2$ AT $(x_1, x_2) = (0.5, 0.5)$ FOR PROBLEM 1.

Solution c				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	0.022183	0.022239	0.022240	0.022235
$t = 1$	0.157699	0.156461	0.156275	0.156237
$t = 2$	0.222929	0.222948	0.223058	0.223014
$t = 3$	0.249984	0.251094	0.251588	0.251556
$t = 4$	0.261986	0.263315	0.263802	0.263755
$t = 5$	0.267656	0.268779	0.269050	0.268970
$t = 6$	0.270467	0.271270	0.271304	0.271198
$t = 7$	0.271906	0.272406	0.272262	0.272151
$t = 8$	0.272653	0.272910	0.272658	0.272558
$t = 9$	0.273040	0.273115	0.272822	0.272732
$t = 9.9$	0.273219	0.273176	0.272884	0.272801
Solution $\partial c/\partial x_1$				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	-0.000158	-0.000159	-0.000159	-0.000159
$t = 1$	-0.001125	-0.001116	-0.001114	-0.001116
$t = 2$	-0.001590	-0.001590	-0.001592	-0.001593
$t = 3$	-0.001783	-0.001791	-0.001795	-0.001797
$t = 4$	-0.001869	-0.001878	-0.001881	-0.001884
$t = 5$	-0.001909	-0.001917	-0.001918	-0.001921
$t = 6$	-0.001929	-0.001935	-0.001933	-0.001937
$t = 7$	-0.001940	-0.001943	-0.001945	-0.001944
$t = 8$	-0.001945	-0.001947	-0.001949	-0.001947
$t = 9$	-0.001948	-0.001948	-0.001946	-0.001948
$t = 9.9$	-0.001949	-0.001949	-0.001937	-0.001949
Solution $\partial c/\partial x_2$				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	-0.013041	-0.013074	-0.013075	-0.013076
$t = 1$	-0.092708	-0.091980	-0.091873	-0.091882
$t = 2$	-0.131056	-0.131067	-0.131131	-0.131154
$t = 3$	-0.146961	-0.147613	-0.147902	-0.147939
$t = 4$	-0.154017	-0.154798	-0.155083	-0.155113
$t = 5$	-0.157350	-0.158010	-0.158173	-0.158180
$t = 6$	-0.159003	-0.159474	-0.159496	-0.159490
$t = 7$	-0.159848	-0.160143	-0.160056	-0.160051
$t = 8$	-0.160288	-0.160439	-0.160292	-0.160290
$t = 9$	-0.160515	-0.160559	-0.160384	-0.160392
$t = 9.9$	-0.160620	-0.160595	-0.160424	-0.160433

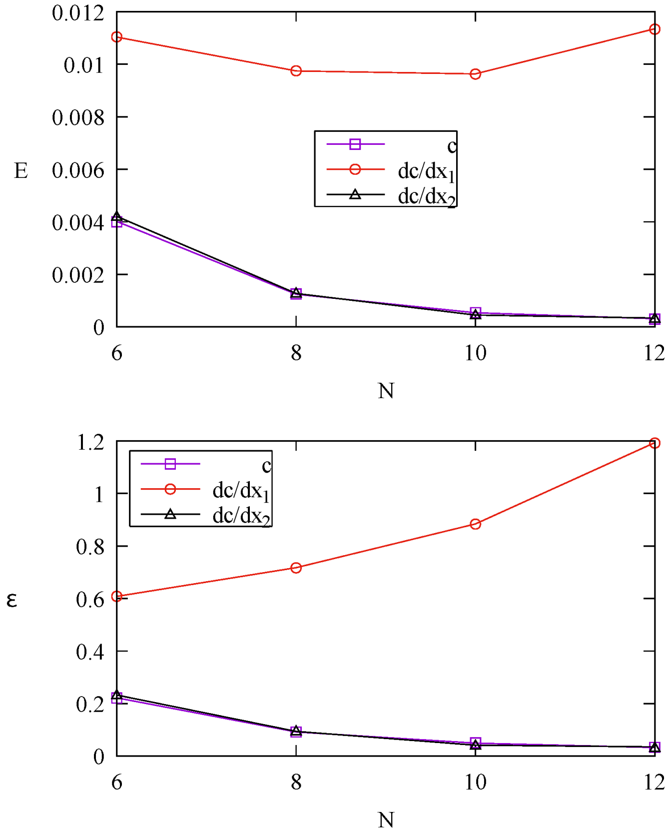

Fig. 5. The global average error E and efficiency number $\varepsilon = \tau E$ for Problem 1.

TABLE V
THE TOTAL ELAPSED CPU TIME τ, THE GLOBAL AVERAGE ERROR E, THE EFFICIENCY NUMBER $\varepsilon = \tau E$ FOR PROBLEM 2

N		6	8	10	12
τ		607.500	807.172	1005.766	1197.688
c	E	0.00192582	0.00037054	0.00025343	0.00022137
	ε	0.10664241	0.02733299	0.02323679	0.02293305
$\frac{\partial c}{\partial x_1}$	E	0.01055651	0.00960582	0.00964427	0.01032717
	ε	0.58456684	0.70857930	0.88425937	1.06982981
$\frac{\partial c}{\partial x_2}$	E	0.00235693	0.00023174	0.00028444	0.00030845
	ε	0.13051517	0.01709471	0.02607957	0.03195328

Problem 2:: Next, we suppose that the time variation function is

$$f(t) = 0.1t$$

The convergence and the efficiency may be seen from Figures 6 – 9 and Table V. In general the numerical solutions c and $\partial c/\partial x_2$ converge steadily to the analytical solutions, and their time efficiency also slightly become better (smaller) as N increases from $N = 6$ to $N = 12$ (see Figures 6, 8, 9 or Table V). As shown in Figures 7 and 9 (or Table V), the numerical solution $\partial c/\partial x_1$ on the other hand, converges slowly when $N = 6$ to $N = 10$ but it gets divergent when $N = 12$. The decrease of its error when N changes form $N = 6$ to $N = 10$ is not significant, whereas the elapsed CPU time gets bigger significantly. This gives inefficiency as N moves from $N = 6$ to $N = 12$. The optimized value of N for obtaining the numerical solutions $c, \partial c/\partial x_1, \partial c/\partial x_2$ of best error E and efficiency number ε can be seen in Table VI. Table VII shows solutions c, $\partial c/\partial x_1$ and $\partial c/\partial x_2$ at $(x_1, x_2) = (0.5, 0.5)$.

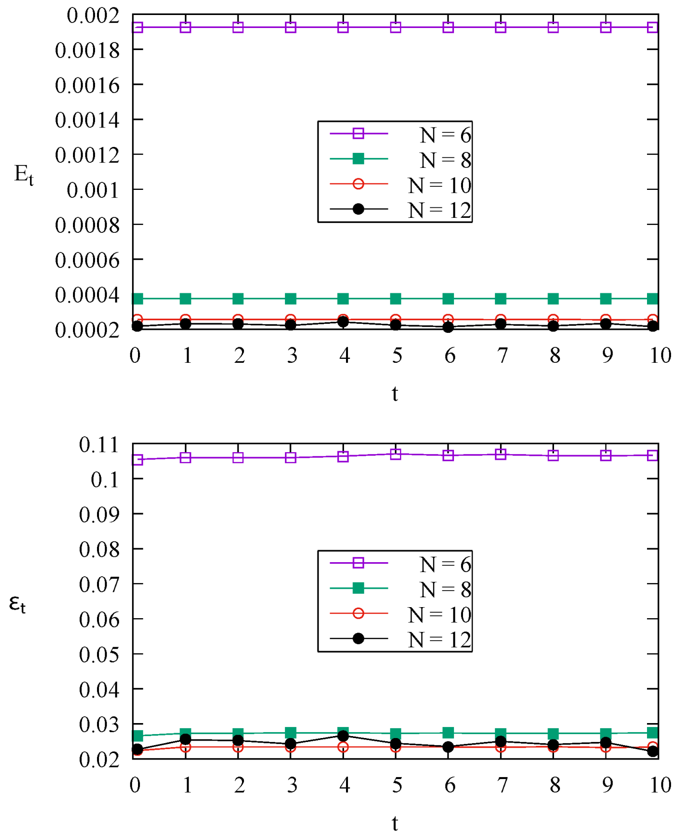

Fig. 6. The average error E_t and the CPU time efficiency ε_t of the numerical solution c for Problem 2.

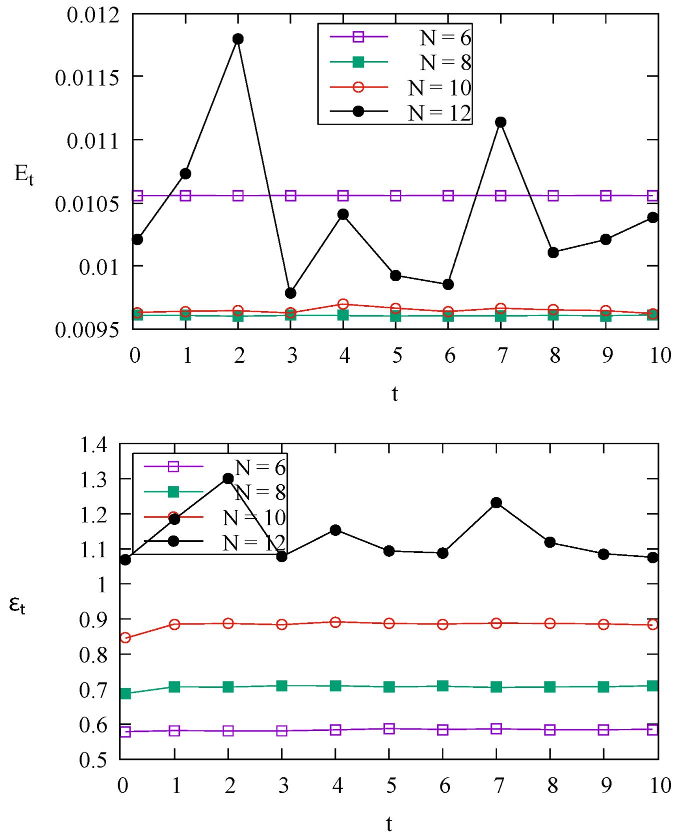

Fig. 7. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_1$ for Problem 2.

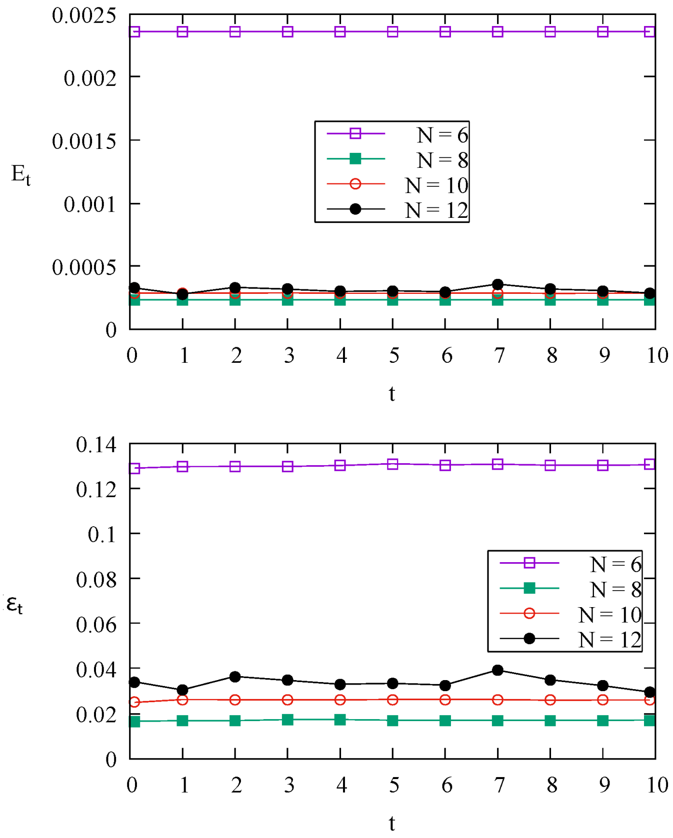

Fig. 8. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_2$ for Problem 2.

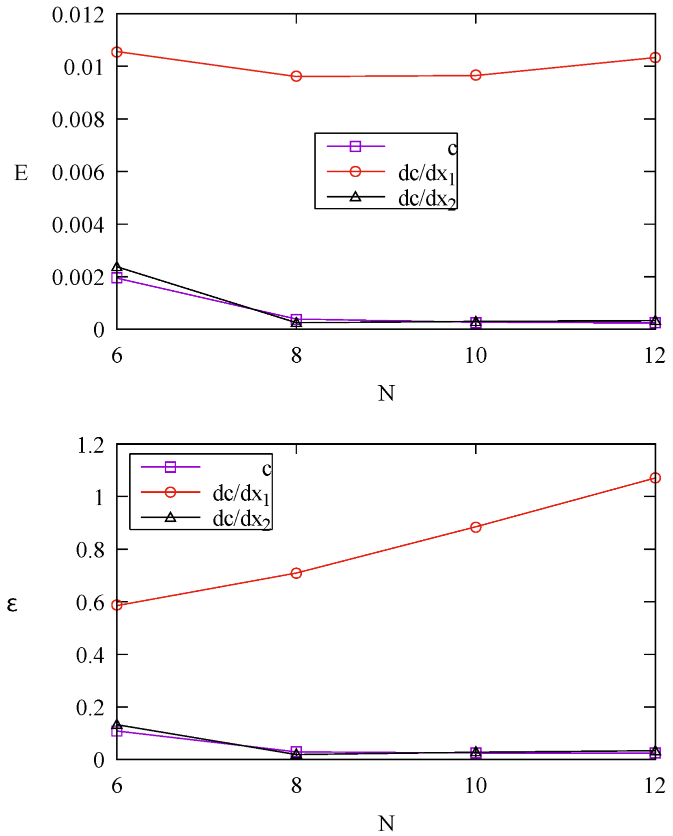

Fig. 9. The global average error E and efficiency number $\varepsilon = \tau E$ for Problem 2.

TABLE VI
THE OPTIMIZED VALUE OF N FOR OBTAINING THE NUMERICAL SOLUTIONS $c, \partial c/\partial x_1, \partial c/\partial x_2$ OF BEST ERROR E AND EFFICIENCY NUMBER ε FOR PROBLEM 2

	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$
E	$N = 12$	$N = 8$	$N = 8$
ε	$N = 12$	$N = 6$	$N = 8$

TABLE VII
THE SOLUTIONS c, $\partial c/\partial x_1$ AND $\partial c/\partial x_2$ AT $(x_1, x_2) = (0.5, 0.5)$ FOR PROBLEM 2.

Solution c				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	0.002723	0.002730	0.002729	0.002729
$t = 1$	0.027234	0.027297	0.027293	0.027286
$t = 2$	0.054468	0.054593	0.054585	0.054572
$t = 3$	0.081702	0.081890	0.081877	0.081859
$t = 4$	0.108937	0.109187	0.109172	0.109145
$t = 5$	0.136171	0.136483	0.136462	0.136431
$t = 6$	0.163405	0.163780	0.163753	0.163717
$t = 7$	0.190639	0.191077	0.191048	0.191003
$t = 8$	0.217873	0.218373	0.218339	0.218289
$t = 9$	0.245107	0.245670	0.245635	0.245576
$t = 9.9$	0.269618	0.270237	0.270193	0.270133
Solution $\partial c/\partial x_1$				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	-0.000019	-0.000019	-0.000019	-0.000019
$t = 1$	-0.000194	-0.000195	-0.000194	-0.000195
$t = 2$	-0.000389	-0.000389	-0.000389	-0.000390
$t = 3$	-0.000583	-0.000584	-0.000584	-0.000585
$t = 4$	-0.000777	-0.000779	-0.000777	-0.000780
$t = 5$	-0.000971	-0.000974	-0.000973	-0.000975
$t = 6$	-0.001166	-0.001168	-0.001169	-0.001169
$t = 7$	-0.001360	-0.001363	-0.001363	-0.001364
$t = 8$	-0.001554	-0.001558	-0.001559	-0.001559
$t = 9$	-0.001749	-0.001753	-0.001750	-0.001754
$t = 9.9$	-0.001923	-0.001928	-0.001929	-0.001930
Solution $\partial c/\partial x_2$				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	-0.001601	-0.001605	-0.001604	-0.001605
$t = 1$	-0.016010	-0.016047	-0.016045	-0.016047
$t = 2$	-0.032021	-0.032094	-0.032090	-0.032094
$t = 3$	-0.048031	-0.048142	-0.048134	-0.048141
$t = 4$	-0.064042	-0.064189	-0.064180	-0.064187
$t = 5$	-0.080052	-0.080236	-0.080225	-0.080234
$t = 6$	-0.096063	-0.096283	-0.096268	-0.096281
$t = 7$	-0.112073	-0.112330	-0.112311	-0.112328
$t = 8$	-0.128084	-0.128378	-0.128357	-0.128375
$t = 9$	-0.144094	-0.144425	-0.144404	-0.144422
$t = 9.9$	-0.158503	-0.158867	-0.158842	-0.158864

Problem 3:: Now, we suppose that the time variation function is

$$f(t) = t(10 - t)/25$$

The convergence and the efficiency may be seen from Figures 10 – 13 and Table VIII. In general the numerical solutions c, $\partial c/\partial x_1$ and $\partial c/\partial x_2$ converge quickly to the analytical solutions, and their time efficiency also become better (smaller) as N changes from $N = 6$ to $N = 8$. From $N = 8$ to $N = 12$, the accuracy and the efficiency steadily get better. See Figures 10, 11, 12, 13 (or Table VIII). The optimized value of N for obtaining the numerical solutions $c, \partial c/\partial x_1, \partial c/\partial x_2$ of best error E and efficiency number ε can be seen in Table IX. Table X shows solutions c, $\partial c/\partial x_1$ and $\partial c/\partial x_2$ at $(x_1, x_2) = (0.5, 0.5)$.

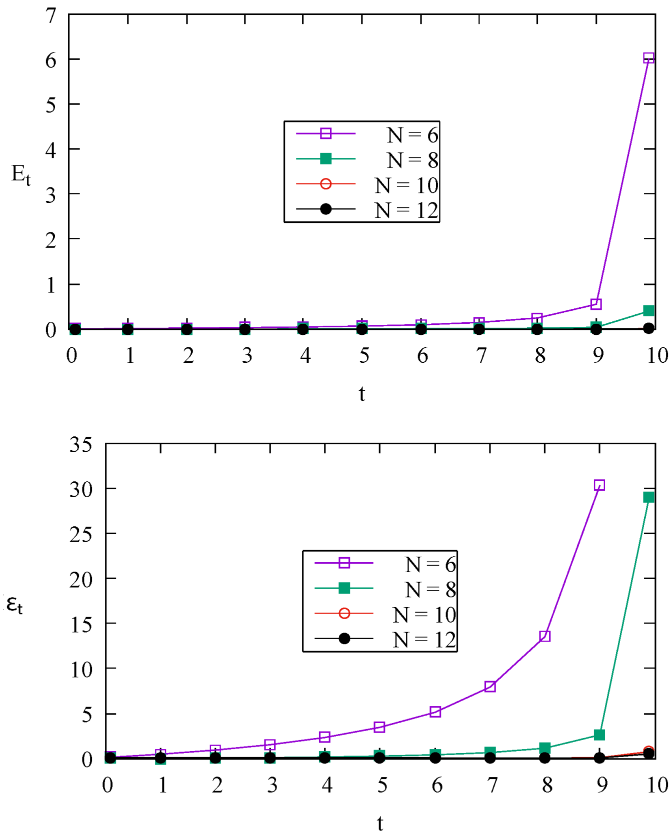

Fig. 10. The average error E_t and the CPU time efficiency ε_t of the numerical solution c for Problem 3.

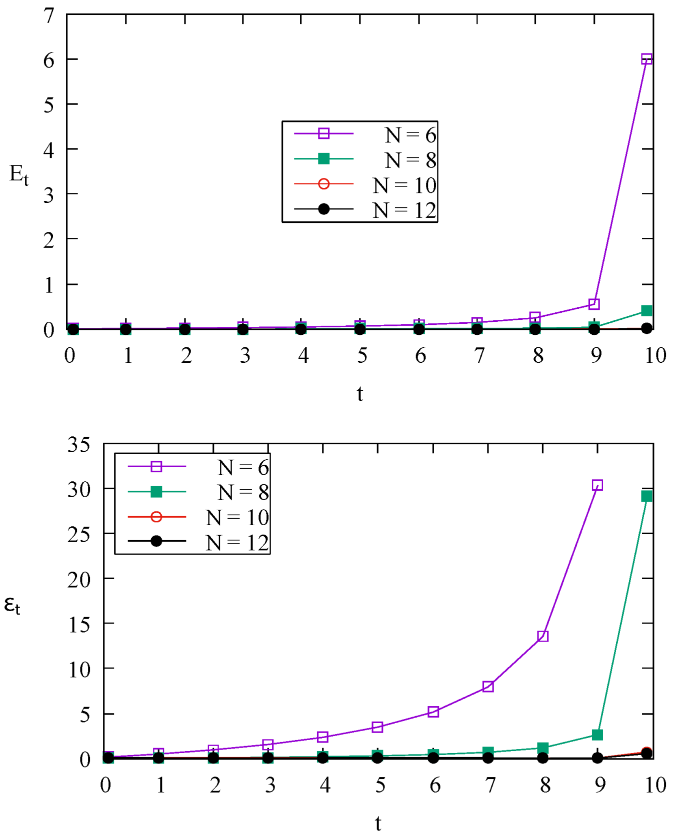

Fig. 12. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_2$ for Problem 3.

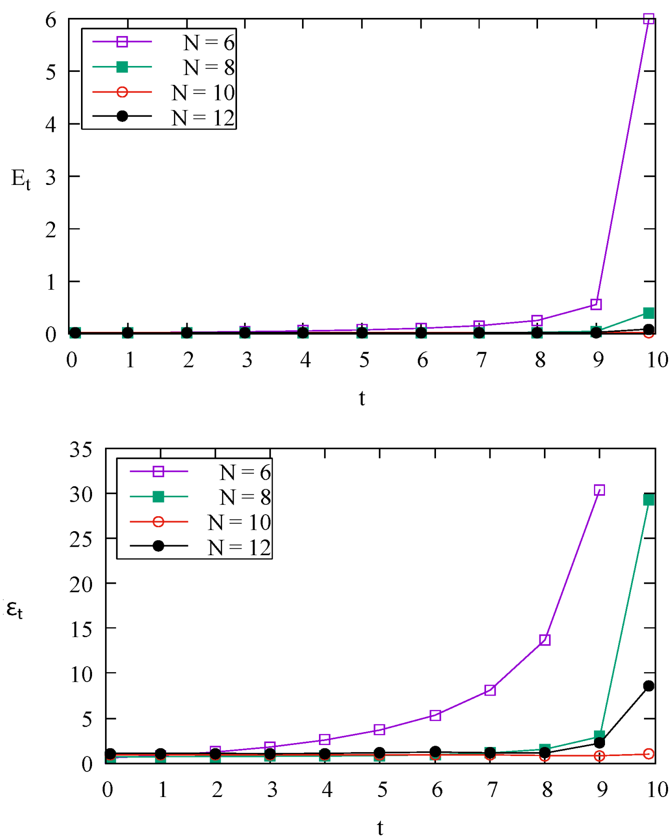

Fig. 11. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_1$ for Problem 3.

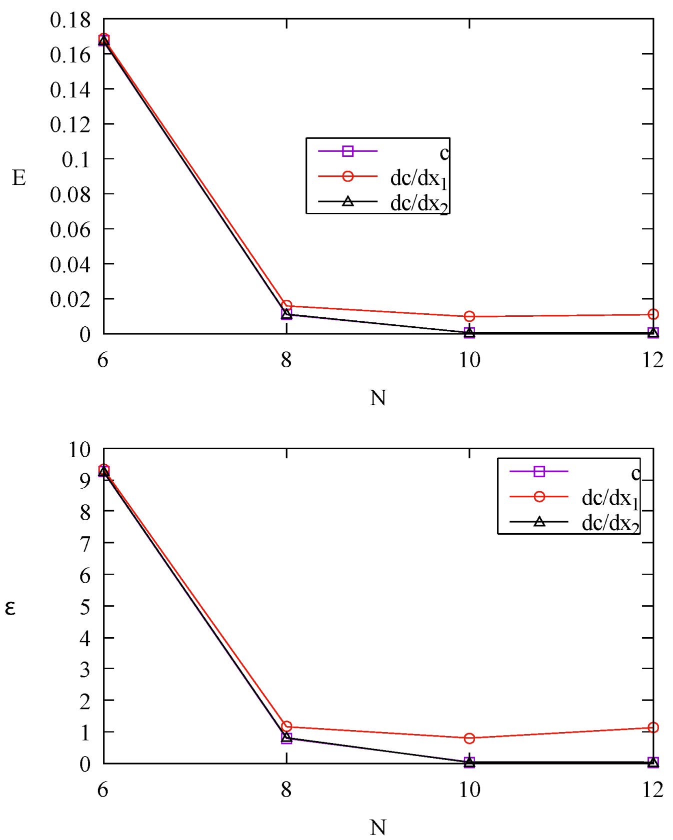

Fig. 13. The global average error E and efficiency number $\varepsilon = \tau E$ for Problem 3.

TABLE VIII
THE TOTAL ELAPSED CPU TIME τ, THE GLOBAL AVERAGE ERROR E, THE EFFICIENCY NUMBER $\varepsilon = \tau E$ FOR PROBLEM 3

N		6	8	10	12
τ		607.359	809.094	995.578	1204.875
c	E	0.16720984	0.01075569	0.00043951	0.00031011
	ε	9.26185734	0.79003892	0.03650706	0.03249397
$\frac{\partial c}{\partial x_1}$	E	0.16881112	0.01575362	0.00960039	0.01076889
	ε	9.35055361	1.15715279	0.79743235	1.12837806
$\frac{\partial c}{\partial x_2}$	E	0.16737521	0.01098110	0.00030840	0.00030683
	ε	9.27101754	0.80659613	0.02561687	0.03214955

TABLE IX
THE OPTIMIZED VALUE OF N FOR OBTAINING THE NUMERICAL SOLUTIONS $c, \partial c/\partial x_1, \partial c/\partial x_2$ OF BEST ERROR E AND EFFICIENCY NUMBER ε FOR PROBLEM 3

	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$
E	$N = 12$	$N = 10$	$N = 12$
ε	$N = 12$	$N = 10$	$N = 10$

TABLE X
THE SOLUTIONS c, $\partial c/\partial x_1$ AND $\partial c/\partial x_2$ AT $(x_1, x_2) = (0.5, 0.5)$ FOR PROBLEM 3.

Solution c				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	0.010778	0.010809	0.010808	0.010805
$t = 1$	0.097380	0.098224	0.098253	0.098230
$t = 2$	0.171646	0.174524	0.174673	0.174631
$t = 3$	0.222799	0.228898	0.229262	0.229204
$t = 4$	0.250838	0.261348	0.262019	0.261947
$t = 5$	0.255763	0.271874	0.272942	0.272862
$t = 6$	0.237575	0.260474	0.262019	0.261947
$t = 7$	0.196273	0.227150	0.229283	0.229204
$t = 8$	0.131858	0.171901	0.174703	0.174631
$t = 9$	0.044329	0.094727	0.098296	0.098230
$t = 9.9$	-0.054209	0.006525	0.010858	0.010805
Solution $\partial c/\partial x_1$				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	-0.000077	-0.000077	-0.000077	-0.000077
$t = 1$	-0.000695	-0.000701	-0.000701	-0.000702
$t = 2$	-0.001224	-0.001245	-0.001247	-0.001247
$t = 3$	-0.001589	-0.001633	-0.001635	-0.001637
$t = 4$	-0.001789	-0.001864	-0.001867	-0.001871
$t = 5$	-0.001825	-0.001939	-0.001943	-0.001949
$t = 6$	-0.001695	-0.001858	-0.001875	-0.001871
$t = 7$	-0.001400	-0.001620	-0.001634	-0.001637
$t = 8$	-0.000941	-0.001226	-0.001248	-0.001247
$t = 9$	-0.000316	-0.000676	-0.000698	-0.000702
$t = 9.9$	0.000387	-0.000047	-0.000075	-0.000077
Solution $\partial c/\partial x_2$				
	$N = 6$	$N = 8$	$N = 12$	Analytical
$t = 0.1$	-0.006336	-0.006354	-0.006354	-0.006355
$t = 1$	-0.057248	-0.057744	-0.057761	-0.057769
$t = 2$	-0.100907	-0.102599	-0.102687	-0.102700
$t = 3$	-0.130979	-0.134565	-0.134779	-0.134794
$t = 4$	-0.147463	-0.153642	-0.154036	-0.154050
$t = 5$	-0.150358	-0.159829	-0.160457	-0.160469
$t = 6$	-0.139666	-0.153128	-0.154036	-0.154050
$t = 7$	-0.115385	-0.133537	-0.134790	-0.134794
$t = 8$	-0.077517	-0.101057	-0.102705	-0.102700
$t = 9$	-0.026060	-0.055688	-0.057787	-0.057769
$t = 9.9$	0.031868	-0.003836	-0.006386	-0.006355

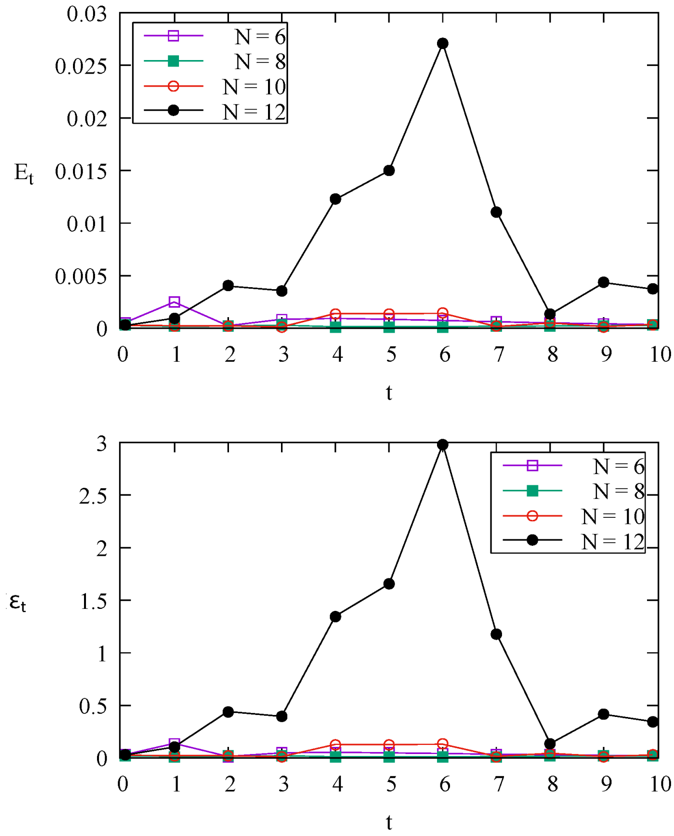

Fig. 14. The average error E_t and the CPU time efficiency ε_t of the numerical solution c for Problem 4.

TABLE XI
THE TOTAL ELAPSED CPU TIME τ, THE GLOBAL AVERAGE ERROR E, THE EFFICIENCY NUMBER $\varepsilon = \tau E$ FOR PROBLEM 4

N		6	8	10	12
τ		608.656	803.063	989.922	1170.953
c	E	0.00076897	0.00017493	0.00079946	0.01190908
	ε	0.04241371	0.01223397	0.06411907	1.10605568
$\frac{\partial c}{\partial x_1}$	E	0.00991336	0.00969678	0.00975808	0.01621108
	ε	0.54678372	0.67816821	0.78262875	1.50560434
$\frac{\partial c}{\partial x_2}$	E	0.00109352	0.00042362	0.00093485	0.01194531
	ε	0.06031440	0.02962697	0.07497827	1.10942109

Problem 4:: Now, we suppose that the time variation function is

$$f(t) = t/(t+1)$$

In general the numerical solutions c and $\partial c/\partial x_2$ converge to the analytical solutions, and their time efficiency also become better (smaller) as N increases from $N = 6$ to $N = 8$ (see Figures 14, 16, 17 or Table XI). On the other hand, as shown in Figures 15 and 17 or Table XI the numerical solution $\partial c/\partial x_1$ converges slowly when $N = 6$ to $N = 8$ but it gets divergent when $N = 10, 12$. The decrease of its error when N changes form $N = 6$ to $N = 8$ is not significant, whereas the elapsed CPU time gets bigger significantly. This gives inefficiency as N moves from $N = 6$ to $N = 12$. The optimized value of N for obtaining the numerical solutions $c, \partial c/\partial x_1, \partial c/\partial x_2$ of best error E and efficiency number ε can be seen in Table XII. In addition, Figure 18 shows solutions c, $\partial c/\partial x_1$ and $\partial c/\partial x_2$ at $(x_1, x_2) = (0.5, 0.5)$.

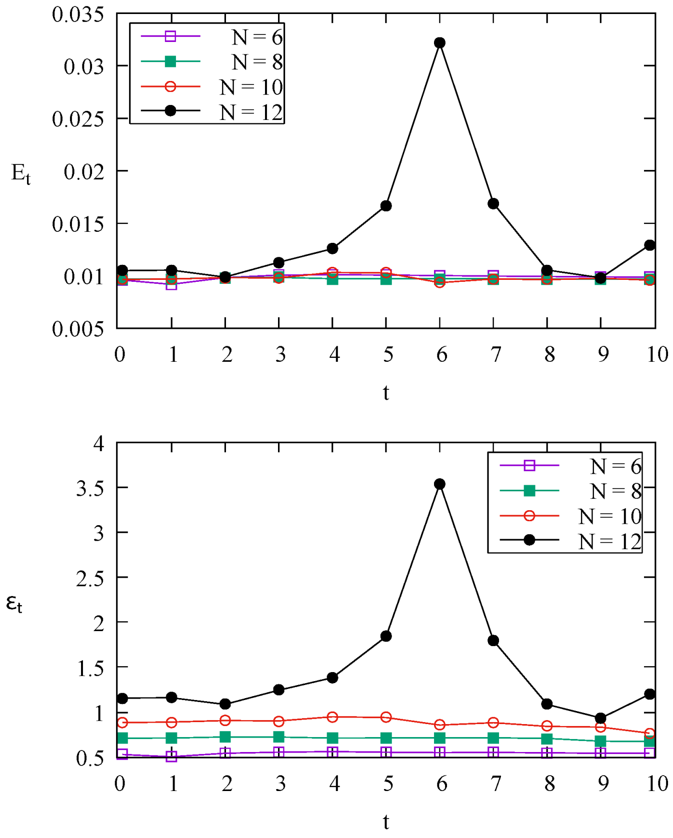

Fig. 15. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_1$ for Problem 4.

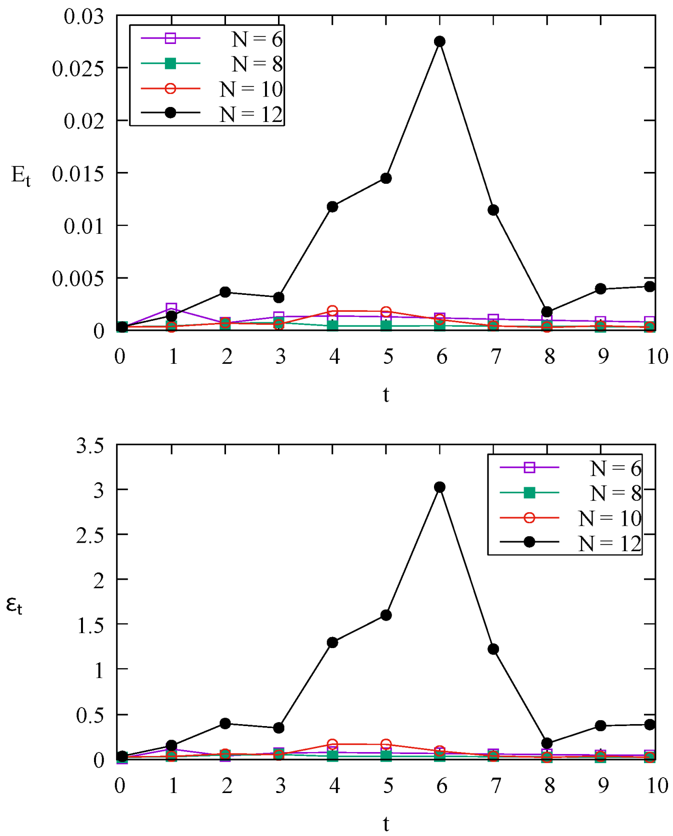

Fig. 16. The average error E_t and the CPU time efficiency ε_t of the numerical solution $\partial c/\partial x_2$ for Problem 4.

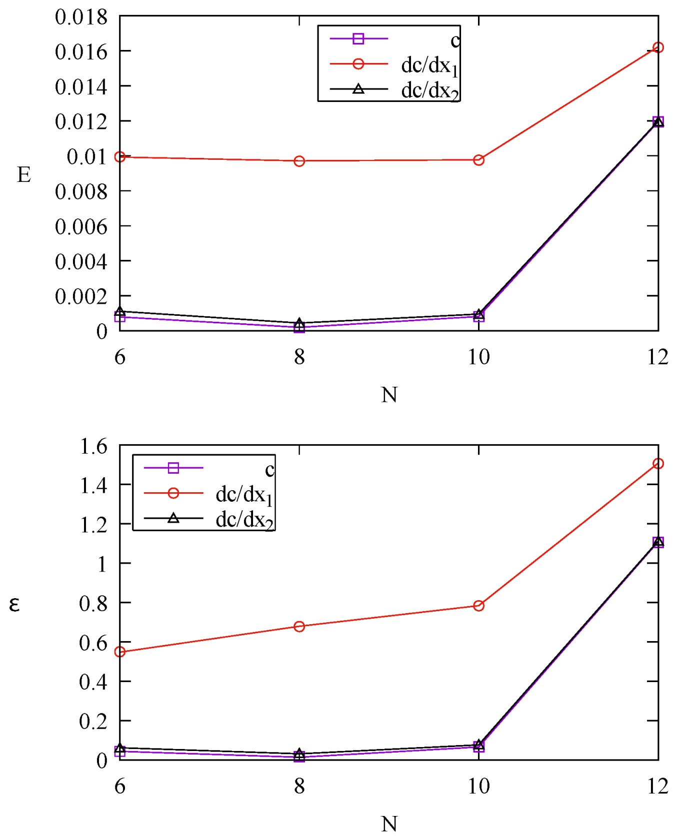

Fig. 17. The global average error E and efficiency number $\varepsilon = \tau E$ for Problem 4.

TABLE XII
THE OPTIMIZED VALUE OF N FOR OBTAINING THE NUMERICAL SOLUTIONS $c, \partial c/\partial x_1, \partial c/\partial x_2$ OF BEST ERROR E AND EFFICIENCY NUMBER ε FOR PROBLEM 4

	c	$\frac{\partial c}{\partial x_1}$	$\frac{\partial c}{\partial x_2}$
E	$N = 8$	$N = 8$	$N = 8$
ε	$N = 8$	$N = 6$	$N = 8$

B. Problems without analytical solutions

Problem 5:: Furthermore, we will show the impact of the anisotropy and the inhomogeneity of the material under consideration on the solution c. Based on the results for the test problems in Section IV-A where the errors are small enough when $N = 10$ is used, then for this problem we will use $N = 10$.

Again, we choose the velocity $\hat{v}_i$ and rate of change $\hat{\alpha}$

$$\hat{v}_i = (0.5, 0.3)\,, \hat{\alpha} = 0.341625/s$$

For this problem the medium is supposed to be inhomogeneous or homogeneous with function of gradation $g(\mathbf{x})$ respectively

$$\begin{aligned} g^{1/2}(\mathbf{x}) &= (1 - 0.15x_1 + 0.25x_2) \\ g^{1/2}(\mathbf{x}) &= 1 \end{aligned}$$

and anisotropic or isotropic with constant coefficients

$$\hat{d}_{ij} = \begin{bmatrix} 1 & 0.45 \\ 0.45 & 0.75 \end{bmatrix} \quad \text{Anisotropic}$$

$$\hat{d}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{Isotropic}$$

The boundary conditions are that (see Figure 19)

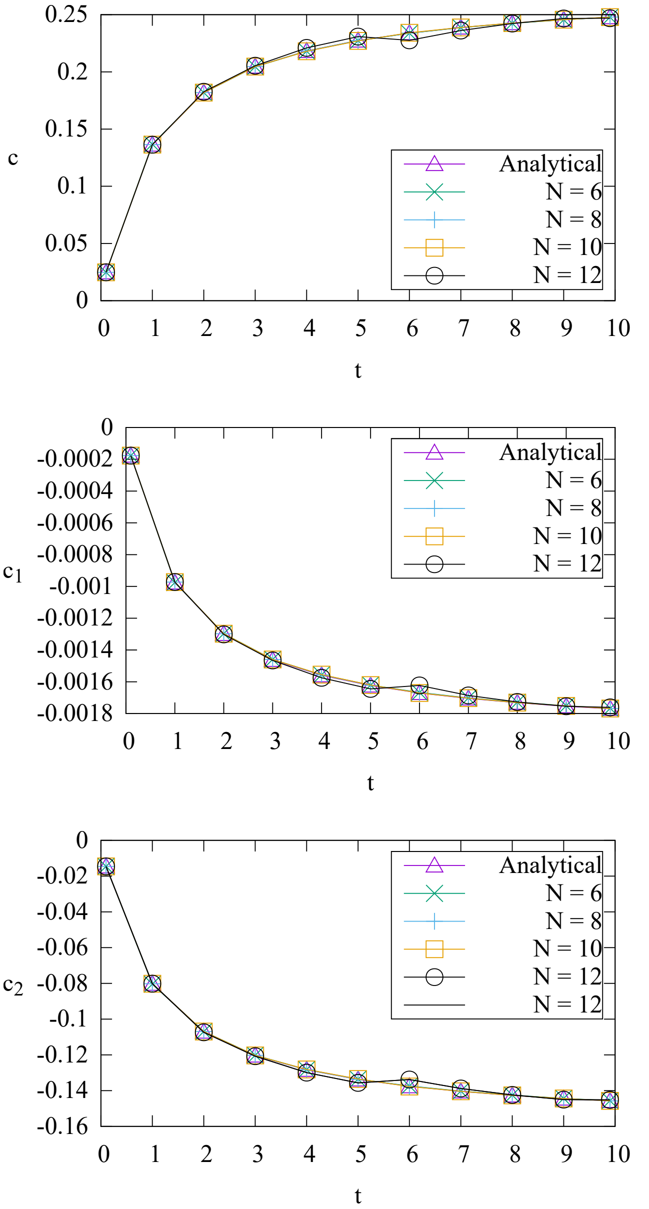

Fig. 18. The solutions c, $c_1 = \partial c/\partial x_1$ and $c_2 = \partial c/\partial x_2$ at $(x_1, x_2) = (0.5, 0.5)$ for Problem 4.

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

where $P(t)$ takes several forms, namely

$$
\begin{aligned}
&\text{Form 1:} \quad P(t) = 1\\
&\text{Form 2:} \quad P(t) = 1 - \exp(-0.85t)\\
&\text{Form 3:} \quad P(t) = 0.1t\\
&\text{Form 4:} \quad P(t) = t(10 - t)/25\\
&\text{Form 5:} \quad P(t) = t/(t + 1)
\end{aligned}
$$

There is no simple analytical solution for the problem. In fact the set of boundary conditions is geometrically symmetric about the axis $x_2 = 0.5$.

Figure 20 shows that the solution c varies with time t following the variation of function $P(t)$ as the boundary condition on the side AD. This verifies the consistency of the solution. Figure 20 also shows that for forms 1, 2 and 5 of

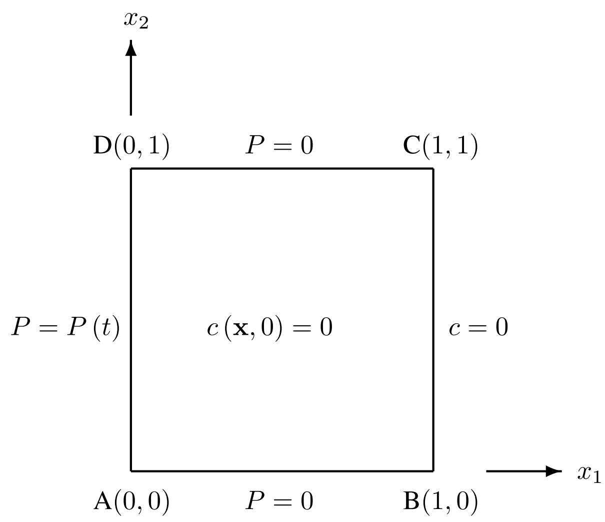

Fig. 19. The boundary conditions for the problems in Section IV-B

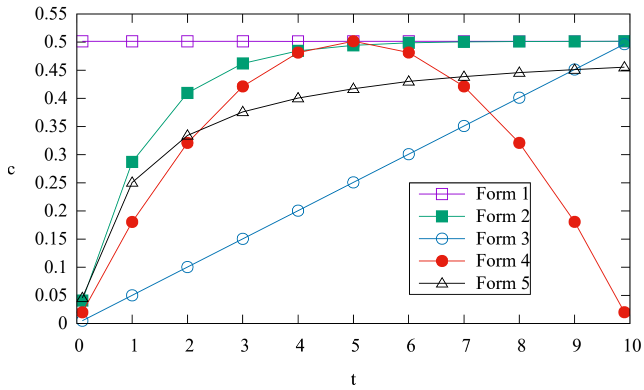

Fig. 20. The solutions c at $(x_1, x_2) = (0.5, 0.25)$ for all forms of $P(t)$ of Problem 5.

$P(t)$ the solution c will approach a same steady value as the time t goes to infinity. This is expected as the corresponding $P(t)$ will tend to 1 as the time t goes to infinity. Figure 21 indicates that as expected the values c coincide at points $(x_1, x_2) = (0.5, 0.25), (0.5, 0.75)$ (symmetric about the line $x_2 = 0.5$) when the material is isotropic homogeneous. Otherwise the values c differ which means that the anisotropy and inhomogeneity of the material contribute impact on the values of c.

V. Conclusion

Several problems for an unsteady anisotropic diffusion-convection equation of incompressible flow with a class of quadratically variable coefficients have been solved using a combined BEM and Laplace transform. From the results of the considered problems in Section IV, we may conclude that the analysis of reduction to constant coefficients equation (in Section III) for deriving the boundary-only integral equation (18) is valid, and the BEM and Stehfest formula is appropriate for solving such problems as defined in Section II. Moreover, the results of the test problem in Section IV-A show the accuracy of the method, whereas the results of the problem in Section IV-B exhibit the consistency of the numerical solutions. The effect of the inhomogeneity and anisotropy of materials as well as the obtained steady-state solutions are as expected.

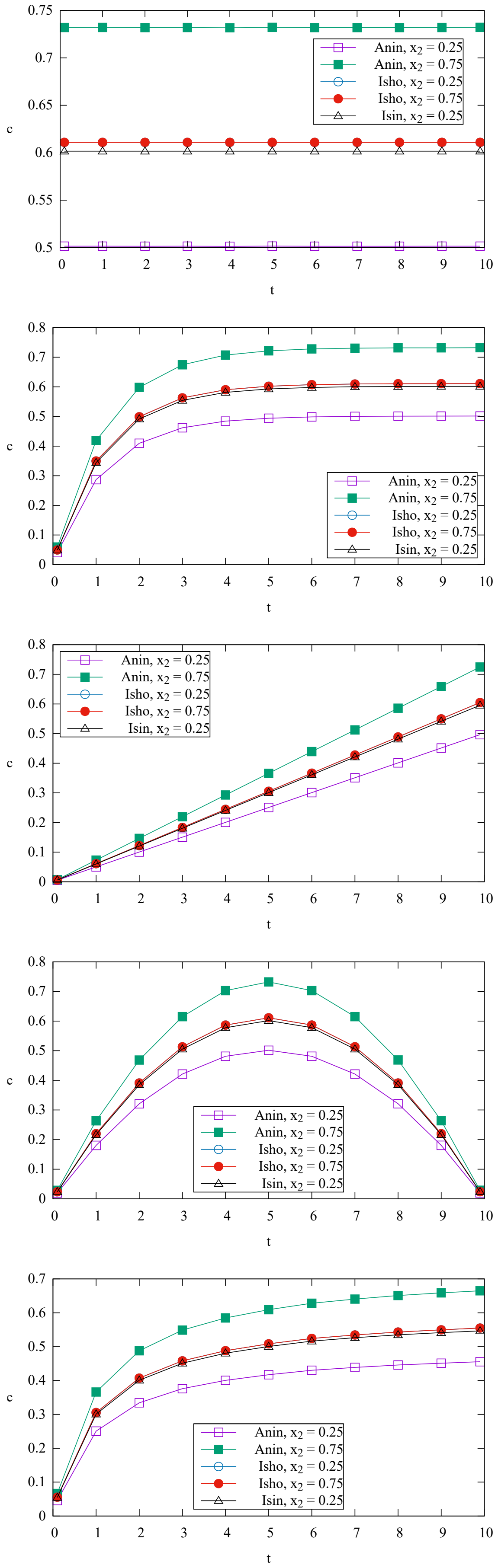

Fig. 21. The solutions c at $(x_1, x_2) = (0.5, 0.25), (0.5, 0.75)$ when the material is anisotropic inhomogeneous (Anin), isotropic homogeneous (Isho), isotropic inhomogeneous (Isin) for every form of $P(t)$ of Problem 5.

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