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AN OPERATOR-SPLITTING ALGORITHM FOR THREE-DIMENSIONAL CONVECTION-DIFFUSION PROBLEMS

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ABSTRACT

An operator-splitting algorithm for the three-dimensional convection-diffusion equation is presented. The flow region is discretized into tetrahedronal elements which are fixed in time. The transport equation is split into two successive initial value problems: a pure convection problem and a pure diffusion problem. For the pure convection problem, solutions are found by the method of characteristics. The solution algorithm involves tracing the characteristic lines backwards in time from a vertex of an element to an interior point. A cubic polynomial is used to interpolate the concentration and its derivatives within each element. For the diffusion problem, an explicit finite-element algorithm is employed. Numerical examples are given which agree well with the analytical solutions.

INTRODUCTION

The operator-splitting technique has been developed by many researchers for solving the two-dimensional convection-diffusion problems (e. g. Holly and Preissmann 1977, Sobey 1983, Ding and Liu 1989). The basic concept of the operator-splitting approach is to split the convection-diffusion problems into two successive initial value problems: a pure convection problem and a pure diffusion problem. Most suitable numerical schemes can be selected to solve each sub-problem so as to minimize the numerical damping and oscillations.

In this paper, the operator-splitting approach developed by Ding and Liu (1989) is extended to three-dimensional problems. Tetrahedronal elements are employed to discretize the flow domain. The finite element mesh is fixed in time. The algorithm for solving the pure convection problem involves tracing the characteristic lines backwards in time from a vertex of an element to an interior point which is in the same element. A cubic polynomial is used to interpolate the concentration in an element using the values of concentration and its higher derivations at nodal points. For the pure diffusion problem an explicit finite element algorithm is employed. Since the values of first and second derivatives of the concentration are needed in the interpolation procedure, a similar set of initial value problems for these derivative must also be solved using the same operator-splitting algorithm.

Numerical results are obtained for two problems with uniform flows. Agreement between the numerical solutions and analytical solutions is good.

GOVERNING EQUATIONS AND OPERATOR-SPLITTING METHOD

The transport equation for a three-dimensional convection-diffusion problem can be written as:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial c}{\partial x} + D_{xy}\frac{\partial c}{\partial y} + D_{xz}\frac{\partial c}{\partial z}\right) + \frac{\partial}{\partial y}\left(D_{yx}\frac{\partial c}{\partial x} + D_{yy}\frac{\partial c}{\partial y} + D_{yz}\frac{\partial c}{\partial z}\right) + \frac{\partial}{\partial z}\left(D_{zx}\frac{\partial c}{\partial x} + D_{zy}\frac{\partial c}{\partial y} + D_{zz}\frac{\partial c}{\partial z}\right), \quad (1)$$

where C denotes the concentration of a dispersive substance and (u, v, w) repesent the flow velocity components in the (x, y, z) -directions, respectively. The dispersion coefficient tensor can be expressed as:

$$\underline{\underline{D}} = \begin{bmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{bmatrix} \quad (2)$$

which is, in general, a function of the velocity field. In the present study, the velocity components assumed to be known and are not affected by the changes in concentration.

The solution for the concentration is sought in a region R bounded by boundaries Γ. The initial conditions are specified as:

$$C(x, y, z, t=0) = C_o(x, y, z) \text{ in R and on } \Gamma. \quad (3)$$

Two types of boundary conditions are used. Along the inflow boundaries, Γ_1, the time history of concentration is prescribed, i. e.,

$$C(x, y, z, t) = f(x, y, z, t), \text{ along } \Gamma_1 \quad (4)$$

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

$$(\underline{\underline{D}} * \nabla C) * \bar{n} = g(x, y, z, t), \text{ along } \Gamma_2, \quad (5)$$

where $\bar{n}$ represents the unit outward normal along the boundary Γ_2. If $g=0$, the boundary Γ_2 represents a solid boundary and Eq. (5) becomes the no-flux condition.

An operator-splitting method is employed here to integrate the transport equation. The numerical solution of Eq. (1) over a time step Δt is obtained by two fractional steps, each of duration $\Delta t/2$, seeking solutions of the consecutive initial-boundary-value-problems:

$$\frac{1}{2}\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = 0,$$

$$n\Delta t \leqslant t \leqslant (n+\frac{1}{2})\Delta t, \quad (6)$$

$$\frac{1}{2}\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}(D_{xx}\frac{\partial c}{\partial x} + D_{xy}\frac{\partial c}{\partial y} + D_{xz}\frac{\partial c}{\partial z}) + \frac{\partial}{\partial y}(D_{yx}\frac{\partial c}{\partial x} + D_{yy}\frac{\partial c}{\partial y} + D_{yz}\frac{\partial c}{\partial z}) + \frac{\partial}{\partial z}(D_{zx}\frac{\partial c}{\partial x} + D_{zy}\frac{\partial c}{\partial y} + D_{zz}\frac{\partial c}{\partial z}),$$

$$(n+\frac{1}{2})\Delta t \leqslant t \leqslant (n+1)\Delta t, \quad (7)$$

where $n=0, 1, 2, \cdots\cdots$. The operator-splitting method separates the convection processes from the diffusion processes. This allows one to choose the most suitable numerical scheme for different physical processes.

NUMERICAL PROCEDURES

During the fractional step $n\Delta t \leqslant t \leqslant (n+1/2)\Delta t$ only the convection is considered. The concentration is invariant along the characteristic lines which are determined by

$$\frac{dx}{dt} = 2u, \quad \frac{dy}{dt} = 2v, \quad \frac{dz}{dt} = 2w. \quad (8)$$

For the present problem, tetrohedronal elements are used to discretize the flow domain and the element mesh is fixed in time. There are two tasks to be performed to find the concentration at all element nodes at $t=(n+1/2)\Delta t$: (1) Find the location of an interior point D from which a characteristic line travels to a vertex of the same element, B, during the time interval $n\Delta t \leqslant t \leqslant (n+1/2)\Delta t$. The concentration at point B at $t=(n+1/2)\Delta t$ is the same as that at point D at $t=n\Delta t$. (2) Calculation of the concentration at point D at $t=n\Delta t$.

One may find the characteristic line connecting points B and D and the location of point D at $t=n\Delta t$ by integrating Eq. (8) numerically. Because the location of point D is unknown a priori, an iterative scheme is needed. However, if the time step size and the element size are sufficiently small, the velocity components can be approximated as linear functions in time. Eq. (8) can be written approximately as:

$$x_D = x_B - \frac{1}{2}[u_D^n + u_B^{n+1/2}]\Delta t \quad (9a)$$

$$y_D = y_B - \frac{1}{2}[v_D^n + v_B^{n+1/2}]\Delta t \quad (9b)$$

$$z_D = z_B - \frac{1}{2}[w_D^n + w_B^{n+1/2}]\Delta t \quad (9c)$$

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

Denoting $(\bar{x}, \bar{y}, \bar{z})$ as the local coordinate for a tetrahedronal element. The concentration at an interior point is approximated as a cubic polynomial:

$$c = a_1 + a_2\bar{x} + a_3\bar{y} + a_4\bar{z} + a_5\bar{x}^2 + a_6\bar{y}^2 + a_7\bar{z}^2 + a_8\bar{x}^3 + a_9\bar{y}^3 + a_{10}\bar{z}^3 + a_{11}\bar{x}\bar{y} + a_{12}\bar{y}\bar{z} + a_{13}\bar{z}\bar{x} + a_{14}\bar{x}^2\bar{y} + a_{15}\bar{x}\bar{y}^2 + a_{16}\bar{y}^2\bar{z} + a_{17}\bar{y}\bar{z}^2 + a_{18}\bar{x}\bar{z}^2 + a_{19}\bar{x}^2\bar{z} + a_{20}\bar{x}\bar{y}\bar{z} \quad (10)$$

where $a_1, a_2, \cdots\cdots, a_{20}$ are coefficients to be determined. For convenience, the nodal points of the element are numbered in such a way that the origin of the local cooridnates is positioned at the fourth node. The $\bar{x}$-, $\bar{y}$-, and $\bar{z}$- axis are parallel to the global x-, y-, and z- axis, respectively. To determine the 20 unknown coefficients, the concentration and its first derivatives at each node of the elements are treated are treated as known quantities. Furthermore, the cross derivatives, C_{xy}, C_{yz}, C_{zx} and C_{xyz} at the origin of the local coordinates of each element are also used.

The governing equations for the derivatives of the concentration during the convection step can be obtained by taking derivatives of Eq. (6). For example, to find the equation for

$\partial C/\partial x$ one takes the derivative of Eq. (6) with respect to x. Thus

$$\frac{\partial}{\partial t}\left(\frac{\partial C}{\partial x}\right)+2u\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right)+2v\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial x}\right)+2w\frac{\partial}{\partial z}\left(\frac{\partial C}{\partial x}\right)=-2\left[\frac{\partial u}{\partial x}\frac{\partial C}{\partial x}+\frac{\partial v}{\partial x}\frac{\partial C}{\partial y}+\frac{\partial w}{\partial x}\frac{\partial C}{\partial z}\right] \quad (11)$$

The characteristic lines for $\partial C/\partial x$ are the same as those for C, which have been determined. Eq. (11) can be integrated directly from point D (at $t=n\Delta t$) to point B (at $t=(n+1/2)\Delta t$). Similar equations can be obtained for other derivatives. The characteristic lines all remain the same, but the inhomogeneous terms become more complicated for higher derivatives.

For the diffusion problem, an explicit finite element scheme is adopted for its efficiency. Within each element the concentration is represented by :

$$C(x,y,z,t)=\sum_{i=1}^{4}L(x,y,z)C_i(t), \quad (12)$$

where $L_i(x,y,z)$ are the linerar shape functions. Consider a nodal point B which is surrounded by M elements. For the convenience of discussion, without loosing the generality, point B is designated as the node facing side 1 in each element. Multiplying Eq. (7) by L_i, and integrating over an element, one obtains

$$\iiint_{A_e}\frac{L_1}{2}\frac{\partial C}{\partial t}dv=\iiint_{A_e}L_1\left[\frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}+D_{xy}\frac{\partial C}{\partial y}+D_{xz}\frac{\partial C}{\partial z}\right)+\frac{\partial}{\partial y}\left(D_{yx}\frac{\partial C}{\partial x}+D_{yy}\frac{\partial C}{\partial y}+D_{yz}\frac{\partial C}{\partial z}\right)+\frac{\partial}{\partial z}\left(D_{zx}\frac{\partial C}{\partial x}+D_{zy}\frac{\partial C}{\partial y}+D_{zz}\frac{\partial C}{\partial z}\right)\right]dV \quad (13)$$

Substituting Eq. (12) into Eq. (13) yields an explicit equation for the concentration at the nodal point B at the time step $t=(n+1)\Delta t$:

$$C_B^{n+1}=C_B^{n+1/2}+\frac{\Delta t}{V_G}\sum_{e=1}^{M}V_e\left\{\frac{\partial L_1}{\partial x}\left[D_{xx}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial x}C_i^{n+1/2}\right)+\bar{D}_{xy}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial y}C_i^{n+1/2}\right)+\bar{D}_{xz}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial z}C_i^{n+1/2}\right)\right]+\frac{\partial L_i}{\partial y}\left[\bar{D}_{yx}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial x}C_i^{n+1/2}\right)+\bar{D}_{yy}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial y}C^{n+1/2}\right)+\bar{D}_{yz}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial z}C_i^{n+1/2}\right)\right]+\frac{\partial L_i}{\partial z}\left[\bar{D}_{zx}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial x}C^{n+1/2}\right)+\bar{D}_{zy}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial y}C_i^{n+1/2}\right)+\bar{D}_{zz}\left(\sum_{i=1}^{4}\frac{\partial L_i}{\partial z}C^{n+1/2}\right)\right]\right\}+\frac{\Delta t}{VG}\sum_{i=1}^{N_0}R_s^{n+1/2} \quad (14)$$

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 $0<z<800m$, $0<y<800m$ and $0<x<6000m$. The fluid moves in the x-direction with a speed 0.5m/sec. Thus

$$u=0.5m/sec,\ v=w=0 \quad (15)$$

Two element networks are used. The first one is a regular mesh. The flow domain is discretized into 480 cubic elements ($200^m\times200^m\times200^m$) first. Each cubic element is then divided into five tetrahedra. Therefore, there is a total of 2400 tetrahedronal elements with 775 nodal points. The second element mesh has an irregular shape, but the total number of elements remains the same.

The initial condition is given as

$$C_0(x,y,z)=\exp\left[-\frac{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2}{2\sigma_0^2}\right] \quad (16)$$

where ($x_0=1200m$, $y_0=400m$, $z_0=400m$) are the coordinates for the center of the initial concentration distribution and $\sigma_0=264$ m characterizes the size of the concentration. The dispersion coefficients are assumed to be zero; only the convection problem is considered. In the numerical computations, the no-flux boundary condition is applied on the lateral boundaries. The Dirichlet boundary conditions ($C=0$) are used on both up-stream and down-stream boundaries. The time step $\Delta t=96$ sec is used.

To check the effects of different element mesh designs on the solutions, numerical results using the regular and irregular elements are shown in Figure 1. Again, the agreement among the numerical solutions and analytical solution is quite good.

The effects of using the cubic polynomial as an interpolation function for the concentration in the mehtod of characteristics are very significant. Nnumerical computations were carried out using the linear interpolation function. Numerical results at t =9600 sec for the same physical problem are shown in Figure 2. The numerical results are very inaccurate; significant numerical damping has been introduced.

In the second numerical example, the same flow domain and the flow field as the first example are assumed. The initial concentration distribution is, however, a plane source on $x = x_0$. Thus

$$C_0(x, y, z) = \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right] \quad (17)$$

where $x_0 = 1200m$ and $\sigma_0 = 264m$. The dispersion coefficients are assumed to be

$$D_{xx} = 50m^2/s, \; D_{xy} = D_{xz} = D_{yz} = D_{yy} = D_{zz} = 0$$

Usi ng the irregular element mesh described in Figure 1, numerical results are obtaied at $t = 4800$ sec. with $\Delta t = 96sec$ The agreement between analytical solution and the numerical data is excellent and is shown is Figure 3.

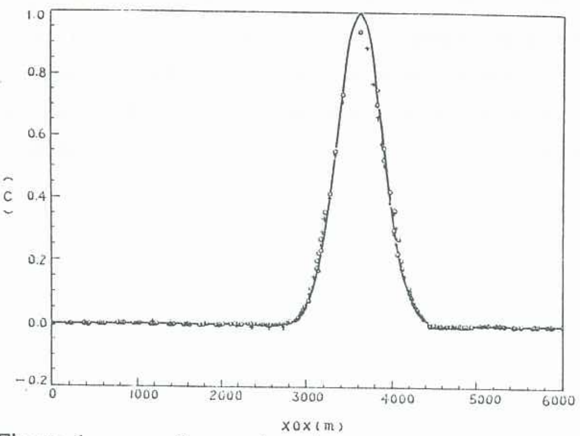

Figure 1. Comparison between numerical results and analytical solutions : — anslytical solutions , + + + numerical results using the irregular mesh , 000 numerical results using the regular mesh .

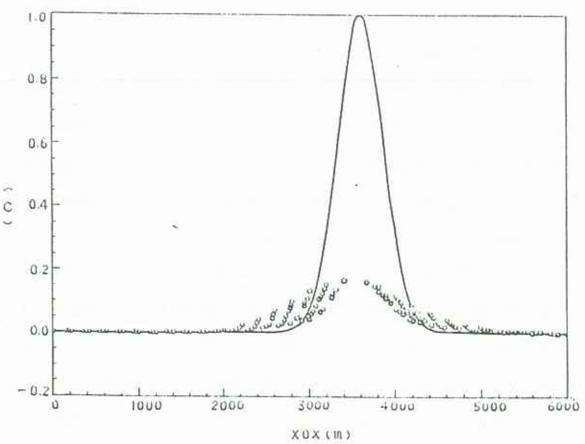

Figure 2. Comparison between numerical results using linear interpolation functions and analytical solutions for concentration at $t = 9600s$: — analytical solution , 000 numerical data .

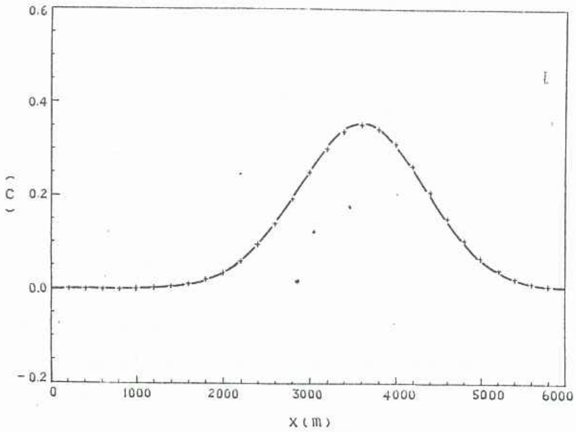

Figure 3. Comparison between numerical data and analytical results for concentration at $t = 4800s$: —analytical solution and + + + numerical data .

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