An Explicit Characteristic-based Finite Volume-Element Method for Convection-Diffusion-Reaction Equation with Source Term

Phongthanapanich S.

Department of Mechanical Engineering Technology, College of Industrial Technology,King Mongkut's University of Technology North Bangkok, Bangkok 10800, Thailand
E-mail address: sutthisakp@kmutnb.ac.th

Abstract

A second-order accurate characteristic-based finite volume method for analyzing time-dependent scalar convection-diffusion-reaction equation in two dimensions is presented. The concept of the characteristic-based scheme is applied to solve the convection-diffusion-reaction equation. The finite volume method is employed to establish the discretized equations for the spatial domain, while the weighted residuals finite element technique is used to estimate the gradient quantities at the cell faces and cell-centered of the control volume. Numerical test cases have shown that the method reduces spurious oscillations and does not require an explicit artificial diffusion for improving the solution stability. The efficiency, robustness and convergence order of the method are investigated by using available analytical and numerical solutions of pure convection, convection-diffusion and convection-diffusion-reaction problems.

Keywords*: Convection-diffusion-reaction equation, Characteristic-based scheme, Explicit scheme, Finite volume-element method*

1 Introduction

Transport phenomena of the convection-diffusion problem in fluid dynamics is a basis for explaining behaviors for a broad class of problems in physical, chemical, biological sciences and engineering [1-4]. Because these problems are related to the hyperbolic conservation law for which their solutions always contain discontinuity and high gradient, accurate numerical solutions are very difficult to obtain. For the convection-dominated diffusion problems, sharp fronts may form up and move throughout the computational domain. In such situation, a spurious non-physical oscillation, known as the Gibbs' phenomenon, can develop and deteriorate the accuracy of the numerical solution obtained from using the standard finite difference and finite element methods. Many special treatments have been developed and applied to suppress such spurious oscillation that occurs in the computed solutions for the convection and convection-dominated diffusion problems. At present, improved methods for approximating the convection term are still needed. Development of accurate numerical methods for the convection-diffusion equations remains a challenging task in computational fluid dynamics [5-10].

It is well-known that the standard Galerkin finite element method usually yields oscillatory solution for convection-dominated diffusion problem. Many techniques have been proposed to overcome the method instability in order to improve the solution accuracy [11-15,7]. As an example of a flow in the boundary layer, the use of a single stabilizing parameter is insufficient to provide smooth flow distribution in the vicinity of sharp solution gradient that is not aligned with the velocity direction. The shock-capturing procedure [16] is a usual remedy for this situation. Among several stabilizing schemes, the characteristic Galerkin scheme has been developed by using the time stepping as the basis [17,18,13,19]. The scheme, which is based on Taylor's series expansion, is attractive due to the ease of implementation that can be written in a fully explicit form [18,20]. Many second-order time-integration finite element methods have been proposed by combining the standard Galerkin spatial discretization with the second-order accurate time stepping scheme. These second-order methods include the Lax-Wendroff, leap frog, and Crank-Nicolson methods. These methods, however, fail to produce satisfactory numerical solutions for convection dominated problems [23]. Many multi-step explicit schemes have also developed to provide higher-order solution accuracy but are suffered from severe restriction of the allowable time step in both convection and diffusion-dominated problems. Some methods can provide high solution accuracy by using the graded meshes for capturing detailed solutions [24,25]. For example, the subgrid scale stabilized method [26] is a technique that can provide high solution accuracy in all physical regimes. Its solution stability for the advection-diffusion-reaction equation is examined by using the Fourier analysis as presented in Ref. [27].

Computational techniques for solving the hyperbolic equation are generally classified into the explicit and implicit (or semi-implicit) methods. The explicit method is simple to implement and can provide acceptable solution accuracy. However, the method is constrained by the CFL condition in order to stabilize the spatial error from growing without bound. Attempts to relief the constraint have been developed, such as the one proposed by Wang and Liu [28]. On the other hand, the implicit method provides a more stable solution. However, a large time step size may not be used because the solution accuracy degrades with time. The inversion of the coefficient matrix is another weakness of the method since it is a time consumable process and requires a large block of memory.

The objective of this work is to develop an explicit characteristic-based finite volume method that provides stabilized numerical solutions for two-dimensional convection-diffusion-reaction problems. The combination of the conventional finite element and finite volume methods for solving fluid flow problems is of interest by many researchers recently [29-32]. However, the idea of using the finite volume scheme to discretize the characteristic-based convection-diffusion-reaction equation has never been investigated. In this paper, the concept of characteristic-based scheme [13,20], for approximating the Lagrangian derivatives in time, is used to derive the discretized convection-diffusion-reaction equation. An explicit finite volume method is employed to derive the discretized equations for the spatial domain. The cell-face and cell-centered gradient quantities implemented in the present scheme is obtained by using the weighted residuals finite element method. The robustness and efficiency of the proposed method are examined by analyzing the pure convection, convection-dominated diffusion, and convection-diffusion-reaction problems. The presentation of the paper starts from explaining the theoretical formulation and the corresponding characteristic-based scheme in Section 2. The finite volume discretization of the characteristic equations is presented in Section 3. Finally, the proposed method is examined and evaluated in Section 4 by using five examples. These examples are: (1) the Gaussian distribution flow in a square problem, (2) the Codina's test cases, and (3) the skew flow problem.

2 Characteristic convection – diffusion – reaction formulation

The characteristic-based scheme for convection-diffusion-reaction equation is presented in this section. The governing differential equation of a typical transport process with an unknown scalar quantity ϕ for the transient convection-diffusion-reaction problem with source term on a two-dimensional domain is [33],

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

The differential equation is subjected to the boundary conditions

$$\phi = g_D \quad \text{on} \quad \partial\Omega_D \tag{2}$$

$$\varepsilon \frac{\partial \phi}{\partial \mathbf{n}} = g_N \quad \text{on} \quad \partial\Omega_N \tag{3}$$

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

$$\phi(\mathbf{x},0) = \phi_0(\mathbf{x}) \tag{4}$$

where ϕ is the scalar quantity, $\mathbf{v} = \mathbf{v}(\mathbf{x})$ is the given convection velocity vector, $\varepsilon \geq 0$ is the diffusion coefficient, κ is the reaction coefficient, $q = q(\mathbf{x},t)$ is the prescribed source term, and for $T < \infty$.

By following the step described in Refs.[13,20], the convection-diffusion-reaction equation along the characteristic can be written by

$$\frac{\partial \phi}{\partial t} + \phi\nabla' \cdot \mathbf{v} - \nabla' \cdot (\varepsilon \nabla' \phi) + \kappa\phi = q \tag{5}$$

where all terms are evaluated at $\mathbf{x}' = \mathbf{x}'(t)$. The finite difference method is then applied to the temporal term and the spatial term is approximated by the quantities at time n (by backward tracing along the characteristic). Finally, the fully explicit semi-discrete form of Eq. (5) can be written in the form

$$\frac{1}{\Delta t}\left(\phi^{n+1}\Big|_{\mathbf{x}} - \phi^{n}\Big|_{\mathbf{x}-\Delta\mathbf{x}}\right) = \left(-\phi\nabla\cdot\mathbf{v} + \nabla\cdot(\varepsilon\nabla\phi) - \kappa\phi + q\right)^{n}\Big|_{\mathbf{x}-\Delta\mathbf{x}} \tag{6}$$

where $\phi = \phi(\mathbf{x}', t)$ and $\mathbf{x}'$ is the path of the characteristic wave. The incremental time period Δt is from n to $n+1$, and the incremental distance $\Delta\mathbf{x}$ is from $\mathbf{x}-\Delta\mathbf{x}$ to $\mathbf{x}$. The local Taylor's series expansion in space is applied to the second term on the left-hand side and to all the right-hand side terms of the equation. The incremental distance $\Delta\mathbf{x}$ along the characteristic path is then approximated by $\Delta\mathbf{x} = \overline{\mathbf{v}}\Delta t$, where $\overline{\mathbf{v}}$ is the average velocity along the characteristic [20]. To obtain a fully explicit scheme, $\overline{\mathbf{v}}$ is approximated by

$$\begin{aligned}\overline{\mathbf{v}} &= \frac{1}{2}\left(\mathbf{v}^{n+1}\Big|_{\mathbf{x}} + \mathbf{v}^{n}\Big|_{\mathbf{x}-\Delta\mathbf{x}}\right) \\ &\approx \Delta t\left(\mathbf{v}^{n} - \frac{\Delta t}{2}\mathbf{v}^{n}\cdot\nabla\mathbf{v}^{n}\right)\Bigg|_{\mathbf{x}}\end{aligned} \tag{7}$$

Finally Eq. (6) can be written in the form

$$\begin{aligned}\phi^{n+1} - \phi^{n} = &-\Delta t\left[\nabla\cdot(\mathbf{v}\phi - \varepsilon\nabla\phi) + \kappa\phi - q\right]^{n} \\ &+ \frac{(\Delta t)^2}{2}\left[\nabla\cdot(\mathbf{v}\nabla\cdot(\mathbf{v}\phi)) - \nabla\cdot\mathbf{v}\nabla\cdot(\mathbf{v}\phi)\right. \\ &\left.+ \kappa\mathbf{v}\cdot\nabla\phi - \mathbf{v}\cdot\nabla q\right]^{n}\end{aligned} \tag{8}$$

3 Explicit finite volume formulation

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

$$\Omega = \cup_{i=1}^{N}\Omega_i,\ \Omega_i \neq 0, \text{and}\ \Omega_i \cap \Omega_j = 0 \ \text{ if } i \neq j \tag{9}$$

Equation (8) is then integrated over the control volume Ω_i [34] to obtain

$$\begin{aligned}\int_{\Omega_i}\left(\phi^{n+1} - \phi^{n}\right)d\mathbf{x} = &\int_{\Omega_i} -\Delta t\left[\nabla\cdot(\mathbf{v}\phi - \varepsilon\nabla\phi) + \kappa\phi - q\right]^{n} \\ &+ \frac{(\Delta t)^2}{2}\left[\nabla\cdot(\mathbf{v}\nabla\cdot(\mathbf{v}\phi)) - \nabla\cdot\mathbf{v}\nabla\cdot(\mathbf{v}\phi)\right. \\ &\left.+ \kappa\mathbf{v}\cdot\nabla\phi - \mathbf{v}\cdot\nabla q\right]^{n} d\mathbf{x}\end{aligned} \tag{10}$$

Then the divergence theorem is applied to the spatial terms to yield

$$\begin{aligned}\int_{\Omega_i}\phi^{n+1}d\mathbf{x} = &\int_{\Omega_i}\phi^{n}d\mathbf{x} \\ &- \Delta t\int_{\partial\Omega_i}\left[n_i(\nu)\cdot(\mathbf{v}(\nu)\phi(\nu,t^n) - \varepsilon\nabla\phi(\nu,t^n))\right]d\nu \\ &+ \frac{(\Delta t)^2}{2}\int_{\partial\Omega_i} n_i(\nu)\cdot\left[(\mathbf{v}(\nu)\nabla\cdot(\mathbf{v}(\nu)\phi(\nu,t^n)) - \right. \\ &\qquad \left.\mathbf{v}(\nu)\phi(\nu,t^n)\nabla\cdot(\mathbf{v}(\mathbf{x}))\right]d\nu \\ &- \Delta t\int_{\Omega_i}\left[\kappa\phi(\mathbf{x},t^n) - q(\mathbf{x},t^n)\right]d\mathbf{x} \\ &+ \frac{(\Delta t)^2}{2}\int_{\Omega_i}\left[\kappa\mathbf{v}(\mathbf{x})\cdot\nabla\phi(\mathbf{x},t^n) - \right. \\ &\qquad \left.\mathbf{v}(\mathbf{x})\cdot\nabla q(\mathbf{x},t^n)\right]d\mathbf{x}\end{aligned} \tag{11}$$

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} are represented by

$$\phi_i^{n} = \frac{1}{|\Omega_i|}\int_{\Omega_i}\phi^{n}d\mathbf{x} \tag{12}$$

$$\phi_i^{n+1} = \frac{1}{|\Omega_i|}\int_{\Omega_i}\phi^{n+1}d\mathbf{x} \tag{13}$$

where $|\Omega_i|$ is the measure of Ω_i. For any control volume, the flux integral over $\partial\Omega_i$ appearing on the right-hand side of Eq. (11) could be approximated by the summation of fluxes passing through all adjacent cell faces. Hence, by applying the midpoint quadrature integration rule on the spatial domain terms, the flux integral over $\partial\Omega_i$ may be approximated by

$$\int_{\partial\Omega_i}\left[n_i(\nu)\cdot(\mathbf{v}(\nu)\phi(\nu,t^n)-\varepsilon\nabla\phi(\nu,t^n))\right]d\nu \approx \sum_{j=1}^{NF}\left|\Gamma_{ij}\right|\mathbf{n}_{ij}\cdot\left[\mathbf{v}_{ij}\phi_{ij}(t^n)-\varepsilon\nabla\phi_{ij}(t^n)\right] \tag{14}$$

$$\int_{\partial\Omega_i} n_i(\nu)\cdot\left[(\mathbf{v}(\nu)\nabla\cdot(\mathbf{v}(\nu)\phi(\nu,t^n))- \mathbf{v}(\nu)\phi(\nu,t^n)\nabla\cdot(\mathbf{v}(\mathbf{x}))\right]d\nu \approx \sum_{j=1}^{NF}\left|\Gamma_{ij}\right|\mathbf{n}_{ij}\cdot\mathbf{v}_{ij}\left[\nabla\cdot(\mathbf{v}\phi_i(t^n))-\phi_{ij}(t^n)\nabla\cdot\mathbf{v}\right] \tag{15}$$

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

$$\partial\Omega_i = \cup_{j=1}^{NF}\Gamma_{ij} \text{ and } \Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j \tag{16}$$

The integrations of the other terms can then be approximated by

$$\int_{\Omega_i}\kappa\phi(\mathbf{x},t^n)d\mathbf{x} \approx \left|\Omega_i\right|\kappa\phi_i(t^n) \tag{17}$$

$$\int_{\Omega_i} q(\mathbf{x},t^n)d\mathbf{x} \approx \left|\Omega_i\right| q_i(t^n) \tag{18}$$

$$\int_{\Omega_i}\kappa\mathbf{v}(\mathbf{x})\cdot\nabla\phi(\mathbf{x},t^n)d\mathbf{x} \approx \left|\Omega_i\right|\kappa\mathbf{v}\cdot\nabla\phi_i(t^n) \tag{19}$$

$$\int_{\Omega_i}\mathbf{v}(\mathbf{x})\cdot\nabla q(\mathbf{x},t^n)d\mathbf{x} \approx \left|\Omega_i\right|\mathbf{v}\cdot\nabla q_i(t^n) \tag{20}$$

By substituting Eqs. (12)-(20) into Eq.(11), a fully explicit characteristic-based finite volume scheme for solving Eq. (1) is obtained in the form

$$\phi_i^{n+1} = \phi_i^n - \frac{\Delta t}{\left|\Omega_i\right|}\sum_{j=1}^{NF}\left|\Gamma_{ij}\right|\mathbf{n}_{ij}\cdot\left[\mathbf{v}_{ij}\phi_{ij}^{n+1/2} + \frac{\Delta t}{2}\mathbf{v}_{ij}\phi_{ij}^n\nabla\cdot\mathbf{v} - \varepsilon\nabla\phi_{ij}^n\right] + \frac{(\Delta t)^2}{2}\left[\kappa\mathbf{v}\cdot\nabla\phi_i^n - \mathbf{v}\cdot\nabla q_i^n\right] - \Delta t\left[\kappa\phi_i^n - q_i^n\right] \tag{21}$$

where the quantities at time $t = n$ are $\phi_{ij}^n = \phi_{ij}(t^n)$, $\phi_i^n = \phi_i(t^n)$, and $q_i^n = q_i(t^n)$. Finally, the scalar quantity at the half time step $t = n + 1/2$, $\phi_{ij}^{n+1/2}$ is expressed by

$$\phi_{ij}^{n+1/2} = \phi_i^n + (\mathbf{x}_{ij} - \mathbf{x}_i)\cdot\nabla\phi_i^n - \frac{\Delta t}{2}\nabla\cdot(\mathbf{v}\phi_i^n) \tag{22}$$

where $\mathbf{x}_i$ and $\mathbf{x}_{ij}$ are the cell centroid and the face centroid locations, respectively. For the opposite direction of velocity, the values of $\phi_{ij}^{n+1/2}$ could be computed from Eq. (22) by using the values from the neighboring control volumes according to the upwinding direction.

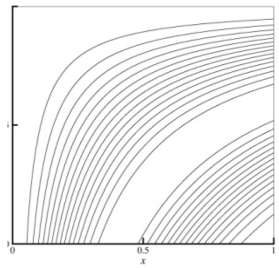
4 Numerical experiments

To evaluate the performance of the proposed finite volume method, three examples of the pure-convection, convection-diffusion and convection-diffusion-reaction problems are examined. These examples are: (1) the Gaussian distribution flow in a square problem, (2) the Codina's test cases problem, and (3) the skew flow problem. Because the proposed method (CFVM) is developed using the concept of the characteristic-based finite element method (CBSFEM) [20], thus, the solutions from the CBSFEM will be used to compare with those obtained from the CFVM.

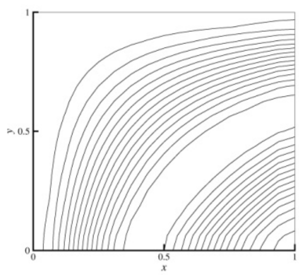
4.1 *Gaussian distribution flow in a square*

The first example is adopted from the paper presented by Waterson and Deconinck [35] for testing the solution convergence to the steady-state solution. The example is a convection problem with unknown of a scalar quantity from a non-uniform flow field in a unit square domain, $\Omega = (0,0)\times(1,1)$. The initial condition $\phi(\mathbf{x},0)$ is set to be zero and the inflow boundary condition along $y = 0$ is given by $\phi(\mathbf{x}, t \ge 0) = \exp(-2x)\sin^2(\pi x)$. The steady-state velocity field is specified by $u(\mathbf{x}) = x$ and $v(\mathbf{x}) = 1 - y$.

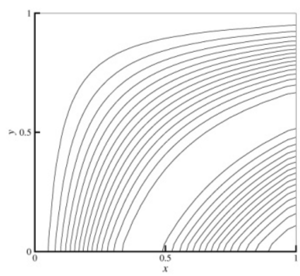
The uniform grids S0 to S4 consisting of 8×8 ($\Delta x = \Delta y = 1/8$), 16×16, 32×32, 64×64, 128×128 cells, respectively, are used in this test case. Figures 1(a)-(d) show the exact and numerical solutions of the three uniform grids, S1 to S3. Figure 3 shows the computed profiles at the outlet boundary $x = 1$ obtained from grids S1 to S3 as compared to the exact solution. The computed profiles obtained from these grids approach the exact solution as the grid is refined.



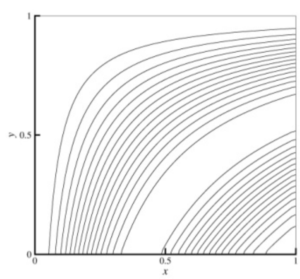
(a) Exact solution



(b) Grid S1



(c) Grid S2



(d) Grid S3

Figure 1: Comparison of exact and numerical solutions on grids S1, S2, and S3.

The exact solution for this problem is $\phi(\mathbf{x}) = \exp(-2x(1-y))\sin^2(\pi x(1-y))$. The steady-state solution is defined by the value of the solution when the residual $\frac{1}{NE}\sqrt{\left(\phi_i^{n+1} - \phi_i^n\right)^2}$ is less than 10^{-6}. Figure 3 shows the plot of the L_2-norm errors of the solutions versus grid sizes. By comparing the computed solutions with the exact minimum and maximum values of 0 and 0.4064, respectively, the proposed method provides solution that converges to the exact solution as the grid is refined. It is noted that the experimental order of convergence (EOC) of the L_2-norm error for this problem is about two.

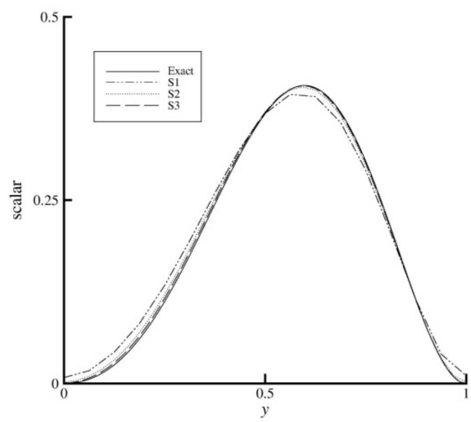


Figure 2: Comparison of exact and numerical solutions along the boundary $x = 1$.

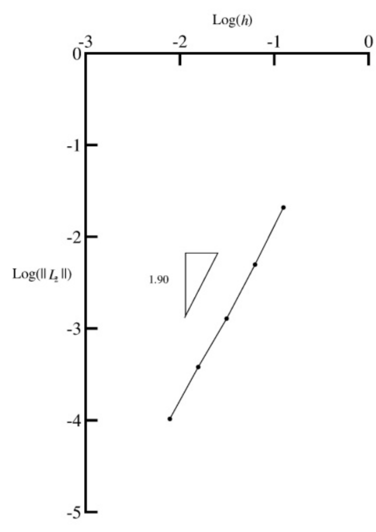


Figure 3: Plot of L_2-error norms versus grid sizes.

4.2 *Codina's test cases*

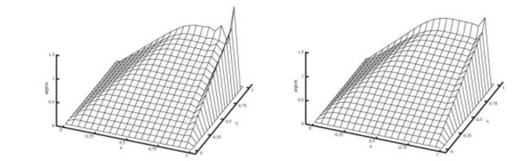
The next example is the oblique inflow convection-diffusion-reaction problem which was presented by Codina [36]. The domain size is a unit square of $\Omega = (0,0) \times (1,1)$ and the initial condition $\phi(\mathbf{x},0)$ is set to be zero. The steady velocity field,

$$u(\mathbf{x}) = V\cos(\pi/3)$$
$$v(\mathbf{x}) = V\sin(\pi/3) \tag{23}$$

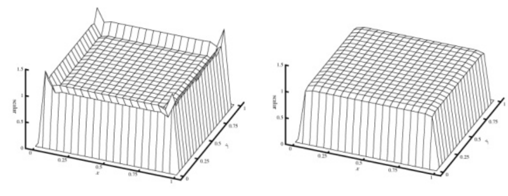
with $q = 1$, and $\varepsilon = 10^{-4}$. Three different cases have been tested, with the given parameters as follows;

(I) $V = 1, \kappa = 10^{-4}$ (convection-dominated), (II) $V = 10^{-4}, \kappa = 1$ (reaction-dominated) and (III) $V = 0.5, \kappa = 1$ (combined effect). The steady-state analyses of these test cases are performed on a 20×20 grid size.

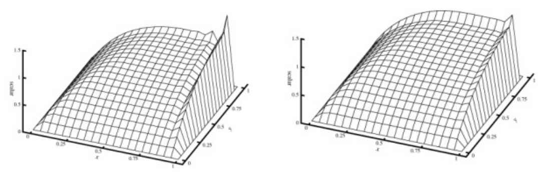
For case I with a small reaction effect, the scalar quantity profile flows across the domain with an increasing amount of its height until it approaches the outflow boundaries as shown by Figure 4(a). Both methods yield overshooting solutions along the outflow boundaries. However, the magnitude of the overshooting solution obtained from the CFVM is less than those of the CBSFEM and SUPG methods [37]. For case II with a large reaction effect, the scalar quantity profile also flows across the domain with an increasing amount of its height uniformly through out the domain. Figure 4(b) shows that the CBSFEM yields oscillation along all fronts of the scalar quantity profile as well as the SUPG and GLS methods. Solutions obtained from the CFVM and the SGS methods do not produce any oscillation along the fronts of the scalar quantity profile on this grid size. For case III with the combined convection and reaction effect, the scalar quantity profile represents a superposition of the solutions from cases (a) and (b) together. In this case, all methods yield oscillation along all fronts of the scalar quantity profile as shown by Figure 4(c). To eliminate the overshooting of the computed solution along such outflow boundaries of cases I and II, the Barth and Jespersen limiter function [38] is applied to the gradient terms in Eqs.(26) and (27). With the limiter function, the solution overshooting disappears along such outflow boundaries as shown by Figures 12(a)-(b).



(a) Case I

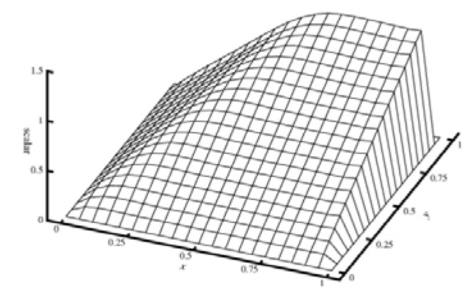


(b) Case II

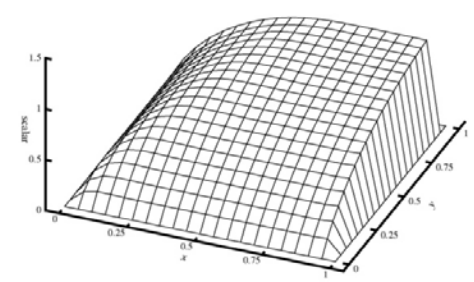


(c) Case III

Figure 4: Comparison of numerical solutions (Left=CBSFEM, Right=CFVM).



(a) Case I



(b) Case III

Figure 5: Numerical solutions with limiter function.

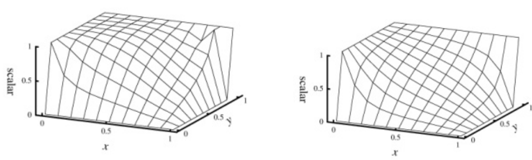
4.3 *Skew flow*

The last example is a skew flow problem presented by Hauke [26]. This example considers the behavior of the numerical solutions in different flow regimes in a square domain $\Omega = (0,0) \times (1,1)$, with the initial condition $\phi(\mathbf{x},0)$ of zero. Four boundary conditions are $\phi(x=0,t) = \phi(y=1,t) = 1$, and $\phi(x=1,t) = \phi(y=0,t) = 0$. The velocity field is given by

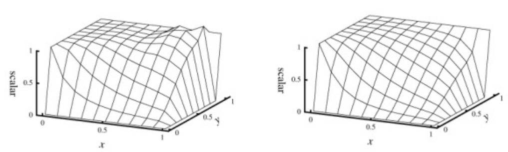
$$u(\mathbf{x}) = \cos(\pi/6) \quad v(\mathbf{x}) = \sin(\pi/6) \tag{24}$$

with $q = 0$. Three different cases have been tested with the given parameters of; (I) $\varepsilon = 0.5, 0.05, 0.005; \kappa = 0$, and (II) $\varepsilon = 0.005; \kappa = 100, 10, 1$.

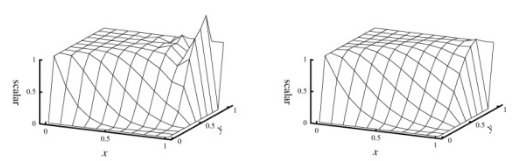
The analyses of these test cases are performed on the 10×10 grid size as were used in Ref.[26]. The numerical solutions are examined at the steady-state condition.



(a) $\varepsilon = 0.5, \kappa = 0$



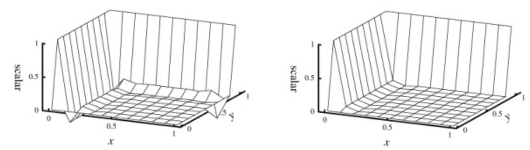
(b) $\varepsilon = 0.05, \kappa = 0$



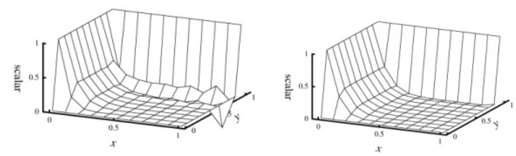
(c) $\varepsilon = 0.005, \kappa = 0$

Figure 6: Case I, comparison of numerical solutions (Left=CBSFEM, Right=CFVM).

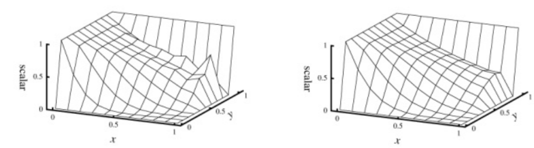
For case I, Figures 6(a)-(c) show that the CBSFEM produces overshooting solutions along boundary $x = 1$ for all values of ϵ, whereas the CFVM yields good stable solutions. For case II, Figures 7(a)-(c) show that the CBSFEM still produces oscillations near the boundary $y = 1$ for all values of κ, whereas the CFVM provides good stable solutions. The CBSFEM yields oscillated and incorrect solutions especially in the sub-cases (b) and (c), even though these solutions converge to steady-state condition. It should also be noted that for all tested cases, the solutions obtained by CFVM are comparable with those from the SGS method presented in Ref.[26].



(a) $\varepsilon = 0.005, \kappa = 100$



(b) $\varepsilon = 0.005, \kappa = 10$



(c) $\varepsilon = 0.005, \kappa = 1$

Figure 7: Case II, comparison of numerical solutions (Left=CBSFEM, Right=CFVM).

5 Conclusions

This paper presents an explicit second-order characteristic-based finite volume method for solving the convection-diffusion-reaction equation in two-dimensional domain. The theoretical formulation of the proposed method was explained in details. The computational procedure is based on the application of characteristic-based scheme to the convection-diffusion-reaction equation. The finite volume method was applied to derive the discretized equations for the spatial domain. Three numerical examples were used to evaluate the performance and to determine the order of accuracy of the proposed method. These examples showed that the method provides converged solution with improved solution accuracy as the grid is refined. The examples also showed that the method does not require any explicit artificial diffusion for improving the solution stability.

Acknowledgments

The author is pleased to acknowledge the College of Industrial Technology, King Mongkut's University of Technology North Bangkok (KMUTNB) and the National Metal and Materials Technology Center (MTEC) for supporting this research work.

References

[1] Mazzia A., Bergamaschi L. and Putti M., 2000. A Time-splitting Technique for the Advection-Dispersion Equation in Groundwater, *Journal of Computational Physics*, 157: 181-198.

[2] Frolkovic P. and De Schepper H., 2001. Numerical Modelling of Convection Dominated Transport coupled with Density Driven Flow in Porous Media, *Advances in Water Resources*, 24: 63-72.

[3] Bertolazzi E. and Manzini G., 2004. Least Square-based Finite Volumes for Solving the Advection-Diffusion of Contaminants in Porous Media, *Applied Numerical Mathematics*, 49: 277-289.

[4] Man C. and Tsai CW., 2007. A Higher-order Predictor-Corrector Echeme for Two-dimensional Advection-Diffusion Equation, *International Journal for Numerical Methods in Fluids*, 56: 401-418.

[5] Li X., Wu W., and Zienkiewicz O.C., 2000. Implicit Characteristic Galerkin Method for Convection-Diffusion Equations, *International Journal for Numerical Methods in Engineering*, 47: 1689-1708.

[6] Rui H.X. and Yang D.P., 2001. Multiplicative Schwarz Algorithm with Time Stepping along Characteristic for Convection-Diffusion Equations, *Journal of Computational Mathematics*, 19: 501-510.

[7] Nesliturk A. and Harari I., 2003. The Nearly-optimal Petrov-Galerkin Method for Convection-Diffusion Problems, *Computer Methods in Applied Mechanics and Engineering*, 192: 2501-2519.

[8] Chertock A., Kurganov A. and Petrova G., 2009. Fast Explicit Operator Splitting Method for Convection-Diffusion Equations, *International Journal for Numerical Methods in Fluids*, 59: 309-332.

[9] Smolianski A., Shipilova O. and Haario H., 2007. A Fast High-resolution Algorithm for Linear Convection Problems: Particle Transport Method, *International Journal for Numerical Methods in Engineering*, 70: 655-684.

[10] Gomez H., Colominas I., Navarrina F. and Casteleiro M., 2007. A discontinuous Galerkin method for a Hyperbolic Model for Convection-Diffusion Problems in CFD, *International Journal for Numerical Methods in Engineering*, 71: 1342-1364.

[11] Brooks A.N. and Hughes T.J.R., 1982. Streamline Upwind Petrov-Galerkin Formulation for Convection Dominated Flows with Particular Emphasis on the Incompressible Navier-Stokes Equation, *Computer Methods in Applied Mechanics and Engineering*, 32: 199-259.

[12] Codina R., 1994. Stability Analysis of the Forward Euler Scheme for the Convection-Diffusion Equation using SUPG Formulation in Space, *International Journal for Numerical Methods in Engineering*, 36: 1445-1464.

[13] Zienkiewicz O.C. and Codina R., 1995. A General Algorithm for Compressible and Incompressible Flow - part I The Split, Characteristic based Scheme, *International Journal for Numerical Methods in Fluids*, 20: 869-885.

[14] Wang H., Gahle H.K., Ewing R.E., Espedal M.S., Sharpley R.C. and Man S., 1999. An ELLAM Scheme for Advection-Diffusion Equations in Two Dimensions, *SIAM Journal on Scientific Computing*, 20: 2160-2194.

[15] Franca L.P. and Valentin F., 2001. On an Improved Unusual Stabilized Finite Element Method for the Advection-Reactive-Diffusive Equation, *Computer Methods in Applied Mechanics and Engineering*, 190: 1785-1800.

[16] Codina R., 1993. A Discontinuity-Capturing Crosswind Dissipation for the Finite Element Solution of the Convection-Diffusion Equation, *Computer Methods in Applied Mechanics and Engineering*, 110: 325-342.

[17] Douglas J. and Russell T.F., 1982. Numerical Methods for Convection Dominated Diffusion problems based on Combining the Method of Characteristics with Finite Element or Finite Difference Procedures, *SIAM Journal on Numerical Analysis*, 19: 871-885.

[18] Morton K.W., 1985. Generalised Galerkin Methods for Hyperbolic Problems, *Computer Methods in Applied Mechanics and Engineering*, 52: 847-871.

[19] Nithiarasu P., Codina R. and Zienkiewicz O.C., 2006. The Characteristic-Based Split (CBS) Scheme-a Unified Approach to Fluid Dynamics,

International Journal for Numerical Methods in Engineering, 66: 1514-1546.

[20] Zienkiewicz O.C., Taylor R.L. and Nithiarasu P., 2005. *The Finite Element Method for Fluid Dynamics*, Sixth Edition, Elsevier Butterworth-Heinemann, Burlington.

[21] Richtmyer R.D. and Morton K.W., 1967. *Difference Methods for Initial-value Problems*, Wiley-Interscience, New York.

[22] Roache P.J., 1976. *Computational Fluid Dynamics*, Hermosa, Albuquerque.

[23] Donea J., Roig B. and Huerta A., 2000. High-order Accurate time-stepping Schemes for Convection-Diffusion Problems, *Computer Methods in Applied Mechanics and Engineering*, 182: 249-275.

[24] Stynes M. and O'Riordan E., 1997. A Uniformly Convergent Galerkin Method on a Shishkin Mesh for a Convection-Diffusion Problem, *Journal of Mathematical Analysis and Applications*, 214: 36-54.

[25] Duran R.G. and Lombardi A.L., 2006. Finite Element Approximation of Convection Diffusion Problems using Graded Meshes, *Applied Numerical Mathematics*, 56: 1314-1325.

[26] Hauke G., 2002. A Simple Subgrid Scale Stabilized Method for the Advection-Diffusion-Reaction Equation, *Computer Methods in Applied Mechanics and Engineering*, 191: 2925-2947.

[27] Hauke G. and Doweidar M.H., 2005. Fourier Analysis of Semi-Discrete and Space-Time Stabilized Methods for the Advection-Diffusion-Reaction Equation: II. SGS, *Computer Methods in Applied Mechanics and Engineering*, 194: 691-725.

[28] Wang H. and Liu J., 2001. Development of CFL-free, Explicit Schemes for Multidimensional Advection-Reaction Equations, *SIAM Journal on Scientific Computing*, 23: 1418-1438.

[29] Swaminathan C.R. and Voller V.R., 1992. Streamline Upwind Scheme for Control-Volume Finite Elements, part 1. Formulations, *Numerical Heat Transfer: Part B*, 22: 95-107.

[30] Gallo C. and Manzini G., 2003. Finite Volume/Mixed Finite Element Analysis of Pollutant Transport and Bioremediation in Heterogeneous Saturated Aquifers, *International Journal for Numerical Methods in Fluids*, 42:1-21.

[31] Aboubacar M. and Webster M.F., 2003. Development of an Optimal Hybrid Finite Volume/Element Method for Viscoelastic Flows, *International Journal for Numerical Methods in Fluids*, 41: 1147-1172.

[32] Chandio M.S., Sujatha K.S. and Webster M.F., 2004. Consistent Hybrid Finite Volume/Element Formulations: Model and Complex Viscoelastic Flows, *International Journal for Numerical Methods in Fluids*, 45: 945-971.

[33] Chandio M.S., Sujatha K.S. and Webster M.F., 2004. Consistent Hybrid Finite Volume/Element Formulations: Model and Complex Viscoelastic Flows, *International Journal for Numerical Methods in Fluids*, 45: 945-971.

[34] Theeraek P., Phongthanapanich S. and Dechaumphai P., 2009. Combined Adaptive Meshing Technique and Finite Volume Element Method for Solving Convection-Diffusion Equation, *AIJSTPME*, 2: 51-58.

[35] Phongthanapanich S., 2012. Second-order Finite Volume Method for Two-dimensional Convection-Reaction Equation, *The Journal of King Mongkut's University of Technology North Bangkok*, 22: 16-23.

[36] Waterson N.P. and Deconinck H., 2007. Design Principles for Bounded Higher-order Convection Schemes - A Unified Approach, *Journal of Computational Physics*, 224: 182-207.

[37] Codina R., 2000. On Stabilized Finite Element methods for Linear Systems of Convection-Diffusion-Reaction Equations, *Computer Methods in Applied Mechanics and Engineering*, 199: 61-82.

[38] Codina R., 1998. Comparison of Some Finite Element Methods for Solving the Diffusion-Convection-Reaction Equation, *Computer Methods in Applied Mechanics and Engineering*, 156: 185-210.

[39] Barth T.J. and Jespersen D.C., 1989. The Design and Application of Upwind Schemes on Unstructured Meshes, *AIAA paper 89-0366*.