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모멘트법에 의한 이송방정식의 수치해석

Numerical Analysis for Advection Equation Based on the Method of Moments

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Abstract

The method of moments, a Lagrangian scheme, considers the zeroth, first, and second moments of the grid cell spatial distributions of the concentration and then advects the concentration by maintaining conservation of the moments. The reasonable initial description of the first and second moments as well as the mean concentration, the zeroth moments, in grid element is important in the method of moments. In this study, the description methods of each initial moment are reviewed, and the method of moments is extended to overcome the restrictions of Courant number. Its performance is compared with those of available Eulerian and Lagrangian schemes. As the results, the method is successfully extended to overcome the stability restriction and is an accurate scheme for the advection simulation of concentration distribution, especially of which the gradient is steep. In addition, the method is very promising scheme in terms of computational efficiency when the mixing is confined in a relatively small region to the entire domain in two-dimensional problem.

Keywords: method of moments, Lagrangian scheme, advection, limitation of Courant number

요 약

모멘트법은 Lagrangian 방법으로서 격자요소 내에서의 농도의 공간분포에 대한 0차, 1차, 2차 모멘트를 고려하고 각 모멘트의 보존성을 유지하면서 농도분포의 이송을 계산하는 방법이다. 따라서 각 격자요소에서의 0차 모멘트, 즉 평균농도 뿐만 아니라 1차 및 2차 모멘트 값의 합리적인 초기 설정이 요구된다. 본 연구에서는 각 모멘트들의 초기값 설정방법을 검토하고, 기존 모멘트법의 Courant 수에 대한 제약조건을 극복하기 위하여 모멘트법을 개선하였다. 모멘트법에 의한 모의 결과를 유용한 Eulerian 및 Lagrangian 기법에 의한 모의 결과와 비교 검토하여 모멘트법의 계산 능력을 분석하였다. 분석 결과 모멘트법은 농도분포의 이송 모의시 농도가 급변하는 구간에서도 정확한 해석결과를 발생시키는 기법이며, 본 연구에서 제시한 Courant 수 제약조건의 극복에 관한 연구는 성공적으로 이루어진 것으로 나타났다. 한편, 모멘트법은 농도가 전체 계산영역의 일부에 분포하는 2차원 영역에서의 이송 모의시 계산시간에 있어서 매우 효율적인 것으로 나타났다.

핵심용어 : 모멘트법, Lagrangian 방법, 이송, Courant 수의 제약

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1. Introduction

Large efforts have been invested by many researchers to develop appropriate numerical schemes for the advection-diffusion equation. These schemes are basically grouped into two categories: the Eulerian and the Lagrangian. Eulerian discretization methods for advective transport suffer from troublesome numerical errors, of which the magnitude sometimes exceeds that of physical dispersion. Thus, attention has been repeatedly given to Lagrangian methods that appear to provide a more natural approach to solutions of the advection equation (Abbott and Basco, 1989).

The first-order Upwind approximation to the advection problem tends to be overly diffusive with the results. The QUICKEST(Leonard, 1979), a third-order Upwind scheme, provides better results, even if it produces over- and under-estimation in the region of steep gradient, but causes some difficulties in the region of boundary. Davis and Moore (1982) generalized QUICKEST scheme to two dimensions in which certain cross-difference term was excluded, which required small time step to minimize the error associated with the neglected second time derivative. These Eulerian schemes using the Upwind differencing or first-order time differencing too can suffer significant errors for multidimensional problems, especially when the velocity vector is at 45° to each coordinate direction (Fletcher, 1991).

Holly and Preissmann (1977) developed a semi-Lagrangian scheme that uses the method of characteristics and a Hermite interpolation to approximate concentrations between grid points. This scheme is not conservative itself, and its accuracy depends on the degree of conservation of the flow field. It gives better results at a Courant number of about 1.0. In the low physical diffusion regions, it generates small negative concentrations (Holly and Usseglio-Polatera, 1984). Jun and Lee (1994a, 1994b) successfully simulated the longitudinal dispersion equation by a split-operator method based on forth-order and sixth-order Holly-Preissmann scheme for advection term and by a hybrid method based on Holly-Preissmann scheme with fifth-degree Hermite interpolating polynomial for advection term, respectively. Lee et al. (1995) compared the performances of Eulerian-Lagrangian methods using Lagrangian interpolation scheme and cubic spline interpolation scheme for advection term with those of Eulerian methods, Stone-Brian, and QUICKEST methods, in one-dimensional problems.

The method of moments, a Lagrangian scheme, was developed by Egan and Mahoney (1972) for determining atmospheric dispersion of pollutants. This method considers the moments over the entire solution domain and uses Lagrangian description for the time evolution of the moments. The computational efficiency of the method of moments depends on the magnitude of the mixing region in the computational domain. Since it maintains subgrid scale resolution, the method of moments is free of numerical oscillation but suffers from some numerical dissipations when complicated distributions are advected. In order to reduce numerical dissipation, Pepper and Long (1978) modified the method of moments with a width correction technique to solve the advection of a passive scalar. Pepper and Baker (1980) used the method of moments in atmosphere pollution transport. Nassiri and Babarutsi (1997) successfully used the method to simulate the dye concentration in turbulent recirculating flow generated in a shallow open channel by a sudden widening of flow in the transverse direction. The method of moments considers the zeroth, first, and second central moments of the grid cell spatial distributions of the concentration and then advects the concentration by maintaining conservation of the moments. It is important to specify the reasonable initial values of the first and second moments as well as the zeroth moment, mean concentration, in each element. In this study, the description method of each initial moments is reviewed. Since the method of moments by previous studies (Egan and Mahoney, 1973; Pepper and Baker, 1980; Nassiri and Babarutsi, 1997) is an explicit scheme, the stability limitation requires that the Courant number be less than or equal to unity for each specific direction. The subject research attempts to extend the method of moments to overcome such restrictions of the Courant number. The performance of the method of moments is compared with those of the Eulerian schemes of first-order Upwind and QUICKEST, and Lagrangian forth-order Holly-Preissmann scheme for pure advection problems for one- and two-dimensional problems.

2. Description of the Method of Moments to Advection in Two-Dimensions

The concentration distribution due to pure advection in constant-dqpth shallow water flows is computed by solving the depth-averaged mass transport equation with excepting diffusion term

$$\frac{\partial C}{\partial t}+\frac{\partial (UC)}{\partial x}+\frac{\partial (VC)}{\partial y}=0 \tag{1}$$

where C is concentration of a conserved pollutant, and U and V are the depth-averaged velocity components in the x- and y-directions, respectively.

The formulation of the method of moments involves the five parameters. The zeroth moment specifies the mean concentration C_m. The two first moments F_x and F_y denote the center of mass in the x- and y-directions with respect to the grid center. The second moments, R_x and R_y, evaluated about the center of mass define the radius of gyration, or equivalently, the square root of the variance, V^2, in the x- and y-directions, respectively. These relations are defined in x- and y-directions as (Egan and Mahoney, 1972; Nassiri and Babarutsi, 1997)

$$C_m = \int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\, dx\, dy \tag{2}$$

$$F_x = \frac{1}{C_m}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\, x\, dx\, dy \tag{3a}$$

$$F_y = \frac{1}{C_m}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\, y\, dx\, dy \tag{3b}$$

$$R_x^2 = \frac{1}{C_m}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\,(x-F_x)^2\, dx\, dy \tag{4a}$$

$$R_y^2 = \frac{1}{C_m}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\,(y-F_y)^2\, dx\, dy \tag{4b}$$

where x, y denote the relative displacements of concentration within the cell from the center of the cell and vary from −0.5 to +0.5 corresponding to the left- and right-hand extreme boundaries of a cell. For the second moment, however, Papper and Baker (1980) used different relations defined as follows.

$$R_x^2 = \frac{12}{C_m}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\,(x-F_x)^2\, dx\, dy \tag{5a}$$

$$R_y^2 = \frac{12}{C_m}\int_{-0.5}^{0.5}\int_{-0.5}^{0.5} C(x,\ y)\,(y-F_y)^2\, dx\, dy \tag{5b}$$

For a rectangular distribution of length L, the second moment has the value $L/\sqrt{12}$. Thus, a convenient scale of an arbitrary distribution within a grid element is $R=\sqrt{12}\,V$, which means that Eqs. 5(a) and 5(b) are reasonable for the second moments. In this study, comparison of the Eq. (5) with Eq. (4) is carried out by numerical tests.

For the simple rectangular concentration distributions, rectangular mesh geometry, the integrals can be readily evaluated by summation for each grid element in terms of the concentration distributions of the portions remaining and newly advected for each successive time step. Fig. 1 illustrates the scaling parameters involved in the advection of a block-shape concentration distribution in one time step.

The downwind transfer of concentration by advection depends on the values of scaling parameters, P_x and P_y , as follows:

$$P_x = \frac{1}{R_x}\left(F_x + \gamma_x + \frac{R_x}{2} - 0.5\right) \qquad (6a)$$

$$P_y = \frac{1}{R_y}\left(F_y + \gamma_y + \frac{R_y}{2} - 0.5\right) \qquad (6b)$$

where γ_x and γ_y are the Courant numbers in x- and y-directions, respectively, which are the ratios of the advection distances per time step to the grid element dimensions.

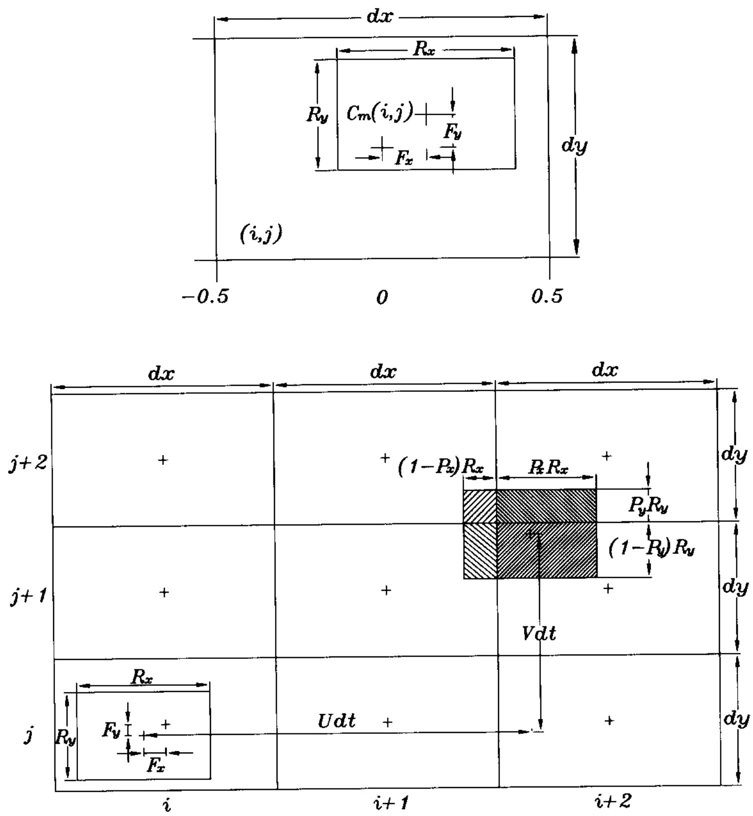

Fig. 1. Scaling Parameters used in the Advection of Block-Shape Mass Concentration from a Position within i, j cell to a Position Partially within Four Adjacent Cells.

In this study, the method of moment is extended to overcome the stability restrictions of Courant numbers. Consider the general case of concentration distribution superposed on a rectangular grid system of specified time interval Δt shown in Fig. 1. If the concentration distribution is advected beyond adjacent grid cells, the following relationship holds

$$U\Delta t/\Delta x = \beta_x + \gamma_x \tag{7a}$$

$$V\Delta t/\Delta y = \beta_y + \gamma_y \tag{7b}$$

where β_x and β_y are the integer portion of Courant numbers and γ_x and γ_y are the decimal portion of Courant numbers in the x-and y-directions, respectively.

The zeroth through second moments at each cell are calculated from concentration distributions advected from more than one adjacent cell. The computational procedure then determines the neighboring cells which contribute to the moment calculation and compute the new values for each cell. For $P_x \leq 0$ and $P_y \leq 0$, none of the concentrations are advected into the downwind cell. If $P_x \geq 1$ and $P_y \geq 1$, all concentrations are advected into the downwind cell. For $0 < P_x < 1$ and $0 < P_y < 1$, the contributions to the new concentrations at each of the four elements sharing the concentration after advection are given by

$$C_{a\,m+1,\,n}^{T+1} = C_{i,j}^{T} P_x (1 - P_y) \tag{8a}$$

$$C_{a\,m+1,\,n+1}^{T+1} = C_{i,j}^{T} P_x P_y \tag{8b}$$

$$C_{a\,m,\,n+1}^{T+1} = C_{i,j}^{T} (1 - P_x) P_y \tag{8c}$$

$$C_{a\,m,\,n}^{T+1} = C_{i,j}^{T} (1 - P_x)(1 - P_y) \tag{8d}$$

where C_a is the concentration at each of the neighboring cells and itself after advection, the subscripts m and n indicate the computational points in each direction which are defined as $i+\beta_x$ and $j+\beta_y$, respectively and superscript $T+1$ denotes the values at the new time step. The center and scaled variance, F_a and R_a, of concentration distribution advected downwind and remained for two dimensional advection are determined from the scaling parameters, P_x and P_y, using the following rules which follow those derived for the contribution to the new concentrations at each of the four elements:

$$F_{ax\,m+1,\,n}^{T+1} = (P_x R_{x\,i,j}^{T} - 1)/2 \tag{9a}$$

$$F_{ay\,m+1,\,n}^{T+1} = (1 - R_{y\,i,j}^{T} + P_y R_{y\,i,j}^{T})/2 \tag{9b}$$

$$F_{ax\,m+1,\,n+1}^{T+1} = (P_x R_{x\,i,j}^{T} - 1)/2 \tag{9c}$$

$$F_{ay\,m+1,\,n+1}^{T+1} = (P_y R_{y\,i,j}^{T} - 1)/2 \tag{9d}$$

$$F_{ax\,m,\,n+1}^{T+1} = (1 - R_{x\,i,j}^{T} + P_x R_{x\,i,j}^{T})/2 \tag{9e}$$

$$F_{ay\,m,\,n+1}^{T+1} = (P_y R_{y\,i,j}^{T} - 1)/2 \tag{9f}$$

$$F_{ax\,m,\,n}^{T+1} = (1 - R_{x\,i,j}^{T} + P_x R_{x\,i,j}^{T})/2 \tag{9g}$$

$$F_{ay\,m,\,n}^{T+1} = (1 - R_{y\,i,j}^{T} + P_y R_{y\,i,j}^{T})/2 \tag{9h}$$

$$R_{ax\,m+1,\,n}^{T+1} = P_x R_{x\,i,j}^{T} \tag{10a}$$

$$R_{ay\,m+1,\,n}^{T+1} = (1 - P_y) R_{y\,i,j}^{T} \tag{10b}$$

$$R_{ax\,m+1,\,n+1}^{T+1} = P_x R_{x\,i,j}^{T} \tag{10c}$$

$$R_{ay\ m+1,\ n+1}^{\ T+1} = P_y R_{y\ i,\ j}^{\ T} \tag{10d}$$

$$R_{ax\ m,\ n+1}^{\ T+1} = (1 - P_x) R_{x\ i,\ j}^{\ T} \tag{10e}$$

$$R_{ay\ m,\ n+1}^{\ T+1} = P_y R_{y\ i,\ j}^{\ T} \tag{10f}$$

$$R_{ax\ m,\ n}^{\ T+1} = (1 - P_x) R_{x\ i,\ j}^{\ T} \tag{10g}$$

$$R_{ay\ m,\ n}^{\ T+1} = (1 - P_y) R_{y\ i,\ j}^{\ T} \tag{10h}$$

The computational procedure computes the values for each cell which contributes to the moment calculation and then computes the new zeroth, first, and second moments for each cell.

$$C_{i,\ j}^{T+1} = \sum C_{a\ i,\ j}^{\ T+1} \tag{11}$$

$$F_{x\ i,\ j}^{\ T+1} = \frac{1}{C_{i,\ j}^{T+1}} \sum C_{a\ i,\ j}^{\ T+1} F_{ax\ i,\ j}^{\ T+1} \tag{12a}$$

$$F_{y\ i,\ j}^{\ T+1} = \frac{1}{C_{i,\ j}^{T+1}} \sum C_{a\ i,\ j}^{\ T+1} F_{ay\ i,\ j}^{\ T+1} \tag{12b}$$

$$(R_{x\ i,\ j}^{\ T+1})^2 = \frac{1}{C_{i,\ j}^{T+1}} \{\sum C_{a\ i,\ j}^{\ T+1} (R_{ax\ i,\ j}^{\ T+1})^2 + 12[\sum C_{a\ i,\ j}^{\ T+1} (F_{ax\ i,\ j}^{\ T+1} - F_{x\ i,\ j}^{\ T+1})^2]\} \tag{13a}$$

$$(R_{y\ i,\ j}^{\ T+1})^2 = \frac{1}{C_{i,\ j}^{T+1}} \{\sum C_{a\ i,\ j}^{\ T+1} (R_{ay\ i,\ j}^{\ T+1})^2 + 12[\sum C_{a\ i,\ j}^{\ T+1} (F_{ay\ i,\ j}^{\ T+1} - F_{y\ i,\ j}^{\ T+1})^2]\} \tag{13b}$$

3. Numerical Tests

Numerical tests are performed to evaluate the accuracy and the effect of Courant number, Cr, on the numerical solutions from the method of moments and other three schemes, such as the first-order Upwind, QUICKEST and forth-order Holly-Preissmann, in one- and two-dimensional flow fields. Error measures used to assess the accuracy of numerical solutions from those methods are the mass conservation ratio, the maximum and minimum predicted concentrations and normalized sum error, L_1 defined for two-dimensional as

$$L_1 = \frac{\sum_i^n \sum_j^m | C_{i,j} - Ce_{i,j} |}{\sum_i^n \sum_j^m | Ce_{i,j} |} \tag{14}$$

where C is a numerical solution, Ce is an exact solution, and i and j are computational node in the domain[$n \times m$].

3.1 Advection in one-dimensional flow

In this section the results of a comparative study is presented, which focuses on the performance of four numerical schemes including the extended method of moments and the description methods of each initial moment in the method when applied to the prediction of constant velocity advection of one-dimensional block and sine-squared wave.

At t = 0, the initial condition is prescribed as

$$C(x, t=0) = \begin{cases} 100 & 0 \le x \le 15\Delta x \\ 100 \sin^2(\pi x/20/\Delta x) & 50\Delta x \le x \le 70\Delta x \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

which consists of a block and a sine-squared wave of widths $15\Delta x$ and $20\Delta x$, respectively. The flow velocity U = 0.5m/s and Δx = 1m, Δt = 1 s, which yields Courant number Cr = 0.5. In addition, Δt = 5 s (Cr = 2.5) is applied to the extended method of moments to evaluate its performance. The exact and numerical solutions using various numerical schemes are compared at time T = 300 s.

The exact and the predicted solutions using the method of moments based on initial description Eq. (4) and Eq. (5) are shown in Fig. 2(d) and Fig. 2(e), respectively. Comparison of Figs. 2(d) and 2(e) shows that the numerical results based on Eq. (5) is promising for advection simulation. And solutions using the first-order Upwind and QUICKEST schemes are shown in Fig. 2(a) and Fig. 2(b), respectively. The method of moments produces better accuracy for both the block and the sine-squared wave advection. The solution using QUICKEST scheme shows over- and under-estimation in the region of steep gradients in the block-shaped concentration profile. This can be also seen in the solutions using forth-order Holly-Preissmann scheme shown in Fig. 2(c), while the method of moments produces quite accurate solutions without spurious oscillations, as shown in Fig. 2(e). In the case of sine-squared wave advection, the QUICKEST scheme

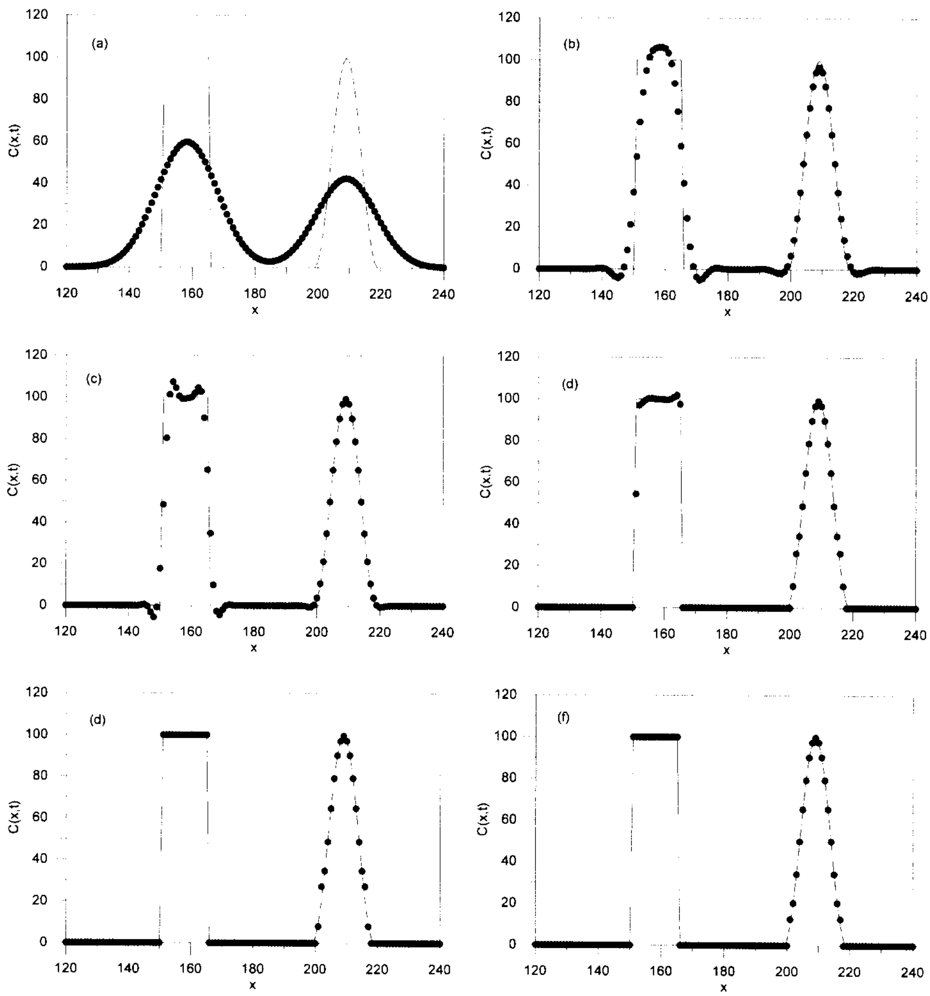

Fig. 2. Analytical and Predicted Solutions Using Various Numerical Schemes in 1D Problem: (a) First-Order Upwind, Cr=0.5; (b) QUICKEST, Cr=0.5; (c) Forth-Order Holly-Preissmann, Cr=0.5; (d) Method of Moments(Eq. 4), Cr=0.5; (e) Method of Moments(Eq. 5), Cr=0.5; (f) Method of Moments(Eq. 5), Cr=2.5

Table 1. Comparison of Numerical Solutions Using Various Numerical Schemes for One-Dimensional Block-Shaped Wave Advection

Numerical Scheme	C_{min}	C_{max}	L_1	$\sum C / \sum C_e$
First-order Upwind (Cr=0.5)	0.00000	59.76492	0.87910	0.9667
QUICKEST (Cr=0.5)	-5.25069	106.08060	0.25840	0.9833
Holly and Preissmann (Cr=0.5)	-5.63550	107.35960	0.14935	0.9667
Method of Moments (Cr=0.5, Eq. 4)	0.00000	101.94710	0.16832	0.9667
Method of Moments (Cr=0.5, Eq. 5)	0.00000	100.00000	0.00000	1.0000
Method of Moments (Cr=2.5, Eq. 5)	0.00000	100.00000	0.00000	1.0000

Table 2. Comparison of Numerical Solutions Using Various Numerical Schemes for One-Dimensional Sine-Squared Wave Advection

Numerical Scheme	C_{min}	C_{max}	L_1	$\sum C / \sum C_e$
First-order Upwind (Cr=0.5)	0.00000	42.41051	0.84829	1.0000
QUICKEST (Cr=0.5)	-1.97905	96.56194	0.07093	1.0000
Holly and Preissmann (Cr=0.5)	-0.65464	99.25913	0.01499	1.0000
Method of Moments (Cr=0.5, Eq. 4)	0.00000	99.17655	0.19918	1.0000
Method of Moments (Cr=0.5, Eq. 5)	0.00000	99.60134	0.02741	1.0000
Method of Moments (Cr=2.5, Eq. 5)	0.00000	99.92152	0.01245	1.0000

produces some dissipation and oscillation, while both method of moments and forth-order Holly-Preissmann scheme give good agreement with exact solution. The predicted solutions using the extended method of moments at Courant number 2.5 shown in Fig. 2(f) produce also good agreement with the exact solution.

Table 1 and 2 give results of four error measures for each numerical scheme for the individual block-shaped wave advection and the sine-squared wave advection, respectively. The used error measures are the minimum predicted concentration, the maximum predicted concentration, standardized sum norm, L_1, and the mass conservation ratio, respectively. The results for block-shaped wave advection demonstrate that the method of moments including the extended version based on Eq. (5) is superior to other schemes for all error measures in Table 1, while the results for sine-squared wave advection show that with the exception of the Eulerian schemes, first-order Upwind and QUICKEST schemes, overall Lagrangian schemes are comparable in Table 2. After all, the results demonstrate that the method of moments based on Eq. (5) is more accurate than that based on Eq. (4). This method is superior to other schemes, especially when the gradient of concentration distribution is steep, and is successfully extended to overcome the restriction of Courant number. In the one-dimensional advection simulation, the efficiency in terms of computational time makes no significant distinction between various schemes.

3.2 Advection in two-dimensional flow

The test problem involves the pure advection of a rectangular parallelpiped in a uniform velocity field. The parallelepiped has a width $10\,\Delta x \times 10\,\Delta x$ and is centered at (6, 6) in a domain[70×70] which has a uniform grid size,

$\Delta x = \Delta y = 1$ m. Its height is 100 units and it is advected in a uniform velocity field, directed at a 45° angle with $U = V = 0.1$m/s to the location (38,38) after $T = 320$ s.

The initial and final locations of the concentration profile are shown in Figs. 3(a) and 3(b), respectively. The predicted concentration profiles for the problem using the

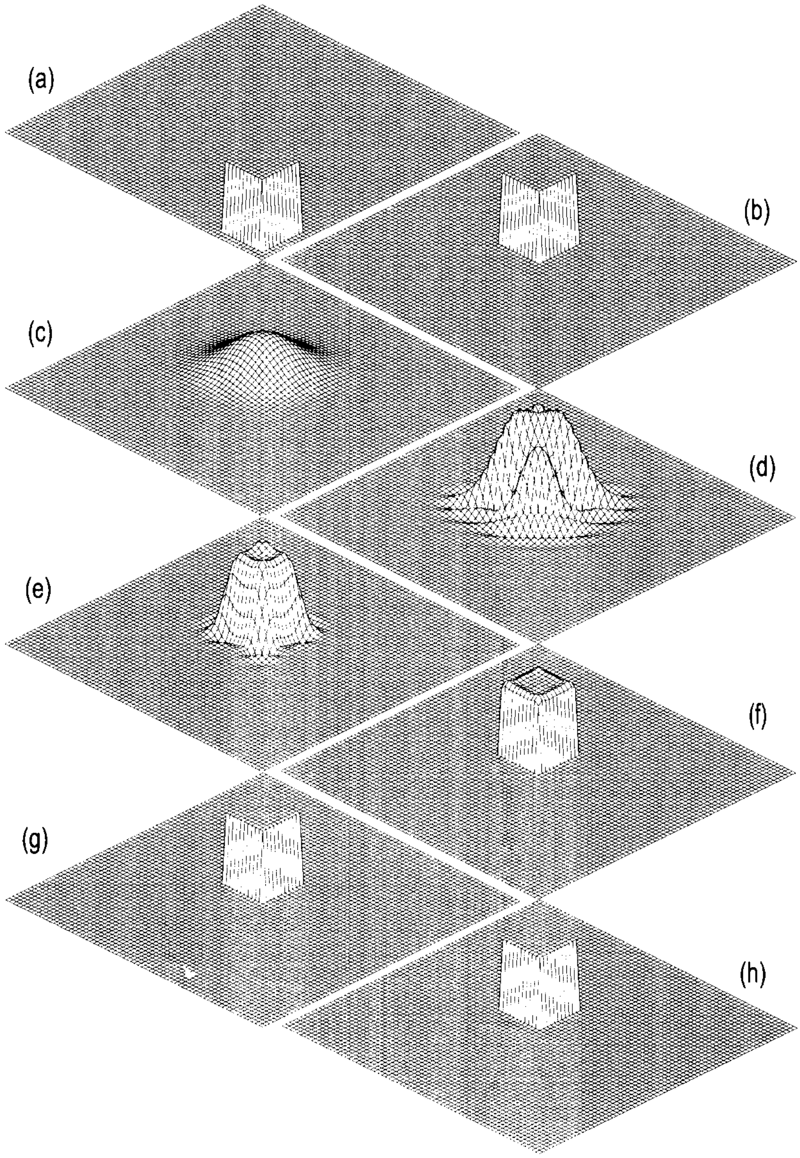

Fig. 3. Initial, Exact, and Predicted Solutions Using Various Numerical Schemes for 2D Problem: (a) Initial Condition; (b) Exact Solution; (c) First-Order Upwind, Cr=0.2; (d) QUICKEST, Cr=0.2; (e) Forth-Order Holly-Preissmann, Cr=0.2; (f) Method of Moments(Eq. 4), Cr=0.2; (g) Method of Moments(Eq. 5), Cr=0.2; (h) Method of Moments(Eq. 5), Cr=1.6

Table 3. Comparison of Numerical Solutions and Computational Time Requirements Using Various Numerical Schemes for Two-Dimensional Problem

Numerical Scheme	$C_{\min}$	$C_{\max}$	L_1	$\sum C / \sum C_e$	CPU Time
First-order Upwind (Cr=0.2)	0.00000	53.05687	1.17714	1.0000	1.00
QUICKEST (Cr=0.2)	-47.48871	130.77360	0.85884	1.0018	3.11
Holly and Preissmann (Cr=0.2)	-19.90277	111.71880	0.33194	1.0000	10.62
Method of Moments (Cr=0.2, Eq. 4)	0.00000	106.55810	0.01734	1.0000	1.53
Method of Moments (Cr=0.2, Eq. 5)	0.00000	100.00000	0.00000	1.0000	1.50
Method of Moments (Cr=1.6, Eq. 5)	0.00000	100.00000	0.00000	1.0000	0.23

first-order Upwind, QUICKEST, forth-order Holly-Preissmann schemes and the method of moments base on Eqs. (4) and Eq. (5) are shown in Figs. 3(c), 3(d), 3(e), 3(f) and 3(g), respectively, where the Courant numbers Cr_x = Cr_y = 0.2 in each direction. In addition, Fig. 3(h) shows the predicted concentration profile for the same problem using the extended method of moments at $Cr_x = Cr_y =$ 1.6. The minimum, maximum, L_1 norm, and the conservation ratio are given in Table 3 for each scheme. The predicted concentration profile using the first-order Upwind scheme shown Fig. 3(c) is overly diffusive with the flatting of concentration peak. The QUICKEST scheme overestimates the concentration peak by 31% and generates negative concentration by about 47% of the initial peak (see Table 3) with severe spurious oscillations as shown in Fig. 3(d). The accuracy of the used QUICKEST scheme (Davis and Moore, 1982) with neglecting some spatial cross-derivative term can be improved by including certain cross-difference terms that appear in the consistent formulation of the multidimensional frame work (Leonard, 1988). The forth-order Holly-Preissmann scheme also overestimates the concentration by about 12% and generates non-physical negative concentration by 20% of the initial peak at the same time as shown in Fig 3(e) and Table 3. The results for the method of moments including the extended version based on Eq. (5) shown in Figs. (2g) and (2h), and Table 3 demonstrate that the method of moments is superior to other schemes for all error measure and is also successfully extended in two-dimensional formulation, as mentioned in one-dimensional test.

The ratio of computational time requirements to the first-order Upwind scheme for each scheme shows that the method of moments is very efficient for the given two-dimensional problem, as shown in Table 3. The Holly-Preissmann scheme requires greater computational effort because the concentration C and its three derivatives $\partial C/\partial x$, $\partial C/\partial y$, and $\partial^2 C/\partial x \partial y$ are advected. The method of moments requires the computation of the concentration only in the grid cells which superposed by any concentration. Its computational efficiency, therefore, depends on the magnitude of the mixing region in the computational domain. It means that the efficiency of the method of moments is high in flow where the mixing is confined to a small region of the domain and low in flows where the mixing is extended in the whole domain.

4. Conclusions

In this study, the method of moments, a Lagrangian scheme, is extended to overcome the restrictions of the Courant number. The method is applied to the prediction of the pure advection of one-dimensional block and sine-squared wave, and a rectangular parallelpiped concentration distribution in one- and two-dimensional uniform flow velocity fields, respectively. Its performance is compared with those of the Eulerian schemes of first-order Upwind and QUICKEST, and Lagrangian forth-order Holly-Preissmann scheme.

The results from the numerical tests demonstrate that the method of moments is an accurate scheme for the advection simulation of concentration distribution, especially of which the gradient is steep, and is very promising scheme in terms of computational efficiency when the mixing is confined in a relatively small region to the entire domain in two-dimensional problem. The numerical tests also show that the method of moments is successfully extended to overcome the stability restriction of the Courant number.

Since the method of moments considers the zeroth, first, and second central moments of the concentration distribution, the reasonable description of each initial moment in grid elements is required. For the initial values of the second moment, it is theoretically reasonable to use Eq. (5) proposed by Pepper and Baker(1980), of which the superior performance is also identified by the numerical tests.

In a fractional step algorithm for advection-diffusion equation the method of moments is easily extended with including an additional term for the conservation of the first and second moments after diffusion simulation at the expense of some computational efficiency. The extension of the method in three-dimension is also straightforward.

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