

Numerical Analysis of a Finite Volume-element Method for Unsteady Diffusion-reaction Equation

Suthisak Phongthanapanich

Department of Mechanical Engineering Technology, College of Industrial Technology, King Mongkut's University of Technology North Bangkok, Bangkok 10800, Thailand

E-mail: sutthisakp@kmutnb.ac.th

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Abstract

The paper presents the numerical analysis of a finite volume-element method for solving the unsteady scalar reaction-diffusion equations. The main idea of the method is to combine the concepts that are employed in the finite volume and the finite element method together. The finite volume method is used to discretize the unsteady reaction-diffusion equation, while the finite element method is applied to estimate the gradient quantities at cell faces. Robustness and efficiency of the combined method have been evaluated on uniform rectangular grids by using available numerical solutions of the two-dimensional reaction-diffusion problems. By implementing one-dimensional analysis, it is showed that the stability of the numerical scheme is given by the condition $\Delta t \leq \Delta x^2 / (2\varepsilon)$, and the scheme is consistent with an order of accuracy of $\mathcal{O}(\Delta x^2, \Delta t^2)$ with respect to $\ell_{2,\Delta x}$ norm.

Keywords: *Finite volume-element method, Numerical analysis, Unsteady diffusion-reaction equation*

1 Introduction

Recent development of several reaction-diffusion analysis schemes in biology, ecology, biochemistry, fluid mechanics and heat transfer has led to physically interesting and mathematically challenging problems related to the non-trivial numerical solution of the singularly perturbed initial/boundary value problem [1-4]. In general, solution of the singularly perturbed problem contains high-gradient boundary layers along the boundary of the domain [2]. Numerical approximation of such boundary layer flow behaviour is not simple, and thus the development of accurate numerical method for analyzing this problem must be done carefully. Some examples of such difficulty are encountered in the cases where the reaction-diffusion equation cannot be satisfied by a globally smooth function. In particular, if the unknown scalar variables vary rapidly within a thin layer, many standard numerical schemes may lead to inaccurate and unstable solutions. A robust and fast numerical method (computation of the full Jacobian matrix should be avoided), in the sense that the error should not deteriorate as the singular perturbation parameter tends to zero, is required.

During the past decade, many techniques of the finite element method for solving the singularly perturbed problems have been proposed and investigated [5,6]. The conventional Galerkin finite element method usually fails to analyze such unsteady reaction-diffusion problems when either the diffusion coefficient becomes small or a small time step is employed in the time discretization. The stabilized finite element method overcame this trouble by employing the balanced residual perturbation term with some stabilization parameters. However, such method has great influence on the solution accuracy. At the same time, some researchers employed the finite difference algorithm to analyze the reaction-diffusion problems [3,7]. Liao [7] proposed an efficient higher-order finite difference algorithm for solving the system of two-dimensional reaction-diffusion equations with nonlinear reaction term. The Pade approximation and Richardson extrapolation are used to achieve high-order solution accuracy in both the spatial and temporal domains. El Salam and Shehata [3] used the implicit Crank-Nicolson technique to linearize the governing equations and then solved the system of algebraic equations by using the LU-decomposition method.

Recently, many researchers proposed some mixed techniques of the finite element and finite volume methods for analyzing the parabolic equation [8-10]. Ma et al. [8] proposed the semi-discrete and full-discrete symmetric finite volume schemes based on the linear finite elements for a class of parabolic problems. The symmetric finite volume schemes are analyzed on dual mesh (cell-vertex scheme) of triangular cells. Wang [9] proposed three schemes of the finite volume element method for solving two-dimensional parabolic equations. The finite volume schemes are also discretized on dual mesh and the nodal value at the center of control volume is approximated by linear finite element interpolation functions. Recently, Phongthanapanich and Dechaumphai [10] proposed a finite volume element method, that combines the finite volume and the finite element methods for analyzing the unsteady scalar reaction-diffusion equation. The cell-centered finite volume method is used to analyze the problem on a uniform control volume. The concept of the finite element method is applied to estimate the gradient quantities herein by employing the method of weighted residuals to determine the nodal gradient quantities. Finally, the trapezoidal rule is used to calculate the gradient quantities at cell faces.

This paper can be considered as the continuation of the previous work [10], where the consistency, the stability, and the convergence of the finite volume-element method for solving the unsteady scalar reaction-diffusion equation are proved. The presentation of the paper starts from explanation of the theoretical formulation in Section 2. The numerical analysis of the proposed scheme is then applied in Section 3. Finally, the robustness and accuracy of the scheme is evaluated by using an example from Ref.[5].

2 Review of Finite Volume-element Method for Diffusion-reaction Equation

In this paper, the finite volume approach is used to discretize the following two-dimensional scalar reaction-diffusion equation,

$$\frac{\partial \varphi}{\partial t} - \varepsilon \nabla^2 \varphi + \kappa \varphi = f, \text{ in } \Omega \times T \quad (1)$$

subject to the boundary conditions

$$\varphi = g_D \text{ on } \partial\Omega_D \quad (2a)$$

$$\varepsilon \frac{\partial \varphi}{\partial \mathbf{n}} = g_N \text{ on } \partial\Omega_N \quad (2b)$$

with $\Omega = \partial\Omega_D \cup \partial\Omega_N$ with $\partial\Omega_D \cap \partial\Omega_N = 0$. The initial condition is defined for $\mathbf{x} \in \Omega$ with $\Omega \subset R^2$ by

$$\varphi(\mathbf{x}, 0) = \varphi_0(\mathbf{x}) \quad (3)$$

where ϕ is the scalar quantity, $\varepsilon > 0$ is the diffusion coefficient, κ is the reaction coefficient, $f = f(\mathbf{x})$ is the prescribed source term, and $T \in [0, T]$ for $T < \infty$.

The computational domain is first discretized into a collection of non-overlapping triangular control volumes $\Omega_i \in \Omega, i = 1, \dots, N$, that completely cover the domain such that

$$\Omega = \cup_{i=1}^N \Omega_i, \Omega_i \neq 0, \text{ and } \Omega_i \cap \Omega_j = 0 \text{ if } i \neq j \quad (4)$$

Equation (1) is then integrated over the control volume Ω_i to obtain

$$\int_{\Omega_i} \left(\frac{\partial \varphi}{\partial t} - \varepsilon \nabla^2 \varphi + \kappa \varphi - f \right) d\mathbf{x} = 0 \quad (5)$$

The finite difference approximation and the divergence theorem are then applied to the temporal and spatial terms [10,11], respectively, of the above equation to yield

$$\begin{aligned} \int_{\Omega_i} \varphi(\mathbf{x}, t^{n+1}) d\mathbf{x} &= \int_{\Omega_i} \varphi(\mathbf{x}, t^n) d\mathbf{x} \\ &+ \Delta t \left[\varepsilon \int_{\partial\Omega_i} n_i(\nu) \cdot \nabla \varphi(\nu, t^n) d\nu \right. \\ &\left. - \int_{\Omega_i} \kappa \varphi(\mathbf{x}, t^n) d\mathbf{x} + \int_{\Omega_i} f(\mathbf{x}) d\mathbf{x} \right] \end{aligned} \quad (6)$$

where $n_i(\nu)$ is the unit outward normal vector of $\partial\Omega_i$. The approximations to the cell average of ϕ over Ω_i at time t^n and t^{n+1} [12,13] are represented by

$$\varphi_i^n = \frac{1}{|\Omega_i|} \int_{\Omega_i} \varphi(\mathbf{x}, t^n) d\mathbf{x} \quad (7a)$$

$$\varphi_i^{n+1} = \frac{1}{|\Omega_i|} \int_{\Omega_i} \varphi(\mathbf{x}, t^{n+1}) d\mathbf{x} \quad (7b)$$

where $|\Omega_i|$ is the measure of Ω_i . For a rectangular control volume, the flux integral over $\partial\Omega_i$ appearing on the right-hand side of Eq.(6) could be approximated by the summation of fluxes passing through all the adjacent cell faces. Hence, by applying the quadrature integration formula on the spatial domain term, the flux integral over $\partial\Omega_i$ may be approximated by

$$\varepsilon \int_{\partial\Omega_i} n_i(v) \cdot \nabla \varphi(v, t^n) dv = \varepsilon \sum_{j=1}^4 |\Gamma_{ij}| \mathbf{n}_{ij} \cdot \nabla \varphi_{ij}(t^n) \quad (8)$$

where Γ_{ij} is the segment of boundary $\partial\Omega_i$ between two adjacent control volumes Ω_i and Ω_j , which is defined by

$$\partial\Omega_i = \cup_{j=1}^4 \Gamma_{ij} \text{ and } \Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j \quad (9)$$

The integrations of the other terms can then be approximated by

$$\int_{\Omega_i} \kappa \varphi(\mathbf{x}, t^n) d\mathbf{x} = |\Omega_i| \kappa \varphi_i(t^n) \quad (10)$$

$$\int_{\Omega_i} f(\mathbf{x}) d\mathbf{x} = |\Omega_i| f(x_i) \quad (11)$$

By substituting Eqs. (7a)-(11) into Eq.(6), a fully explicit finite volume-element scheme for solving Eq. (1) is obtained in the form

$$\varphi_i^{n+1} = \varphi_i^n + \left[\frac{\varepsilon \Delta t}{|\Omega_i|} \sum_{j=1}^4 |\Gamma_{ij}| \mathbf{n}_{ij} \cdot \nabla \varphi_{ij}^n - \Delta t \left[\kappa \varphi_i^n - f_i \right] \right] \quad (12)$$

where the quantities at time $t = n$ are $\varphi_{ij}^n = \varphi_{ij}(t^n)$, and $\varphi_i^n = \varphi_i(t^n)$. And the treatment of boundary conditions in this paper is based on using the concept of ghost cell. The central differencing at the boundary is used for the Neumann boundary condition, while the Dirichlet boundary condition is prescribed at the center of the ghost cell.

In this paper, the gradient term, $\nabla \varphi_{ij}^n$, is approximated by the weighted residuals method which is commonly used in the finite element technique [10-12]. Firstly, the $\nabla \varphi_i^n$ is assumed to distribute linearly over cell Ω_i , in the form

$$\nabla \varphi_i^n = \sum_{k=1}^4 N_k(\mathbf{x}) \nabla \varphi_k^n \quad (13)$$

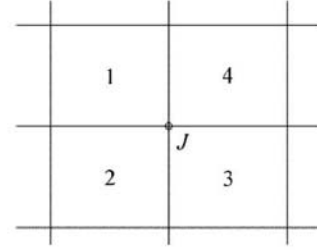


Figure 1: Rectangular cells surrounding point.

where $N_k(\mathbf{x})$ denotes the linear interpolation functions for rectangular cell. By applying the weighted residuals method and the Gauss's theorem to Eq.(13), the gradient quantities at point J are obtained as

$$\nabla \varphi_{J,i}^n = \mathbf{M}^{-1} \left[\int_{\partial\Omega_i} n_i(v) N_J(v) \varphi_i^n dv - \int_{\Omega_i} \frac{\partial N_J(\mathbf{x})}{\partial \mathbf{x}} \varphi_i^n d\mathbf{x} \right] \quad (14)$$

where \mathbf{M} is the consistent mass matrix, and $\nabla \varphi_{J,i}^n$ are the contributions of the gradient quantities in the cell Ω_i to the gradient quantities at point J . As an example, Figure 1 shows four rectangular cells surrounding point J . In order to compute the total gradient quantities at point J , Eq.(14) is applied to all cells surrounding the point J such that

$$\nabla \varphi_J^n = \sum_{i=1}^I \nabla \varphi_{J,i}^n \quad (15)$$

where I is the number of the surrounding cells. Finally, the gradient quantities at Γ_{ij} , $\nabla \varphi_{ij}^n$, are then computed by applying the trapezoidal rule along the common edge of cells i and j .

3 Numerical Analysis

For simplicity, the order of accuracy and stability of the explicit numerical scheme [14,15] given by Eq.(12) will be analyzed on uniform one-dimensional grid cell, $|\Omega_i| = \Delta x$. The numerical equation for i cell, $|\Omega_i| \in (x_{i-1/2}, x_{i+1/2})$, may be written as following

$$\varphi_i^{n+1} = \varphi_i^n + \frac{\varepsilon \Delta t}{\Delta x} \left(\left. \frac{\partial \varphi}{\partial x} \right|_{i+1/2}^n - \left. \frac{\partial \varphi}{\partial x} \right|_{i-1/2}^n \right) - \Delta t \left(\kappa \varphi_i^n - f_i \right) \quad (16)$$

By using one-dimensional linear interpolation function, the gradient quantities at cell faces $i-1/2$ and $i+1/2$ can be written by

$$\left. \frac{\partial \varphi}{\partial x} \right|_{i-1/2}^n = \frac{1}{\Delta x} (\varphi_i^n - \varphi_{i-1}^n) \quad (17a)$$

$$\left. \frac{\partial \varphi}{\partial x} \right|_{i+1/2}^n = \frac{1}{\Delta x} (\varphi_{i+1}^n - \varphi_i^n) \quad (17b)$$

and by using these expressions on the right hand side of Eq.(16) to give

$$\varphi_i^{n+1} = \varphi_i^n + \alpha (\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n) - \Delta t (\kappa \varphi_i^n - f_i) \quad (18)$$

where $\alpha = \varepsilon \Delta t / \Delta x^2$.

Denote the Eq.(1) by $\mathcal{L}v = F$ and the corresponding discretized approximation by $L_k^n u_k^n = G_k^n$ where G_k^n denotes an approximation has been made of the source term. By assuming that there is an approximate solution to this problem, u_k^n which is defined on grid and satisfies the initial condition $u_k^0 = f(k\Delta x)$. If the Eq.(18) is written in the generalized form as

$$\mathbf{u}^{n+1} = Q\mathbf{u}^n + \Delta t \mathbf{G}^n \quad (19)$$

where Q is an operator acting on the appropriate space, then a definition of consistency can be given as follows [15].

Definition 1: The numerical scheme given by Eq.(19) is consistent with the partial differential equation in a norm $\|\cdot\|$ if the solution of the partial differential equation, v , satisfies

$$\mathbf{v}^{n+1} = Q\mathbf{v}^n + \Delta t \mathbf{G}^n + \Delta t \boldsymbol{\tau}^n \quad (20a)$$

and

$$\|\boldsymbol{\tau}^n\| \rightarrow 0 \quad (20b)$$

as $(\Delta x, \Delta t) \rightarrow 0$, where \mathbf{v}^n denotes the vector whose k^{th} component is $v(k\Delta x, n\Delta t)$.

Definition 2: The numerical scheme given by Eq.(19) is said to be accuracy of order (p, q) to the given partial differential equation if

$$\|\boldsymbol{\tau}^n\| = \mathcal{O}(\Delta x^p) + \mathcal{O}(\Delta t^q) \quad (21)$$

Let v denote a solution of Eq.(1). Then by applying definition 1 to Eq.(18) yields

$$\begin{aligned} \Delta t(\tau_i^n) &= v_i^{n+1} - \left[v_i^n + \alpha (v_{i+1}^n - 2v_i^n + v_{i-1}^n) \right. \\ &\quad \left. - \Delta t (\kappa v_i^n - f_i) \right] \\ &= v_i^n + (v_t)_i^n \Delta t + (v_{tt})_i^n \frac{\Delta t^2}{2} - (v_i^n \\ &\quad + \alpha \left[v_i^n + (v_x)_i^n \Delta x + (v_{xx})_i^n \frac{\Delta x^2}{2} \right. \\ &\quad \left. + (v_{xxx})_i^n \frac{\Delta x^3}{6} + (v_{xxxx})_i^n \frac{\Delta x^4}{24} \right. \\ &\quad \left. - 2v_i^n + v_i^n - (v_x)_i^n \Delta x + (v_{xx})_i^n \frac{\Delta x^2}{2} \right. \\ &\quad \left. - (v_{xxx})_i^n \frac{\Delta x^3}{6} + (v_{xxxx})_i^n \frac{\Delta x^4}{24} \right] \\ &\quad - \Delta t (\kappa v_i^n - f_i) \\ &= (v_t)_i^n \Delta t + (v_{tt})_i^n \frac{\Delta t^2}{2} - \alpha (v_{xx})_i^n \Delta x^2 \\ &\quad - (v_{xxxx})_i^n \frac{\Delta x^4}{12} + \Delta t \kappa v_i^n - \Delta t f_i \\ &= (v_{tt})_i^n \frac{\Delta t^2}{2} - \alpha (v_{xxxx})_i^n \frac{\Delta x^4}{12} \end{aligned} \quad (22)$$

and

$$(\tau_i^n) = (v_{tt})_i^n \frac{\Delta t}{2} - \varepsilon (v_{xxxx})_i^n \frac{\Delta x^2}{12} \quad (23)$$

By assuming that v_{tt} and v_{xxxx} satisfy

$$\sum_{i=-\infty}^{\infty} [(v_{tt})_i^n]^2 \Delta x < A < \infty \quad (24a)$$

$$\sum_{i=-\infty}^{\infty} [(v_{xxxx})_i^n]^2 \Delta x < B < \infty \quad (24b)$$

for any Δx and Δt , then the numerical scheme is accurate order $(\Delta x^2, \Delta t)$ with respect to the $\ell_{2, \Delta x}$ norm. To further improve the time accuracy of the scheme, the second-order accurate Runge-Kutta time stepping method [16] is applied to Eq.(12). And by following the idea of Shu and Osher [16], the accurate order of the numerical scheme is increase to $(\Delta x^2, \Delta t^2)$ with respect to the $\ell_{2, \Delta x}$ norm.

Definition 3: The homogeneous part of Eq.(18), $\mathbf{u}^{n+1} = Q\mathbf{u}^n$, is stable with respect to norm $\|\cdot\|$ if there exist positive constant Δx_0 and Δt_0 , and non-negative constants K and β so that

$$\|\mathbf{u}^{n+1}\| \leq Ke^{\beta M} \|\mathbf{u}^0\| \quad (25)$$

for $0 < \Delta x \leq \Delta x_0$ and $0 < \Delta t \leq \Delta t_0$.

Next, to analyze the stability of the numerical scheme, the discrete Fourier transform for the problem of the form

$$\hat{\phi}_i^n = \xi^n e^{ij\pi\Delta x}, \quad 0 \leq j \leq M \quad (26)$$

is applied to the homogeneous part of Eq.(18), term by term, to obtain

$$\begin{aligned} \xi^{n+1} e^{ij\pi\Delta x} &= \xi^n e^{ij\pi\Delta x} + \alpha \left[\xi^n e^{l(i+1)j\pi\Delta x} \right. \\ &\quad \left. - 2\xi^n e^{ij\pi\Delta x} + \xi^n e^{l(i-1)j\pi\Delta x} \right] \\ &\quad - \Delta t (\kappa \xi^n e^{ij\pi\Delta x}) \end{aligned} \quad (27)$$

$$G = \frac{\xi^{n+1}}{\xi^n} = 1 + \alpha \left[e^{lj\pi\Delta x} + e^{-lj\pi\Delta x} - 2 \right] - \Delta t \kappa \quad (28)$$

where G is the amplification factor. Then by using some trigonometric identity to yield

$$\begin{aligned} G &= 1 + \alpha \left[2 \cos(j\pi\Delta x) - 2 \right] - \Delta t \kappa \\ &= 1 - 4\alpha \sin^2 \left(j\pi \frac{\Delta x}{2} \right) - \Delta t \kappa \end{aligned} \quad (29)$$

According to von Neumann condition, the homogeneous part of Eq.(18) is stable with respect to the $\ell_{2,\Delta x}$ norm if and only if there exists positive constant C so that $|G| \leq 1 + C\Delta t$ for all $\xi \in [-\pi, \pi]$. Then by applying von Neumann condition to Eq.(29) to have

$$\left| 1 - 4\alpha \sin^2 \left(j\pi \frac{\Delta x}{2} \right) - \Delta t \kappa \right| \leq 1 + \kappa \Delta t \quad (30)$$

And the maximum time step Δt , is given by

$$\Delta t \leq \frac{\Delta x^2}{2\varepsilon} \quad (31)$$

In order to analyze the consistency of the numerical scheme and by utilizing Eq.(30), it is requires that $\alpha \leq 0.5$ to yield

$$\left| 1 - 4\alpha \sin^2 \left(j\pi \frac{\Delta x}{2} \right) - \Delta t \kappa \right| \leq 1 + \kappa \Delta t \leq e^{\kappa \Delta t} \quad (32)$$

By using the definition of the amplification factor from Eq.(28), then to have

$$\|\hat{\phi}^{n+1}\|_2 \leq e^{\kappa M} \|\hat{\phi}^n\|_2 \quad (33)$$

Lastly, by applying the result of Eq.(33) $n + 1$ times and using the Parseval's identity, to yield

$$\|\hat{\phi}^{n+1}\|_2 \leq e^{\kappa(n+1)\Delta t} \|\hat{\phi}^0\|_2 \quad (34)$$

and

$$\begin{aligned} \|\hat{\phi}^{n+1}\|_{2,\Delta x} &= \sqrt{\Delta x} \|\hat{\phi}^{n+1}\|_2 \\ &\leq \sqrt{\Delta x} e^{\kappa(n+1)\Delta t} \|\hat{\phi}^0\|_2 \\ &= \sqrt{\Delta x} e^{\kappa(n+1)\Delta t} \|\phi^0\|_2 \\ &= e^{\kappa(n+1)\Delta t} \|\phi^0\|_{2,\Delta x} \end{aligned} \quad (35)$$

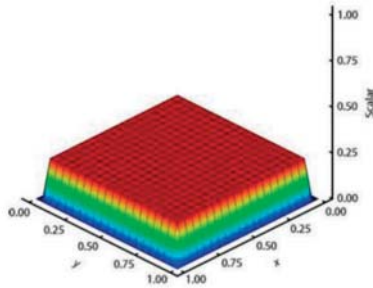
Hence by the definition of stability, Eq.(18) is stable with respect to the discrete energy norm. And by making the appropriate smoothness assumptions on the derivatives of the solution, then the numerical scheme is converge with respect to the discrete energy norm.

4 Numerical Experiments

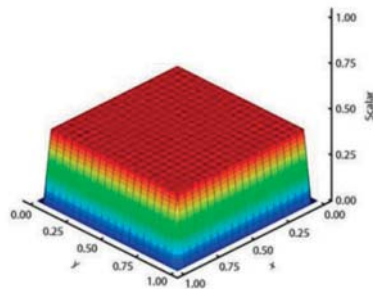
To evaluate the robustness and accuracy of the proposed finite volume element method, one reaction-diffusion problem subjected to homogeneous boundary conditions are examined. The example is used to evaluate the capability of the proposed method for the singularly perturbed problem where the diffusion coefficient is very small as compared to the reaction coefficient. The numerical results obtained from this example will be compared with the finite element solutions presented by Franca et al. [5].

4.1 Reaction-dominated diffusion problem

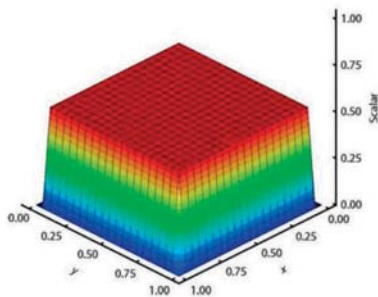
The example is a reaction-dominated diffusion problem, with $\varepsilon = 10^{-6}$, $\kappa = 1$, and $f = 1$. The initial condition is given by $\phi_0(x) = 0$. A unit square domain is divided into 400 uniform square grids (20×20). The problem is analyzed using the fixed time step of $\Delta t = 0.1$. Figures 2(a)-(d) show the numerical solutions of the tested grids at four different times. The four computed profiles show that there is no spurious oscillation along the high-gradient boundary layers. For the purpose of comparison with the solutions presented in Ref.[5] (Variant of the PGEM), the analysis is repeated but at different times of $t = 0.1$, and $t = 7.5$.



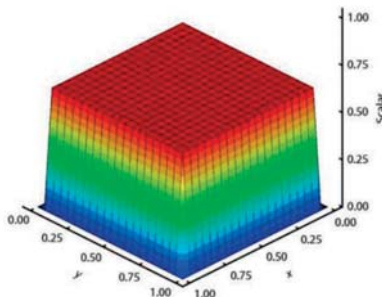
(a) At time $t = 0.25$



(b) At time $t = 0.5$

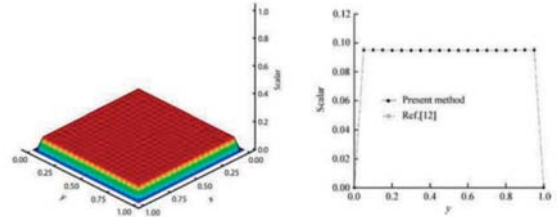


(c) At time $t = 0.75$



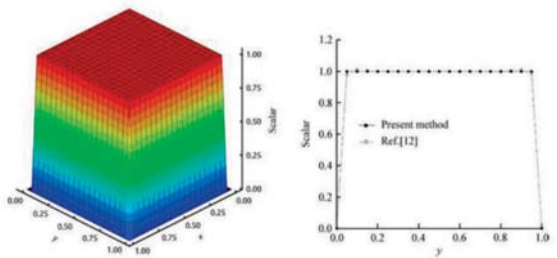
(d) At time $t = 1.0$

Figure 2: Numerical solutions at four different times of problem 4.1.



(a) At time $t = 0.1$ (b) Along the line $x = 0.5$

Figure 3: Comparison of numerical solutions of problem 4.1 ($t = 0.1$).



(a) At time $t = 7.5$ (b) Along the line $x = 0.5$

Figure 4: Comparison of numerical solutions of problem 4.1 ($t = 7.5$).

At time $t = 0.1$, the computed profiles and the solutions at $x = 0.5$ are shown in Figures 3(a) and 3(b), respectively. Figures 4(a) and 4(b) show the similar behavior of the solution at the time of $t = 7.5$. Spurious oscillation does not occur along the high-gradient boundary layers of the solution profiles at these two times. The maximum values are comparable with the solutions from the method presented by Ref.[5].

5 Conclusions

This paper presents an explicit finite volume element method for analyzing the reaction-diffusion equation on two-dimensional domain. The theoretical formulation of the combined finite volume and finite element method was explained in details. The finite volume method was applied for discretizing the computational domain, while the finite element method was used to estimate the gradient quantities at the cell faces. By applying the one-dimensional numerical analysis, the result shown that that the stability of the numerical scheme is given

by the condition $\Delta t \leq \Delta x^2 / (2\varepsilon)$, and the scheme is consistent with an order of accuracy of $\mathcal{O}(\Delta x^2, \Delta t^2)$ with respect to $\ell_{2,\Delta x}$ norm. And by making the appropriate smoothness assumptions on the derivatives of the solution, then the numerical scheme is converge with respect to the discrete energy norm. The numerical test cases have shown that the combined method does not require any special numerical treatment to improve the solution stability.

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