Simulation of 3D Advection-diffusion Equation of Pollutants on Arbitrary Polyhedron Grids

Linghang XING[1]

[1] *Changjiang River Sciendific Research Institute, No.23, Huangpu Road, Wuhan, China*

Email: xinglinghang@yahoo.com.

Abstract: In order to capture the characteristics of pollutant transportation accurately, two modified QUICK schemes fitting for 3D unstructured grids are advised, namely Q-QUICK and NQ-QUICK. The numerical results show that the present two schemes can improve the precision of convective flux approximation efficiently in simulation of 3D unsteady advection-diffusion equation of pollutants. In addition, Q-QUICK and NQ-QUICK have a little higher computational accuracy to CDS and similar numerical stability to UDS/HDS/PDS after applying the deferred correction method. To this end, their corresponding CPU times are approximately equivalent to those of traditional difference schemes. Furthermore, their abilities for adapting high grid deformation are robust. It is so promising to apply the suggested schemes to simulate pollutant transportation on arbitrary 3D natural boundary in environmental engineering.

Keywords: 3D unstructured grid; Q-QUICK; NQ-QUICK; 3D advection-diffusion equation of pollutants;

1 Introduction

The physical processes of pollutant transportation in flowing water are mainly consisting of advection and diffusion, which are usually governed by advection-diffusion equation of pollutants. Generally, the action of advection process would dominate the transportation of pollutants. Thereby, it is so important to improve the precision of convective flux approximation. Till to now, much works have been done for numerical simulation of advection-diffusion equation of pollutants on structured grids. Usually the natural computational boundaries are irregular. If structured grids applied, the workload of CFD pretreatment including domain subdivision, grid connection and boundary fitting would be increased and the numerical precision in the boundaries would be reduced. Unstructured grid can produce arbitrary geometry and can well fit to complex physical boundary. Presently, the computation based on unstructured grid becomes more and more popular. However, many high-precision schemes on uniform grid can not be applied to unstructured grids directly. It is significative to extend them to unstructured grid computation. In the past decade, a number of difference schemes to calculate convective flux were developed for incompressible flow simulation. They include upwind difference scheme (UDS), central differencing scheme (CDS), hybrid differencing scheme (HDS), the quadratic upstream, quadratic upstream extended and quadratic upstream extended revised difference schemes(QUICK,QUDSE,QUDSER as modified by Pollard and Siu[1]), the locally exact scheme (LEDS) (1972), and the power difference schemes (PDS) of Pantankar[2]. The unconditionally convergent schemes UDS/HDS/LEDS/PDS can be significantly inaccurate under coarse grids, thus they require considerable grid refinement to produce acceptable results. This makes them expensive in practical application. Moreover, they implicitly introduce the numerical diffusion term and distort the solution. In term of accuracy and computational efficiency, it appears that the QUICK/QUDSE/QUDSER may offer the best compromise [3]. In uniform grids, they can have over second-order precision for convective flux approximation. However, QUICK/QUDSE/QUDSER needs two nodes upstream. It is not so easy to apply these high-order schemes to unstructured grid directly, especially in three dimensional problems. Moreover, to find the exact locations of the next upwind node would require a very complex pointer system and consume more memory and CPU time. Davidson L. 1996[4] introduced one method where the next upwind node is constructed by intersection from the line of two adjacent central nodes and its corresponding interface. Presently, it is named Q-QUICK. According to the method, another similar scheme named NQ-QUICK is also introduced for comparative investigation.

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2. Two modified schemes of QUICK

QUICK[5] is a third order approximation of the convection term. However, this high-order scheme is not easy to apply to unstructured grid directly. To find the exact location of the next upwind node would increase the geometrical complexity and consume relative more memory and CPU time. In this paper, two modified QUICK schemes are introduced namely Q-QUICK and NQ-QUICK.

2.1 Q-QUICK

Considering Fig. 1(a), the next upwind node U is constructed by intersection of line $\overline{PA}$ and its corresponding interface. A better way is probably to use reconstruction schemes, namely to compute the gradient in node P and use Taylor expansion to obtain the value at point U.

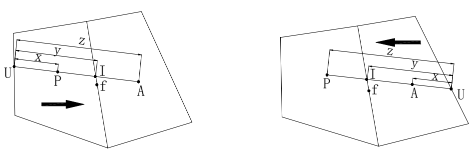
$$\phi_U = \phi_P + \vec{r}_{PU} \cdot (\nabla\phi)_P + \frac{1}{2}(\vec{r}_{PU})^2 : (\nabla\nabla\phi)_P + \cdots + \frac{1}{n!}(\vec{r}_{PU})^n \underbrace{\vdots\vdots\vdots}_{n} (\underbrace{\nabla\nabla \cdot\cdot \nabla}_{n}\phi)_P + \cdots \tag{1}$$

For present study, the second order approximation is considered. Thus the first two terms from the right of the equation are kept. And then, it is imperative to estimate the face value at interface f. In doing this, it is assumed that the flow direction is from right to left. To this end, the face value can be interpolated by QUICK method as the same way acted on the structured grid. So the normal face value ϕ_f is derived according as

$$\phi_f = \phi_P + f_1 \nabla\phi_P \cdot \vec{r}_{PU} + f_2(\phi_A - \phi_P) + \nabla\phi_I \cdot \vec{r}_{If} \tag{2}$$

Where $f_1 = -(z-y)(y-x)/x/z$; $f_2 = y(y-x)/z/(z-x)$

If the flow direction is inverse (see Fig. 1(b)), the same Equation (2) can be derived except f_3 instead of f_1 and f_4 instead of f_2 without any change in formula expression.

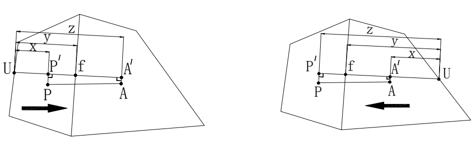


(a) $\vec{u}\cdot\vec{n} > 0$ (b) $\vec{u}\cdot\vec{n} < 0$

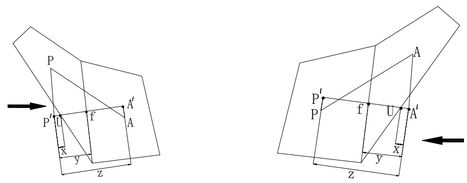
Figure 1 The next upwind node reconstruction for Q-QUICK.

2.2 NQ-QUICK

The reconstruction method of NQ-QUICK has no intrinsic difference to that of Q-QUICK except that the three auxiliary nodes U, P' and A' (seen Fig. 2) in a line are perpendicular to interface f. In addition, the node values of P' and A' should be obtained first before in-



(a) $\vec{u}\cdot\vec{n} > 0$ (b) $\vec{u}\cdot\vec{n} < 0$



(c) $\vec{u}\cdot\vec{n} > 0$ (d) $\vec{u}\cdot\vec{n} < 0$

Figure 2. The next upwind node reconstruction for NQ-QUICK

terpolation by QUICK method. However, a tough problem here is that the relative positions of nodes U, P' and A' are not so simple as those of Q-QUICK. In present study, two cases are summarized as follows.

Case 1: If $\vec{u}\cdot\vec{n} > 0$ (see Fig. 2(a))

$$\phi_f = \phi_{P'} - f_1(\phi_{P'} - \phi_U) + f_2(\phi_{A'} - \phi_{P'}) \tag{3}$$

Where, $f_1 = -(z-y)(y-x)/x/z$; $f_2 = y(y-x)/z/(z-x)$

Case 1: If $\vec{u}\cdot\vec{n} < 0$ (see Fig. 2(b)), similar to that of case 1 except f_3 instead of f_1 and f_4 instead of f_2 without any change in formula expression.

Case 2: If $\vec{u}\cdot\vec{n} > 0$ (see Fig. 2(c))

$$\phi_f = \phi_{P'} - f_1'(\phi_{P'} - \phi_U) + f_2'(\phi_{A'} - \phi_{P'}) \tag{4}$$

Where, $f_1' = 1 - f_1 - f_2$; $f_2' = f_2$, f_1 and f_2 have the same formulas as written in (3).

On high twisted grid, the coefficients of f_1 and f_2 may be much larger, which can cause the face value abnormal and result in the whole computation failure. So some flexible method should be implemented for the whole computational continuity. A better way for mending the defect may use the linear interpolation method for assuring a second-order precision at least. Then, the interface value can be written as

$$\phi_f = \omega\phi_{P'} + (1-\omega)\phi_{A'} \tag{5}$$

Where, ω is the linear interpolation factor. To this end, $f_1' = 0$; $f_2' = 1-\omega$.

Case 2: If $\vec{u}\cdot\vec{n} < 0$ (see Fig. 2(d)), similar to that of case 2 except f_3 instead of f_1 and f_4 instead of f_2 without any change in formula expression.

3. Numerical Verification

In framework of FVM, a 3D advection-diffusion equation of pollutants is discretized by compounds of different time schemes and different convective flux schemes. The former includes UDS and Crank-Nicolson and the later consists of UDS, CDS, HDS, PDS, Q-QUICK and NQ-QUICK. To this end, comprehensive comparisons for their numerical performances are investigated, including relative errors, CPU time and numerical stability.

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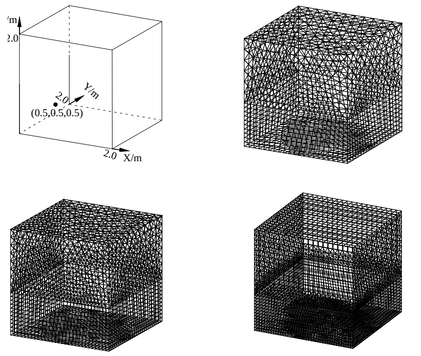


(a)Domain and Initialization (b) Grid1 (c) Grid2 (d) Grid3

Figure 3 Computational domain and grids

3.1 Govering Equation and Initial Condition

In general, a three-dimensional advection-diffusion equation of pollutants can be written as

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)+S_\phi \tag{6}$$

Where, C is concentration of pollutants, u, v and w are velocities along x, y and z directions; D_x, D_y and D_z are diffusive coefficients; S_ϕ is the source item. The initial computational condition is governed by a unit Gauss impulse within a cube. It is depicted as a follow

$$C(x,y,z,0)=\exp\left(-(x-0.5)^2/D_x-(y-0.5)^2/D_y-(z-0.5)^2/D_z\right) \tag{7}$$

Its corresponding resolution is [6]

$$C(x,y,z,t)=\frac{1}{\sqrt[3]{4t+1}}\exp\left(-\frac{(x-0.5-ut)^2}{D_x(4t+1)}-\frac{(y-0.5-vt)^2}{D_y(4t+1)}-\frac{(z-0.5-wt)^2}{D_z(4t+1)}\right) \tag{8}$$

Where, $D_x=D_y=D_z=0.01m^2/s$; $u=v=w=0.8$m/s; x, y and z are defined as $0\le x\le 2$ m, $0\le y\le 2$ m, $0\le z\le 2$ m (see Figure 4(a)); the time step is set as $\Delta t=0.00625$ s.

3.2 Numerical Results

The verification of Q-QUICK/NQ-QUICK has been investigated on three sets of unstructured grids, and the total cells used from grid 1 to grid 3 were 16319, 31959and 64651, respectively (see Fig. 3(b) to (d)). In grid 1 and grid 2, the computational meshes are composed of a group of hybrid grids including tetrahedrons, pyramids and hexahedrons, while in grid 3, further including triangular prism. Correspondingly, the maximal corrected angles from grid 1 to grid 3 are 61.7°, 71.3°and 64.1°. The maximum edge ratios of the tetrahedron, pyramid and hexahedron are 14.8, 10.7 and 8.9, respectively, in grid 1; 11.1, 9.4 and 7.8 in grid 2; and 19.8, 1.9 and 9.3 plus 14.7 for triangular prism in grid 3. Generalized Minimum Residual (GMRES (30)) method with the Incomplete LU (ILUT) precondition is used to accelerate the convergence of the linear equation. The numerical precision is indicated by relative errors defined as a follow

$$\varepsilon=\sum_i\left|C_i-C_{i0}\right|\Big/\sum_i C_{i0} \tag{9}$$

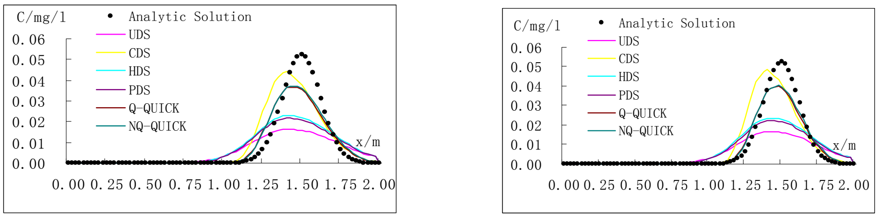
Where, C_{i0} is concentration of analytic solution; C_i is concentration of numerical results

If $t=1.25s$, the relative errors calculated along line $y=x$, $z=0.5m$ and CPU time of each scheme are listed in Table 1, the distributions of concentrations along the line are illustrated in Fig. 4. In framework of Crank-Nicolson scheme, a 3D concentration iso-surface of 0.005mg/l at t=1.0s is depicted in grid 1 for further comparison of advantages and disadvantages of each scheme, their three dimensional renderings are appended in Fig 6.

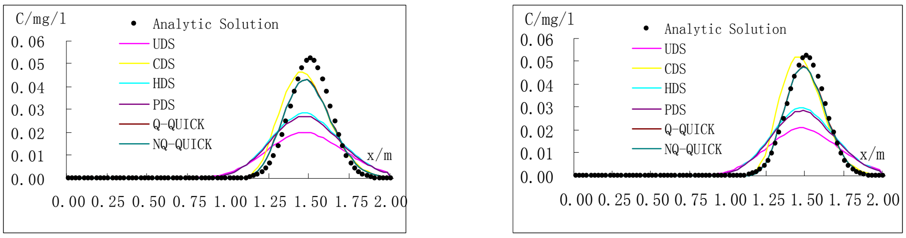
Table 1 Relative errors and CPU time

Time Discretization	**Convective Flux Discretization**	**Grid1**		**Grid2**		**Grid3**	
		Errors	***CPU Time (s)***	***Errors***	***CPU Time (s)***	***Errors***	***CPU Time (s)***
UDS	UDS	0.703	54.14	0.604	117.8	0.501	269.1
	CDS	0.453	51.80	0.273	111.0	0.174	248.2
	HDS	0.611	46.64	0.494	100.9	0.345	231.4
	PDS	0.609	51.23	0.498	112.5	0.364	257.4
	Q-QUICK	0.274	55.31	0.197	120.3	0.170	279.5
	NQ-QUICK	0.265	55.95	0.214	121.6	0.173	284.3
Crank-Nicolson	UDS	0.581	49.41	0.466	105.8	49.41	233.4
	CDS	0.255	47.92	0.091	101.1	47.92	218.8
	HDS	0.454	44.27	0.277	93.52	44.27	203.6
	PDS	0.460	48.04	0.302	102.5	48.04	226.4
	Q-QUICK	0.097	50.80	0.065	108.3	50.80	238.2
	NQ-QUICK	0.127	51.41	0.078	109.2	51.41	239.6

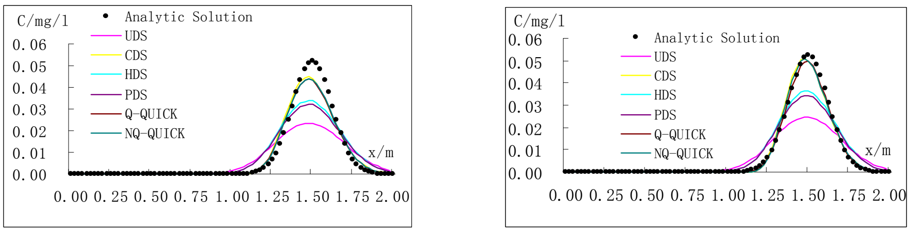
CPU: AMD Athlon(tm) 64 X2 Dual Core Processor 3800+



(a) Grid1, first-order (time) (b) Grid1, Crank-Nicolson (time)

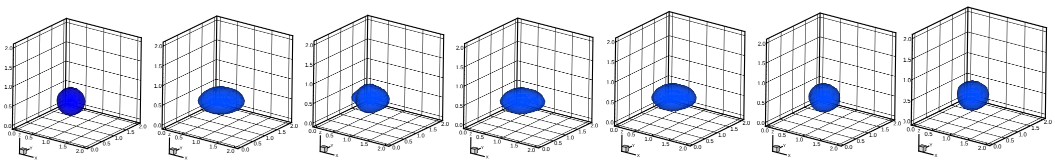


(c) Grid2, first-order (time) (d) Grid2, Crank-Nicolson (time)

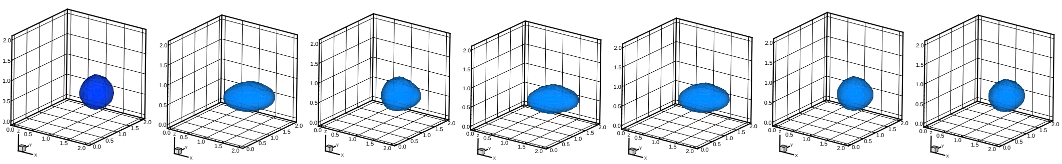


(e) Grid3, first-order (time) (f) Grid3, Crank-Nicolson (time)

Figure 4. Illustration of comparisons of concentration along face y=x,z=0.5m at t=1.25s



Analytic Solution UDS CDS HDS PDS Q-QUICK NQ-QUICK



Analytic Solution UDS CDS HDS PDS Q-QUICK NQ-QUICK

Figure 5 Illustration of comparisons of concentration iso-surface in computational domain. (C=0.005mg/l, first lineat *t*=0.5s and the sencond line at *t*=1.0s)

1) Numerical precision：From Table 2 and Fig. 4, it can be seen that the numerical precision of Q-QUICK/ NQ-QUICK/CDS are much better than UDS/HDS/PDS if fixed scheme of time discretization, as for Q-QUICK/NQ-QUICK/CDS themselves, Q- QUICK/ NQ-QUICK exhibit a little lower relative errors than those of CDS especially in grid 1, In addition, Q-QUICK and NQ-QUICK show a similar numerical precision. Furthermore, with the increasing mesh numbers, Q-QUICK/NQ-QUICK/CDS can fit well to the analytic solution quickly and in grid 3 they can perform a perfectly match. For further clearly representing the numerical precision by each scheme, the shape of the same concentration iso-surface of pollutant is analyzed. As can be seen from Fig. 5, the spherical pollutant in transporting can be maintained well by the suggested scheme Q-QUICK or NQ-QUICK and is almost identical with that of the analytic solution. This situation has been changed a little bye

CDS accounting for the calculated spindle shape and destructed greatly by UDS/HDS/PDS in view of the predicted ellipsoidal pollutant cloud. It is shown that the scheme Q-QUICK or NQ-QUICK has rather the highest calculation accuracy with least false scaling.

2) CPU time：Q-QUICK and NQ-QUICK consume a slight longer CPU times than those of other schemes. In addition, Q-QUICK seems a little economical. This is contributed to its simple reconstruction for up upstream node.

3) Numerical stability：After applying the deferred correction method and over-relaxed approach for cross derivative term approximation, UDS/HDS/PDS/ Q-QUICK/NQ-QUICK can keep a good numerical stability, they are insensitive to high grid deformation. However, in view of CDS, the shape of concentration iso-surface in Fig. 5 has a little distorted and can not retain smoothly on its rear, this exhibits CDS has a little vibration on relative sparse grid.

4. Conclusion

In present study, two modified QUICK namely Q-QUICK and NQ-QUICK are introduced and their verifications were conducted on 3D unsteady advection-diffusion equation of pollutants. The main conclusions are as a follow.1) Q-QUICK and NQ-QUICK show a little higher computational accuracy than that of the central difference scheme; 2) Two modified QUICK schemes have similar numerical stability to upwind difference scheme after applying the deferred correction method; 3) The CPU times consumed by Q-QUICK or NQ-QUICK are approximately equivalent to those of traditional difference schemes and their abilities for adapting high grid deformation are robust; 4) It is so promising to apply the proposed schemes to simulate practical pollutant transportation with the merit of good numerical performances.

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