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Quasi-consistence Hexahedral Element Method for Three-dimensional Convection Problems

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Abstract The key to the numerical solution of three dimensional convection problems is to search for a high-precision interpolating function, which can keep the result stable and damping low. Based on the consistence hexahedral element method, an advanced quasi-consistence hexahedral element method for three-dimensional convection problems is developed in this paper. The flow domain is discretized into arbitrary hexahedral elements, which do not change with time. A cubic polynomial based on three-dimensional Cartesian coordinates (x,y,z) is adopted as the element interpolating function to ensure that variable functions and their first derivatives over the entire domain are continuous. The verified results show that this algorithm is more precise than other methods.

Introduction

The convection-diffusion equation is the main type of governing equations in fluid mechanics. It is composed of convection operator equation and dispersion operator equation and it belongs to the hybrid operator equation. Many numerical methods are presented by many researchers to solve convection-diffusion problem due to their importance in fluid mechanics (Holly and Preissmann 1977, Sobey 1983, Ding and Liu 1989). They try to find out a numerical method for convection-dispersion problems that is of high precision and good stability. However, there are many difficulties to be solved due to the non-linearity of the equation.

The convection operator is the nonlinear part of the convection-diffusion equation that usually results in large numerical damping and oscillation. So it is necessary to seek an algorithm for three dimensional pure-convection problems to minimize numerical damping and oscillation.

A comparison of three finite difference methods, QUICKEST, ULTIMA and ENO schemes, was made by Dorthea *et al* (1990) for the one dimensional pure convection equation with benchmark examples, but it is very difficult to be extended to three dimensional problems. A cubic polynomial function for the two dimensional pure convection equation based on arbitrary triangle element meshes was developed by Ding Daoyang *et al* (1989) and extended to three dimensional problems on the basis of tetrahedron element meshes (Ding and Liu 1992). However, the stability of this scheme was poor. Later, a consistence hexahedral element method for three dimensional convection problems was presented (Ding, Wu and Liu 1997). A cubic polynomial was adopted as the element interpolating function which included C, C_x , C_y , C_z , C_{xy} , C_{yz}, C_{zx} and C_{xyz} of each node of the elements. Numerical damping and oscillation were almost avoided in this way. However, more time would be needed to obtain the result because of too much computational work.

Consequently, a new quasi-consistence hexahedral element method for three dimensional convection problems is developed in this paper, which only includes the quantities of C, C_x, C_y and C_z of each node of the elements. Verification of the algorithm is performed by use of a Gauss-distributed concentration ball at steady flow in an open channel. A comparison with an analytical solution shows that the precision and stability of this algorithm are as good as those of the consistence hexahedral element method, and better than those of the linear interpolating function method.

Governing equation and initial/boundary conditions

The three dimensional pure convection equation can be expressed as

$$\frac{\partial \mathrm{C}}{\partial \mathrm{t}}+\mathrm{u}\frac{\partial \mathrm{C}}{\partial \mathrm{x}}+\mathrm{v}\frac{\partial \mathrm{C}}{\partial \mathrm{y}}+\mathrm{w}\frac{\partial \mathrm{C}}{\partial \mathrm{z}}=0 \quad (1)$$

where C denotes the concentration of a convection substance, and u,v,w represent flow velocity components in (x, y, z) directions, respectively.

The solution to the concentration is sought in a region R with boundaries Γ. The initial condition is specified as

$$C(x,y,z,0)=C_0(x,y,z,0)\text{, in R and on } \Gamma \quad (2)$$

Two types of boundary conditions are used. Along the inflow boundaries Γ_1, the relation between concentration and time is

$$C(x,y,z,t)=f(x,y,z,t)\text{, along } \Gamma_1 \quad (3)$$

Along the outflow boundaries Γ_2, the normal derivative of the concentration is given, i.e.

$$\nabla C\cdot\vec{n}=g(x,y,z,t)\text{, along } \Gamma_2 \quad (4)$$

where $\vec{n}$ represents the unit outward normal along boundary Γ_2. If g=0, boundary Γ_2 represents a solid boundary and Eq.(4) indicates the absence of flux.

Numerical procedure

The method of characteristic line, which is the most suitable numerical scheme, is adopted to solve the convection equation. There are two tasks to be performed to find the concentration at all element nodes for $t=(n+1)\Delta t$. The solution procedures are: (1) to find the location of an interior point D from which a characteristic line travels to the vertex of the same element M during time interval $n\Delta t\le t\le(n+1)\Delta t$. The concentration at point M for $t=(n+1)\Delta t$ is the same as that at point D for $t=n\Delta t$. (2) to calculate the concentration at point D for $t=n\Delta t$.

The characteristic line connecting points M and D can be expressed as:

$$\frac{dx}{d\,\mathrm{t}}=u;\ \frac{dy}{d\,\mathrm{t}}=v;\ \frac{dz}{d\,\mathrm{t}}=w \quad (5)$$

The location of point D for $t=n\Delta t$ can be found by numerical integration of Eq.(5) . Because the location of point D is unknown in advance, an iterative scheme is needed. However, if the time step and the element sizes are sufficiently small, the velocity components can be approximated as linear functions with time. Eq.(5) can be written approximately as:

$$\left.\begin{aligned} x_D&=x_M-\frac{1}{2}(u_D^n+u_M^{n+1})\\ y_D&=y_M-\frac{1}{2}(v_D^n+v_M^{n+1})\\ z_D&=z_M-\frac{1}{2}(w_D^n+w_M^{n+1})\end{aligned}\right\} \quad (6)$$

where subscripts "M" and "D" denote the quantities at points M and D respectively, and superscript "n" represents the time level $n\Delta t$.

(x, y, z) are indicated as the local coordinate for a hexahedral element. The concentration at an interior point is approximated as a cubic polynomial:

$$\begin{aligned} C=&a_1+a_2x+a_3y+a_4z+a_5x^2+a_6y^2\\ &+a_7z^2+a_8xy+a_9yz+a_{10}zx+a_{11}x^3\\ &+a_{12}y^3+a_{13}z^3+a_{14}x^2y+a_{15}y^2z\\ &+a_{16}z^2x+a_{17}xy^2+a_{18}yz^2+a_{19}zx^2\\ &+a_{20}xyz+a_{21}x^4+a_{22}y^5+a_{23}z^4\\ &+a_{24}x^2y^2+a_{25}y^2z^2+a_{26}z^2x^2\\ &+a_{27}xy^3+a_{28}x^3y+a_{29}y^3z+a_{30}yz^3\\ &+a_{31}z^3x+a_{32}zx^3\end{aligned} \quad (7)$$

where a_1, a_2, …,and a_{32} are coefficients to be determined. To determine the 32 unknown coefficients, the concentration and its first derivatives at each node in each element are treated as known quantities.

The governing equations for derivatives of the concentration can be obtained through derivatives of Eq. (1). For example, to find the equation for $\partial C/\partial x$ one takes the derivative of Eq.(1) with respect to x. Thus

$$\frac{\partial}{\partial\,\mathrm{t}}(\frac{\partial C}{\partial x})+\mathrm{u}\frac{\partial}{\partial\,\mathrm{x}}(\frac{\partial C}{\partial x})+\mathrm{v}\frac{\partial}{\partial\,\mathrm{y}}(\frac{\partial C}{\partial x})+\mathrm{w}\frac{\partial}{\partial\,\mathrm{z}}(\frac{\partial C}{\partial x})=0 \quad (8)$$

The characteristic lines for $\partial C/\partial x$ are the same as those for C, which have been determined. Eq.(8) can be integrated directly from point D (when $t=n\Delta t$) to point M (when $t=(n+1)\Delta t$). Similar equations can be obtained for other derivatives.

Numerical examples

To illustrate the accuracy of the present algorithm, numerical results are obtained for the transport of an instantaneous point source in a uniform flow. The computational domain is defined as $0 \le x \le 7200m$, $0 \le y \le 800$m, and $0 \le z \le 800$m. The fluid moves in x-direction with a speed of 0.5m/s. The element network is an irregular mesh with an average mesh size of 100m (Fig.1). There are 4608 hexahedral elements with 5913 nodal points. The initial condition is given as

$$C_0(x,y,z) = \exp[-\frac{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}{2\sigma_0^2}]$$

where (x_0=1200m, y_0=400m, z_0=400m) are the coordinates for the center of initial concentration distribution, and σ_0=264m characterizes the size of concentration. In numerical computations, the no-flux boundary condition is applied to lateral boundaries. The Dirichlet boundary conditions(C=0) are used on both open boundaries. The time step Δt =48s is used.

To check the effect of different interpolation functions in the characteristics method on the solution, a comparison of linear function, consistence and quasi-consistence hexahedral element methods is performed. Numerical results for different time are shown in Figs.2~4. The curve of peak values from three methods is shown in Fig.5. The agreement between numerical solutions of consistence and quasi-consistence hexahedral element methods and analytical solution is quite good, but the result of linear function has large numerical damping and the solution is seriously distorted. However, the present algorithm avoids solving 64×64 linear equations at every time step .The consistence hexahedral element method only needs 1/50 computer time.

The result for the effect of different element sizes on the solution for *T*=9 600s is shown in Fig.6. Again the numerical damping of the consistence and quasi-consistence hexahedral element methods is the same, but lower than that of linear function.

The comparison of the results for σ_0=264m and 528m is shown in Fig.7. The smaller the variable gradient is, the smaller the numerical damping . For variables with a larger gradient, a high-precision interpolating function, such as quasi-consistence hexahedral element method, is naturally necessary to be adopted to obtain physical solution.

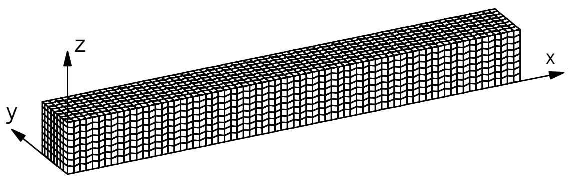

Fig.1 Sketch of computational mesh

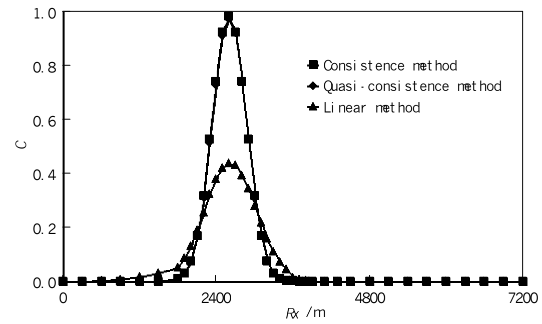

Fig. 2 Calculation of 3D convection for T=2 400s

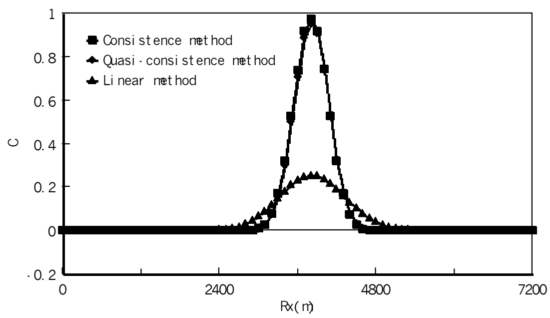

Fig. 3 Calculation of 3D convection for T=4 800s

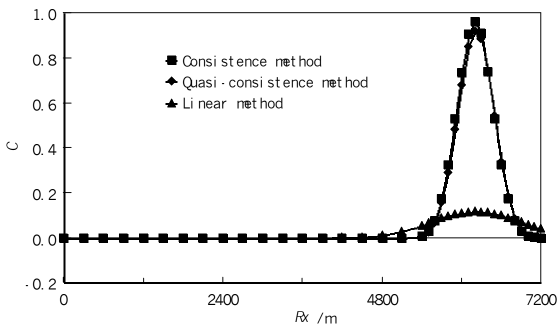

Fig. 4 Calculation of 3D convection for T=9 600s

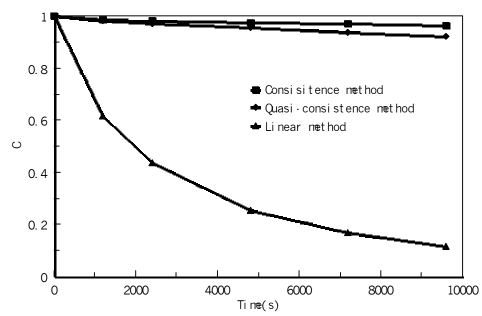

Fig.5 Maximum value comparison of three methods

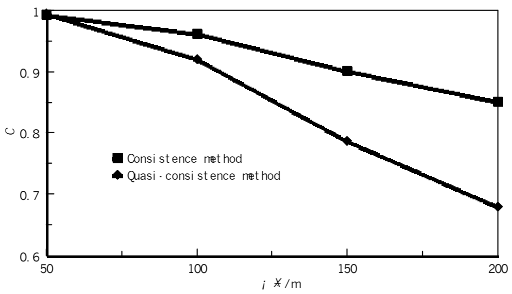

Fig.6 Maximum value comparison of difference mesh distances Δx (T=9 600s)

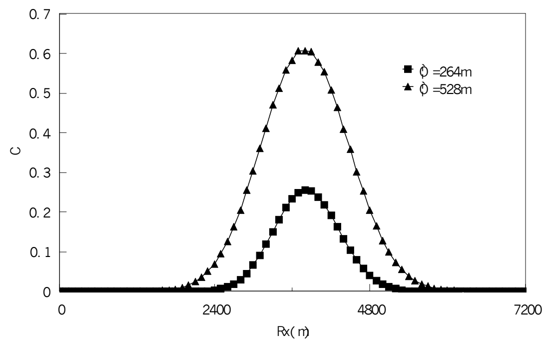

Fig. 7 Calculation of 3D convection for different σ_0 ,for T=4 800s

Conclusions

An advanced quasi-consistence hexahedral element method for three dimensional convection problems is developed. Comparisons of this method with linear interpolating function method and with consistence hexahedral element method are made. The verification of the algorithm is performed by the use of a Gauss-distributed concentration ball at steady flow in an open channel. The comparison with an analytical solution shows that in precision and stability the quasi-consistence hexahedral element method is as good as the consistence hexahedral element method, and better than the linear interpolating function method. For variables with a larger gradient, a high-precision interpolating function, such as the quasi-consistence hexahedral element method, is naturally necessary to be adopted to obtain physical solution. Indeed, it is difficult to apply the quasi-consistence and consistence hexahedral element methods to engineering practice because of the improperly posed boundary conditions for variables and their derivatives.

Acknowledgments

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