Second-order Finite Volume Method
for Two-dimensional Convection-reaction Equation

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บทคัดย่อ

    ระเบียบวิธีไฟไนต์วอลุ่มความถูกต้องลำดับที่สอง สำหรับการแก้สมการการพาและการเกิดปฏิกิริยาในสองมิติบนกริดแบบสามเหลี่ยมได้ถูกนำเสนอ การประมาณพจน์อนุพันธ์ลำดับสูงกว่ากระทำที่ครึ่งช่วงเวลาโดยอาศัยการกระจายอนุกรมของเทย์เลอร์ กรณีทดสอบเชิงตัวเลขได้แสดงให้เห็นว่าระเบียบวิธีที่นำเสนอไม่ต้องการพจน์การนำเทียมเพื่อช่วยให้ผลลัพธ์มีเสถียรภาพ ความแข็งแกร่งและความถูกต้องของระเบียบวิธีที่นำเสนอได้ถูกประเมินผลโดยใช้ผลลัพธ์แม่นตรงและผลลัพธ์เชิงตัวเลข ที่มีอยู่ของปัญหาการพาอย่างเดียว และปัญหาการพาและการเกิดปฏิกิริยาในสองมิติ

คำสำคัญ: สมการการพาและการเกิดปฏิกิริยา ระเบียบวิธีไฟไนต์วอลุ่ม วิธีชัดแจ้ง

Abstract

    A second-order finite volume method for solving two-dimensional convection-reaction equation on triangular grids is presented. Approximation of the higher-order derivative terms is determined at the half time step using the Taylor's series expansion. Numerical test cases have shown that the scheme does not need artificial diffusion term to improve the solution stability. The robustness and accuracy of the proposed scheme have been evaluated by using available analytical and numerical solutions of the two-dimensional pure-convection and convection-reaction problems.

1. Introduction

    The convection-reaction equation is the generalized governing equation for modeling the chemical reactive transport phenomena. The convection-reaction equation admits solutions with moving steep solution gradients. At present, the development of accurate numerical modeling for the convection-reaction equation is still an active research task in computational fluid dynamics [1]-[6]. Many of the current methods, however, suffer from serious numerical difficulties for simulating the reactive transport phenomenon. To alleviate these problems, an upwinding approach has been widely used in the finite difference, finite element and finite volume methods [7], [8]. In solving the hyperbolic

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equation, the numerical techniques may be classified into explicit and implicit (or semi-implicit) methods. The explicit method is popular because it is simple and parallelizable. But the method is limited by the CFL condition, and a small time step is normally required to stabilize the computational procedure. The attempt to relief such constraint is also an active research topic [3]. On the other hand, the implicit method is unconditionally stable, but larger time step may not be used due to its loss of accuracy as solution involved in time. The inversion of the coefficient matrix is another weakness of the method because it is a time consumable process.

In this paper, an explicit high-resolution finite volume method based on a second-order approximation is proposed for solvingthe two-dimensional convection-reaction equation on triangular grids. The robustness and accuracy of the proposed method was eamined by using the convection-dominated problems. For these problems, several schemes become unstable and produce node to node fluctuation [1], [2]. To suppress the fluctuation, artificial diffusion is normally added into the schemes. One of the main objectives of the proposed method is to achieve the numerical stability without adding any artificial diffusion, in order to avoid excessive deterioration of the computed numerical solution. Many current higher-order numerical schemes need some kinds of limiter functions to ensure a bounded solution. The higher-order reconstruction process presented in this paper avoids the use of the limiter function as shown by the numerical examples in Section 3.

The presentation of the paper starts from explanation of the theoretical formulation in Section 2. Evaluation of the proposed method is then examined in Section 3 by using four examples. These examples are: (1) the rotation of cone-shape scalar field, (2) the rotation of slotted cylinder, (3) the oblique inflow convection-reaction (convection-dominated), and (4) the oblique inflow convection-reaction (reaction-dominated) problems.

2. Governing Equation and Finite Volume Formulation

The differential equation for the two-dimensional convection-reaction equation is governed by,

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{v}\phi) + \kappa\phi = q \tag{1}$$

where ϕ is the scalar quantity, t is the time, $\mathbf{v} = \mathbf{v}(\mathbf{x})$ is the given convection velocity vector, κ is the reaction coefficient, and $q = q(\mathbf{x}, t)$ is the prescribed source term. Equation (1) is considered for $\mathbf{x} \in \Omega$ where $\Omega \subset R^2$, and $t \in (0, T)$. The initial condition is defined for $\mathbf{x} \in \Omega$ by $\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x})$. The computational domain is first discretized into a collection of non-overlapping triangular control volumes $\Omega_i \in \Omega, i = 1, \ldots, N$, that completely cover the domain such that $\Omega = \bigcup_{i=1}^{N} \Omega_i$ and $\Omega_i \neq 0$, $\Omega_i \cap \Omega_j = 0$ if $i \neq j$. Equation (1) is then integrated over the control volume Ω_i and in the time interval (t^n, t^{n+1}) to obtain

$$\int_{\Omega_i} \int_{t^n}^{t^{n+1}} \left(\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{v}\phi) + \kappa\phi - q \right) dt d\mathbf{x} = 0 \tag{2}$$

The temporal integration and the divergence theorem are then applied to the first term and the second term, respectively, to yield

$$\int_{\Omega_i} \phi(\mathbf{x}, t^{n+1}) d\mathbf{x} = \int_{\Omega_i} \phi(\mathbf{x}, t^n) d\mathbf{x}$$
$$- \int_{t^n}^{t^{n+1}} \int_{\partial\Omega_i} \mathbf{n}_i(\upsilon) \cdot (\mathbf{v}(\upsilon)\phi(\upsilon, t)) d\upsilon dt$$
$$+ \int_{\Omega_i} \int_{t^n}^{t^{n+1}} \kappa\phi(\mathbf{x}, t) dt d\mathbf{x} - \int_{\Omega_i} \int_{t^n}^{t^{n+1}} q(\mathbf{x}, t) dt d\mathbf{x} \tag{3}$$

where $\boldsymbol{n}_i(\upsilon)$ is the unit normal vector of $\partial\Omega_i$.

In the conventional finite volume method, the approximation to the cell average of ϕ over Ω_i at time t^n and t^{n+1} is represented by [9]

$$\phi_i^n = \frac{1}{|\Omega_i|}\int_{\Omega_i}\phi(\boldsymbol{x},t^n)d\boldsymbol{x} \tag{4a}$$

$$\phi_i^{n+1} = \frac{1}{|\Omega_i|}\int_{\Omega_i}\phi(\boldsymbol{x},t^{n+1})d\boldsymbol{x} \tag{4b}$$

where $|\Omega_i|$ is the measure of Ω_i. For a triangular control volume, the flux integral over $\partial\Omega_i$ appearing on the right-hand side of Eq. (3) could be approximated by the summation of the fluxes passing through the three adjacent cell faces. Hence, by applying the quadrature integration formula on both the temporal and spatial domain terms, the flux integral over $\partial\Omega_i$ may be approximated by

$$\int_{t^n}^{t^{n+1}}\int_{\partial\Omega_i}\boldsymbol{n}_i(\upsilon)\cdot\big(\boldsymbol{v}(\upsilon)\phi(\upsilon,t)\big)d\upsilon dt \tag{5}$$

$$= \Delta t\sum^3\big|\Gamma_{ij}\big|\boldsymbol{n}_{ij}\cdot\boldsymbol{v}_{ij}\phi_{ij}(t^{n+1/2})$$

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 $\partial\Omega_i = \bigcup_{j=1}^3\Gamma_{ij}$ and $\Gamma_{ij} = \partial\Omega_i\cap\partial\Omega_j$.

The integrations of the reaction and source terms could be approximated by

$$\int_{\Omega_i}\int_{t^n}^{t^{n+1}}\kappa\phi(\boldsymbol{x},t)dtd\boldsymbol{x} = \Delta t|\Omega_i|\kappa\phi_i^{n+1/2} \tag{6}$$

and

$$\int_{\Omega_i}\int_{t^n}^{t^{n+1}}q(\boldsymbol{x},t)dtd\boldsymbol{x} = \Delta t|\Omega_i|q_i(t^{n+1/2}) \tag{7}$$

By substituting Eqs. (4)-(7) into Eq. (3), an explicit finite volume scheme for solving Eq. (1) is obtained in the form

$$\phi_i^{n+1} = \phi_i^n - \frac{\Delta t}{|\Omega_i|}\sum_{j=1}^3\big|\Gamma_{ij}\big|\boldsymbol{n}_{ij}\cdot\boldsymbol{v}_{ij}\phi_{ij}^{n+1/2} \tag{8}$$

$$- \Delta t\big(\kappa\phi_i^{n+1/2} - q_i^{n+1/2}\big)$$

where $\phi_{ij}^{n+1/2} = \phi_{ij}(t^{n+1/2})$, $\phi_i^{n+1/2} = \phi_i(t^{n+1/2})$, and $q_i^{n+1/2} = q_i(t^{n+1/2})$.

Finally, the scalar quantities at the half time step $t = n+1/2$ of $\phi_{ij}^{n+1/2}$ and $\phi_i^{n+1/2}$, are approximated by applying the Taylor's series expansion in both space and time. For the explicit formulation, the temporal derivative term may be estimated by adapting the idea for local expansion of unknown along the characteristics [1], [8]. By assuming that velocity is pointed in the direction from Ω_i to Ω_j, the value of $\phi_{ij}^{n+1/2}$ and $\phi_i^{n+1/2}$ and can be written in the form

$$\phi_{ij}^{n+1/2} = \phi_i^n + \big(\boldsymbol{x}_{ij} - \boldsymbol{x}_i\big)\cdot\nabla\phi_i^n - \frac{\Delta t}{2}\big(\boldsymbol{v}_i\cdot\nabla\phi_i^n\big) \tag{9}$$

and

$$\phi_i^{n+1/2} = \phi_i^n - \frac{\Delta t}{2}\big(\boldsymbol{v}_i\cdot\nabla\phi_i^n\big) \tag{10}$$

For opposite direction of the velocity, the value $\phi_{ij}^{n+1/2}$ and $\phi_i^{n+1/2}$ could be computed from Eqs. (9) and (10) but by using the values from the neighboring triangles according to the upwinding direction.

It is well-known that, to ensure the stability of the numerical scheme on triangular grid, the CFL-like stability criterion must be fulfilled. In this paper, the time-step within each control volume is determined from

$$\Delta t = C\min_i\left(\frac{|\Omega_i|}{\max_{j=1,2,3}|\boldsymbol{v}_{n,ij}|}\right) \tag{11}$$

where $\boldsymbol{v}_{n\,ij}$ is the normal velocity at Γ_{ij} and $0 < C \le 1$.

3. Numerical Examples

To evaluate the robustness and accuracy of the proposed second-order finite volume method,

two pure-convection examples and two convection-reaction examples are examined. These examples are: (1) rotation of cone-shaped scalar field, (2) rotation of slotted cylinder, (3) oblique inflow convection-reaction (convection-dominated), and (4) oblique inflow convection-reaction (reaction-dominated) problems.

3.1 Rotation of Cone-shaped Scalar Field

The cone-shaped scalar field is rotated around the domain $\Omega = (-0.5, 0.5) \times (0.5, 0.5)$. The initial condition [10]

$$\phi(\boldsymbol{x}, 0) = \begin{cases} 0 & r > 0.1 \\ 5[1 = \cos(10\pi r)] & r \le 0.1 \end{cases} \quad (12)$$

where r is the distance from the cone center at (0.0, 0.25). The rotating velocity field with the angular velocity of 2π rad/s is imposed as $u(\boldsymbol{x}) = -2\pi y$ and $v(\boldsymbol{x}) = -2\pi x$.

The time step is equal to 1, which is the time period required for one turn rotation. The exact solution at $t=1$ is then equal to initial condition that was given by Eq. (12) above. Figures 1(a)-(b) show the initial grid of 32×32 ($\Delta x = \Delta y = 1/32$), and the exact solution at the time step $t=1$. Figures 2(a)-(c) show the numerical solutions of the three uniform grids S1, S2, and S3 (32×32, 64×64, and 128×128), respectively. The maximum scalar value and the L_2-norm percentage errors (value in parenthesis) obtained from these three grids are 5.04 (2.1%), 8.42(1.11%), and 9.71 (0.57%), respectively. By comparing with the exact solution of 10, the numerical solutions show that the proposed method provides solution that converges to the exact solution as the grid is refined. Figures 2(a)-(c) also highlight the overshoot and undershoot of the numerical solutions that are significantly diminished on the refined grid S3.
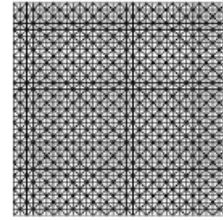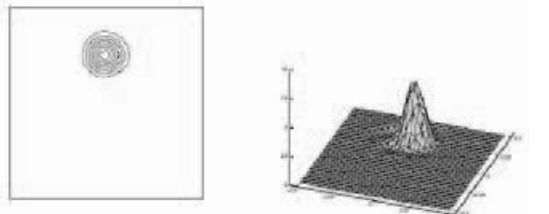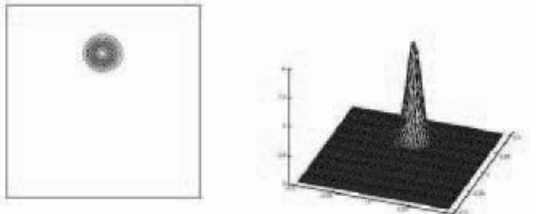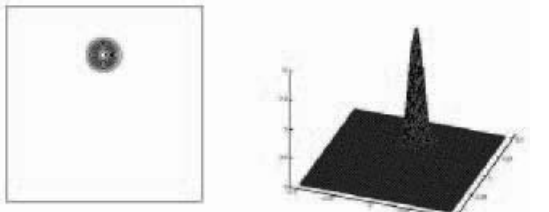

(a) Grid S1
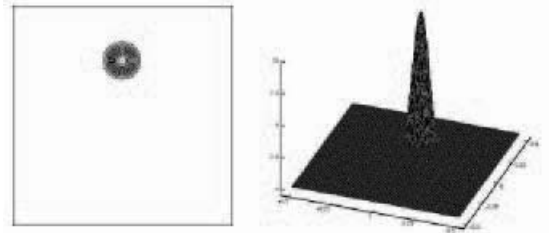
(b) Exact solution

Figure 1 (a)-(b) Example of grid S1 and exact solution of problem 3.1.

(a) Grid S1

(b) Grid S2

(c) Grid S3

Figure 2 (a)-(c) Comparison of numerical solutions on grids S1, S2, and S3 of problem 3.1.

3.2 Rotation of Slotted Cylinder

The rotation of slotted cylinder problem is a popular and challenging convection problem. This is because the sudden change of the initial conditions and the shape of the rectangular slot are difficult to capture by most numerical schemes. The problem was firstly introduced by Zalesak [11], and in this example, the original problem is slightly modified for testing on the domain $\Omega = (0,0) \times (1,1)$. The initial condition $\phi(\boldsymbol{x}, 0)$ is given by

$$\phi(\boldsymbol{x},0) = \begin{cases} 1 & (r > 0.15) \cup (|x - 0.5| \leq 0.025 \\ & \cap (y - 0.5) \leq 0.1) \\ 0 & \text{otherwise} \end{cases} \quad (13)$$

where r is the distance from the center of the domain $(0.5, 0.5)$, and the velocity field is given by $u(\boldsymbol{x}) = y - 0.5$ and $v(\boldsymbol{x}) = 0.5 - x$.

The time step for this example is set to be equal to the time period required for one turn rotation. The exact solution at the final time step is then equal to the initial condition that was given by Eq. (13) above. Figures 3(a)-(d) show the exact and the numerical solutions of the three uniform grids S1, S2, and S3, respectively. The L_2-norm percentage errors obtained from these three grids are 0.26%, 0.09%, and 0.04%, respectively. The numerical comparisons show that the proposed method can provide converged and comparable solution to the exact solution on the finer grid S3. While the shape of slotted cylinder is recovered on the grid S3, the overshoot and undershoot appear slightly as illustrated in Fig. 3(d). To capture the discontinuities efficiently, the adaptive remeshing technique [12]-[14] may be incorporated into the proposed scheme.

3.3 Oblique Inflow Convection-Reaction (Convection-dominated)

The third example is the oblique inflow convection-

(a) Exact solution

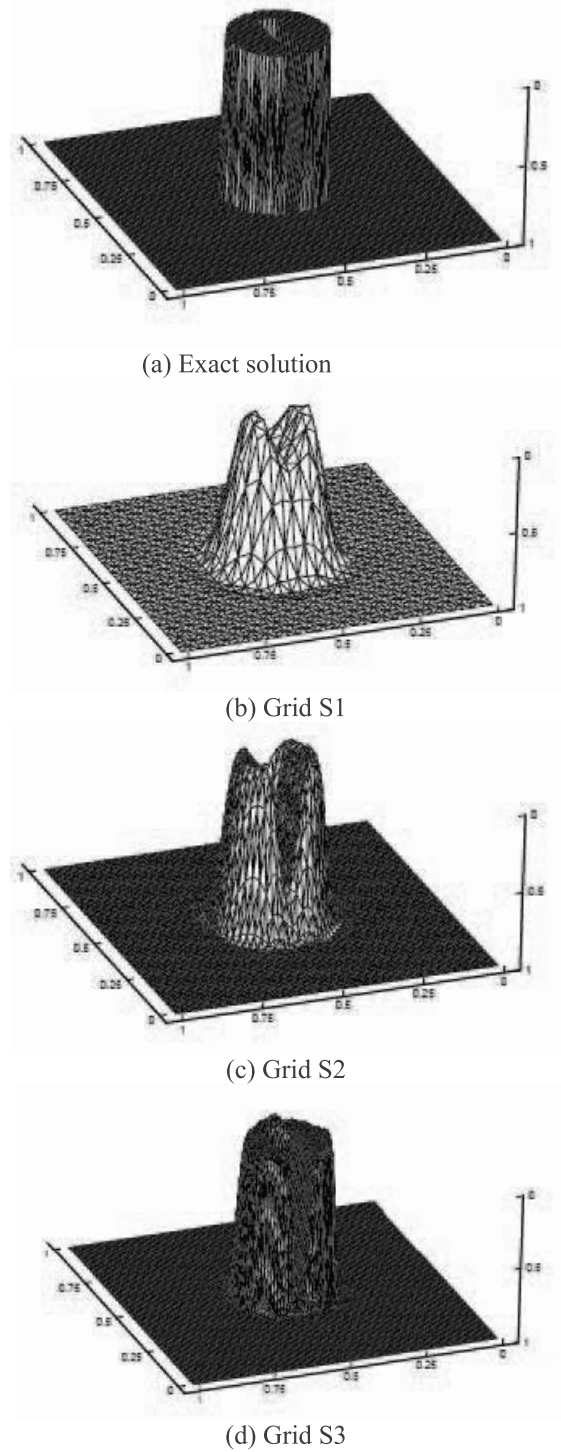(b) Grid S1

(c) Grid S2

(d) Grid S3

Figure 3 (a)-(d) Comparison of exact and numerical solutions on three grids of problem 3.2.

reaction (convection-dominated) problem adapted from Codina [1]. The domain size is the unit square of $\Omega = (0,0) \times (1,1)$. The initial condition $\phi(x,0)$ is set to be zero. The steady velocity field is given by $u(x) = \cos(\pi/3)$ and $v(x) = \sin(\pi/3)$. The source term, q, is given as a constant of 1, and the reaction coefficient, κ is prescribed as a small value of 10^{-4}. With such small reaction effect, the scalar quantities profile flows across the domain with an increasing amount of its height until it approaches the outflow boundaries.

The analysis of this problem is performed on a 16×16 grid size, and the numerical solutions at four time steps, t=0.25, 0.50, 0.75, and 2.0, are shown in Figures 4(a)-(d). It should be noted that this same problem was performed on a uniform grid of 20×20 in Codina [1] and there was oscillation along the fronts of the scalar quantity profile. The oscillation was significantly alleviated by using a finer grid of 52×52 in Codina [1], but the severely overshoot of the solution appeared at the outflow corner. Figures 4(a)-(d) show the solutions from the proposed numerical scheme. Numerical oscillation does not appear along the front of the scalar quantity profile. Without adding any artificial diffusion into the solution, the computed solution thus does not suffer from excessive diffusion as it proceeds in time.

3.4 Oblique Inflow Convection-Reaction (Reaction-dominated)

The last example is similar to example 3.3 above but the reaction effect is dominated. The domain size at four different time steps of problem 3.4 and the initial condition $\phi(x,0)$ is identical to the preceding example but the steady velocity field is
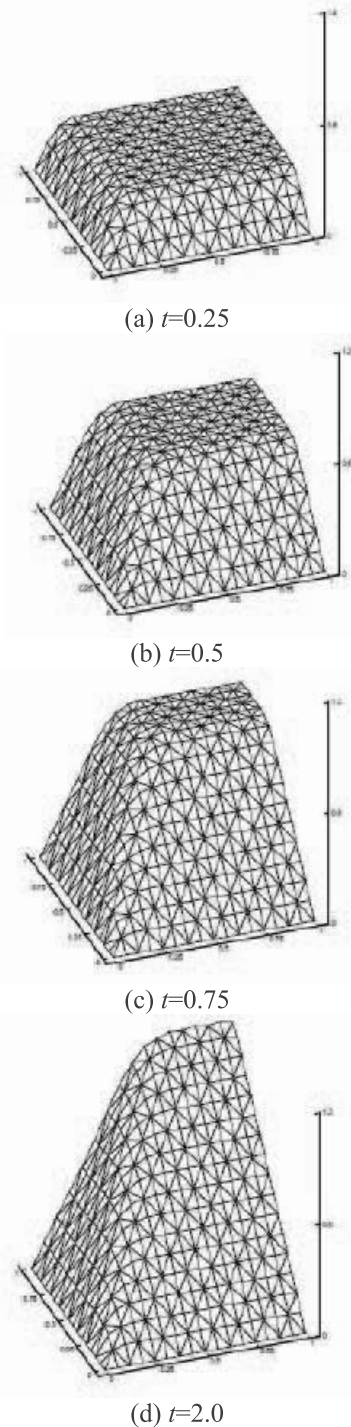

(a) t=0.25

(b) t=0.5

(c) t=0.75

(d) t=2.0

Figure 4 (a)-(d) Numerical solutions on 16×16 grid size at four different time steps of problem 3.3.

(a) t=0.25

(b) t=0.5

(c) t=0.75

(d) t=2.0
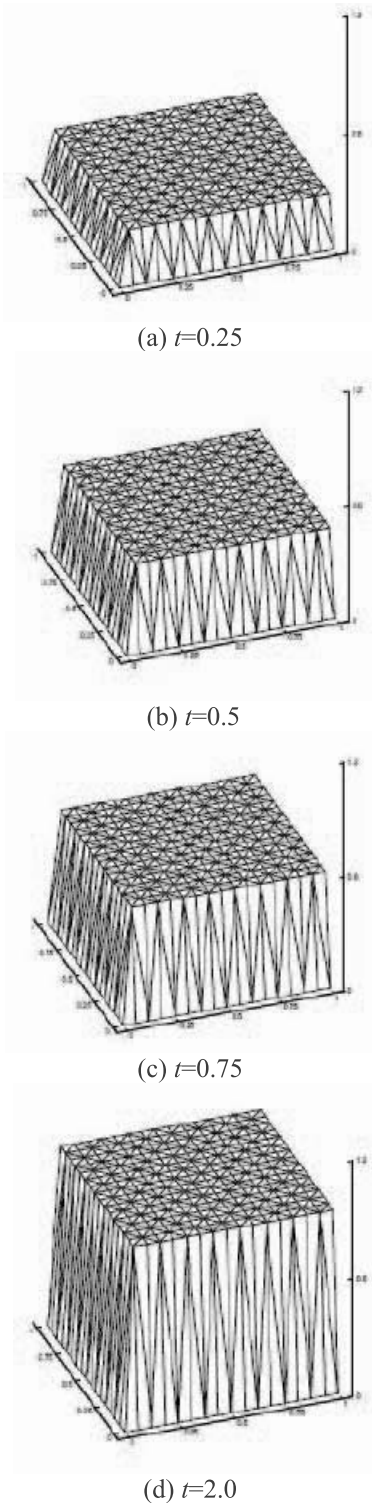
Figure 5   Numerical solutions on 16×16 grid size

given by $u(\boldsymbol{x}) = 10^{-4}\cos(\pi/3)$ and $v(\boldsymbol{x}) = 10^{-4}\sin(\pi/3)$.

The source term, a, is given as a constant of 1, and the reaction coefficient, k is prescribed as a small value of 1. With such a large reaction effect, the scalar quantity profile also flows across the domain with an increasing amount of its height uniformly throughout the domain. Again, the analysis is performed on a 16×16 grid size, and the numerical solution at the four time steps of t=0.25, 0.50, 0.75, and 2.0, are shown in Figures 5(a)-(d). For this problem, the Streamline-Upwind Petrov-Galerkin method (SUPG) [1] using a uniform grid of 20×20 yields some oscillations along all fronts of the scalar quantity profile. Such oscillations disappeared by using a finer grid of 52×52, but all fronts are smeared. Figures 5(a)-(d) show that the proposed numerical scheme does not produce any oscillation along the sharpen fronts of the scalar quantity profile using the 16×16 grid size.

5. Conclusions

An explicit second-order finite volume method for solving the two-dimensional convection-reaction equation on triangular grids is presented. The theoretical formulation of the method was explained in details. The method does not need any kind of limiter functions to ensure the bounded solutions of convection- reaction problems as shown in the examples mentioned above. Four numerical examples were used. The solution behavior and its accuracy are improved as the grid is refined.

6. Acknowledgements

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