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STABILITY OF DIFFERENCE SCHEMES IN SOLVING THREE-DIMENSIONAL MATTER TRANSPORT DIFFUSION EQUATION AND APPLICATIONS

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Abstract. Some algorithms for solving three-dimensional transport diffusion equation are presented. The stability of these difference schemes with the first and second order approximations in time and space steps, and nonnegative property of numerical solutions are proved. As an application, numerical experiments for some test cases and for the water quality of the Cau river in Thai Nguyen City are presented.

Tóm tắt. Bài báo trình bày một số thuật toán tính truyền tải, khuếch tán vật chất và ô nhiễm môi trường bằng phương pháp sai phân hữu hạn. Chứng minh sự ổn định của một số sơ đồ sai phân xấp xỉ phương trình vi phân bậc $O(\tau + h), O(\tau + h^2), O(\tau^2 + h), O(\tau^2 + h^2)$ với τ là bước thời gian, $h = \max\{\Delta x, \Delta y, \Delta z\}$, $\Delta x, \Delta y, \Delta z$ là các bước không gian và tính chất không âm của nghiệm bằng số. Kết quả tính toán thử nghiệm cho các bài toán mẫu và bài toán ô nhiễm nước sông Cầu - thành phố Thái Nguyên.

INTRODUCTION

There are several finite difference schemes for solving the transport diffusion equation. Some of them have the second order approximation (see [2, 3, 5, 7, 10]). Theoretically, a numerical solution of approximation difference scheme of higher order is better than that of lower order one. However, in practice there are some cases, where numerical solutions of lower order approximation difference schemes are better than that of high order ones. For example, the numerical solution of the difference scheme with the weight coefficient $\theta = 0.6$ (i.e the first order approximation in time) is better than that for $\theta = 0.5$ (i.e the second order approximation orders in time). It happens that, may be the time and space steps cannot take very small values or complexity of algorithms can leads to great numerical error etc.

1. MATHEMATICAL MODELING

The mathematical modeling described the matter transport and diffusion processes is given in the form (see [1, 4])

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}+\sigma C-\frac{\partial}{\partial x}\nu\frac{\partial C}{\partial x}-\frac{\partial}{\partial y}\nu\frac{\partial C}{\partial y}-\frac{\partial}{\partial z}\mu\frac{\partial C}{\partial z}=f, \quad (1)$$

The equation (1) can be rewritten in the forms

$$\frac{\partial C}{\partial t}+a_1\frac{\partial C}{\partial x}+a_2\frac{\partial C}{\partial y}+\omega\frac{\partial C}{\partial z}+\sigma C-\nu\Delta C-\frac{\partial}{\partial z}\mu\frac{\partial C}{\partial z}=f, \quad (2)$$

or

$$\frac{\partial C}{\partial t}+a_1\frac{\partial C}{\partial x}+a_2\frac{\partial C}{\partial y}+a_3\frac{\partial C}{\partial z}+\sigma C-\nu\frac{\partial^2 C}{\partial x^2}-\nu\frac{\partial^2 C}{\partial y^2}-\mu\frac{\partial^2 C}{\partial z^2}=f, \quad (3)$$

where $a_1=u-\frac{\partial\nu}{\partial x}$; $a_2=v-\frac{\partial\nu}{\partial y}$; $a_3=w-\frac{\partial\mu}{\partial z}$; $\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}$; $(x,y,z)\in G\subset\mathbb{R}^3$, $t\in(0,T]$; $G=\{(x,y,z):(x,y)\in\Sigma_0\subset\mathbb{R}^2; 0\leqslant z\leqslant H\}$ is a cylinder ; C is the matter concentration; (u,v,w) - the flow velocity vector; $\nu\geqslant 0$ - the horizontal diffusion coefficient; $\mu\geqslant 0$ - the vertical diffusion coefficient; $\sigma\geqslant 0$ - the decay coefficient; f - the source function. Functions u,v,w,σ,ν,μ,f are of the variables x,y,z,t.

The equation (1) or (2) or (3) is one of parabolic type (see [6]).

The initial and boundary conditions are given by

$C(x,y,z,0)=C^0(x,y,z)$ at $t=0$, $C(x,y,z,t)=\varphi(x,y,z,t)$ on Σ if $u_n<0$, $\frac{\partial C}{\partial n}=0$ on Σ if $u_n\geqslant 0$; $\frac{\partial C}{\partial z}=\alpha C,\alpha\geqslant 0$ on Σ_0; $\frac{\partial C}{\partial z}=0$ on Σ_H, where Σ is the bounding cylindrical surface of G, Σ_0 - the bottom face, Σ_H - the top face, $\vec{n}$ - an outside normal vector of Σ and u_n- the projection of velocity vector on the vector $\vec{n}$.

The equation (2) (or (3)) can be rewritten in the form

$$\frac{\partial C}{\partial t}+\Omega C=f, \quad (4)$$

where $\Omega=\sum_{i=1}^{3}\Omega_i$; $\Omega_1=a_1\frac{\partial}{\partial x}-\nu\frac{\partial^2}{\partial x^2}+\frac{\sigma}{3}$, $\Omega_2=a_2\frac{\partial}{\partial y}-\nu\frac{\partial^2}{\partial y^2}+\frac{\sigma}{3}$, $\Omega_3=w\frac{\partial}{\partial z}-\frac{\partial}{\partial z}\mu\frac{\partial}{\partial z}+\frac{\sigma}{3}$; (or $\Omega_3=a_3\frac{\partial}{\partial z}-\mu\frac{\partial^2}{\partial z^2}+\frac{\sigma}{3}$).

2. ALGORITHMS (see [2,3,7])

Let G be overlaid with grid points $G_h=\{(x_m,y_n,z_j); m=0,...,M; n=0,...,N, j=0,...,J\}$, while $[0,T]$ - grid points: $T_h=\{0=t_0<t_1<...<t_K=K.\tau=T\}$ denotes $\varphi^k_{m,n,j}=\varphi(x_m,y_n,z_j,t_k)$.

Differencing equation (4) we obtain

$$\frac{C^{k+1}-C^k}{\tau}+\Omega^{k+1/2}\left[\theta C^{k+1}+(1-\theta)C^k\right]=f^{k+1/2}, \text{with } 0\leqslant\theta\leqslant 1.$$

which implies that

$$(1+\tau\theta\Omega^{k+1/2})C^{k+1}=\tau f^{k+1/2}+[1-\tau(1-\theta)\Omega^{k+1/2}]C^k. \quad (5)$$

We use the following approximation

$$\begin{aligned}(1+\tau\theta\Omega^{k+1/2}) &= (1+\tau\theta)(\Omega_1^{k+1/2}+\Omega_2^{k+1/2}+\Omega_3^{k+1/2})\\ &= (1+\tau\theta\Omega_1^{k+1/2})(1+\tau\theta\Omega_2^{k+1/2})(1+\tau\theta\Omega_3^{k+1/2})+O(\tau^2). \qquad (6)\end{aligned}$$

Substituting (6) in (5) yields that

$$\begin{aligned}(1+\tau\theta\Omega_1^{k+1/2})(1+\tau\theta\Omega_2^{k+1/2})(1+\tau\theta\Omega_3^{k+1/2})C^{k+1} &= \tau f^{k+1/2}\\ &+[1-\tau(1-\theta)\Omega^{k+1/2}]C^k+O(\tau^2). \qquad (7)\end{aligned}$$

The equation (7) can be decomposed as follows

$$(1+\tau\theta\Omega_1^{k+1/2})C^{k+1/3} = \tau f^{k+1/2}+[1-\tau(1-\theta)\Omega^{k+1/2}]C^k, \qquad (8)$$

$$(1+\tau\theta\Omega_2^{k+1/2})C^{k+2/3} = C^{k+1/3}, \qquad (9)$$

$$(1+\tau\theta\Omega_3^{k+1/2})C^{k+1} = C^{k+2/3}. \qquad (10)$$

From (6) we have (8) - (10) approximates (1) or (2) or (3) with the order of approximation $O(\tau^2)$.

The equations (8), (9), (10) are differenced by the two following difference schemes:

a. Upwind difference scheme

$$\begin{aligned}\Omega_1^{k+1/2}C_{m,n,j}^{k+1/3} &= \left(\frac{a_1+|a_1|}{2}\right)_{m,n,j}^{k+1/2}\frac{C_{m,n,j}^{k+1/3}-C_{m-1,n,j}^{k+1/3}}{\Delta x}+\left(\frac{a_1-|a_1|}{2}\right)_{m,n,j}^{k+1/2}\frac{C_{m+1,n,j}^{k+1/3}-C_{m,n,j}^{k+1/3}}{\Delta x}\\ &-\nu_{m,n,j}^{k+1/2}\frac{C_{m+1,n,j}^{k+1/3}-2C_{m,n,j}^{k+1/3}+C_{m-1,n,j}^{k+1/3}}{(\Delta x)^2}+\frac{\sigma_{m,n,j}^{k+1/2}}{3}C_{m,n,j}^{k+1/3}, \qquad (11)\end{aligned}$$

$$\begin{aligned}\Omega_2^{k+1/2}C_{m,n,j}^{k+2/3} &= \left(\frac{a_2+|a_2|}{2}\right)_{m,n,j}^{k+1/2}\frac{C_{m,n,j}^{k+2/3}-C_{m,n-1,j}^{k+2/3}}{\Delta y}+\left(\frac{a_2-|a_2|}{2}\right)_{m,n,j}^{k+1/2}\frac{C_{m,n+1,j}^{k+2/3}-C_{m,n,j}^{k+2/3}}{\Delta y}\\ &-\nu_{m,n,j}^{k+1/2}\frac{C_{m,n+1,j}^{k+2/3}-2C_{m,n,j}^{k+2/3}+C_{m,n-1,j}^{k+2/3}}{(\Delta y)^2}+\frac{\sigma_{m,n,j}^{k+1/2}}{3}C_{m,n,j}^{k+2/3}, \qquad (12)\end{aligned}$$

$$\begin{aligned}\Omega_3^{k+1/2}C_{m,n,j}^{k+1} &= \left(\frac{w+|w|}{2}\right)_{m,n,j}^{k+1/2}\frac{C_{m,n,j}^{k+1}-C_{m,n,j-1}^{k+1}}{\Delta z}+\left(\frac{w-|w|}{2}\right)_{m,n,j}^{k+1/2}\frac{C_{m,n,j+1}^{k+1}-C_{m,n,j}^{k+1}}{\Delta z}\\ &-\frac{\mu_{m,n,j+1/2}^{k+1/2}}{(\Delta z)^2}(C_{m,n,j+1}^{k+1}-C_{m,n,j}^{k+1})+\frac{\mu_{m,n,j-1/2}^{k+1/2}}{(\Delta z)^2}(C_{m,n,j}^{k+1}-C_{m,n,j-1}^{k+1})+\frac{\sigma_{m,n,j}^{k+1/2}}{3}C_{m,n,j}^{k+1}, \qquad (13)\end{aligned}$$

$$\Omega^{k+1/2}C_{m,n,j}^{k} = \Omega_1^{k+1/2}C_{m,n,j}^{k}+\Omega_2^{k+1/2}C_{m,n,j}^{k}+\Omega_3^{k+1/2}C_{m,n,j}^{k}. \qquad (14)$$

Substituting (11) - (14) in (5) and (8) - (10) yields the difference equations approximating the equation (1) or (2) or (3) with the order $O(\tau^2 + h)$ if $\theta = 1/2$ and the one $O(\tau + h)$ if $\theta \neq 1/2$, where $h = \max\{\Delta x, \Delta y, \Delta z\}$.

Substituting (11) and (14) in (8) yields that

$$\alpha_m^x C_{m-1,n,j}^{k+1/3} + \beta_m^x C_{m,n,j}^{k+1/3} + \gamma_m^x C_{m+1,n,j}^{k+1/3} = \delta_m^x, \tag{15}$$

where $\alpha_m^x = -\dfrac{\tau\theta(a_1 + |a_1|)_{m,n,j}^{k+1/2}}{2\Delta x} - \dfrac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta x)^2}$;

$\beta_m^x = 1 + \dfrac{\tau\theta|a_1|_{m,n,j}^{k+1/2}}{\Delta x} + \dfrac{2\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta x)^2} + \dfrac{\tau\theta\sigma_{m,n,j}^{k+1/2}}{3}$;

$\gamma_m^x = -\dfrac{\tau\theta(|a_1| - a_1)_{m,n,j}^{k+1/2}}{2\Delta x} - \dfrac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta x)^2}$;

$\delta_m^x = \tau f_{m,n,j}^{k+1/2} + C_{m,n,j}^k - \tau(1-\theta)\Omega^{k+1/2} C_{m,n,j}^k$.

Similarly, putting (12) in (9) we get

$$\alpha_n^y C_{m,n-1,j}^{k+2/3} + \beta_n^y C_{m,n,j}^{k+2/3} + \gamma_n^y C_{m,n+1,j}^{k+2/3} = \delta_n^y, \tag{16}$$

where $\alpha_n^y = -\dfrac{\tau\theta(a_2 + |a_2|)_{m,n,j}^{k+1/2}}{2\Delta y} - \dfrac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta y)^2}$;

$\beta_n^y = 1 + \dfrac{\tau\theta|a_2|_{m,n,j}^{k+1/2}}{\Delta y} + \dfrac{2\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta y)^2} + \dfrac{\tau\theta\sigma_{m,n,j}^{k+1/2}}{3}$;

$\gamma_n^y = -\dfrac{\tau\theta(|a_2| - a_2)_{m,n,j}^{k+1/2}}{2\Delta y} - \dfrac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta y)^2}$;

$\delta_n^y = C_{m,n,j}^{k+1/3}$.

Combining (13) and (10) yields that

$$\alpha_j^z C_{m,n,j-1}^{k+1} + \beta_j^z C_{m,n,j}^{k+1} + \gamma_j^z C_{m,n,j+1}^{k+1} = \delta_j^z, \tag{17}$$

where $\alpha_j^z = -\dfrac{\tau\theta(w + |w|)_{m,n,j}^{k+1/2}}{2\Delta z} - \dfrac{\tau\theta\mu_{m,n,j-1/2}^{k+1/2}}{(\Delta z)^2}$;

$\beta_j^z = 1 + \dfrac{\tau\theta|w|_{m,n,j}^{k+1/2}}{\Delta z} + \dfrac{\tau\theta(\mu_{m,n,j-1/2}^{k+1/2} + \mu_{m,n,j+1/2}^{k+1/2})}{(\Delta z)^2} + \dfrac{\tau\theta\sigma_{m,n,j}^{k+1/2}}{3}$;

$\gamma_j^z = -\dfrac{\tau\theta(|w| - w)_{m,n,j}^{k+1/2}}{2\Delta z} - \dfrac{\tau\theta\mu_{m,n,j+1/2}^{k+1/2}}{(\Delta z)^2}$;

$\delta_j^z = C_{m,n,j}^{k+2/3}$.

It is easy to verify that the coefficients of the equations (15), (16), (17) satisfy the following conditions $\alpha_m^x < 0, \beta_m^x > 0, \gamma_m^x < 0$ v $\beta_m^x \geqslant |\alpha_m^x| + |\gamma_m^x| + \delta, \quad \delta \geqslant 1; \alpha_n^y < 0, \beta_n^y > 0, \gamma_n^y < 0$ and $\beta_n^y \geqslant |\alpha_n^y| + |\gamma_n^y| + \delta; \alpha_j^z < 0, \beta_j^z > 0, \gamma_j^z < 0$ and $\beta_j^z \geqslant |\alpha_j^z| + |\gamma_j^z| + \delta.$ (18)

b. Central difference scheme

The equation (3) is differenced as follows

$$\Omega_1^{k+1/2}C^{k+1/3} = a_1^{k+1/2}\frac{C_{m+1,n,j}^{k+1/3} - C_{m-1,n,j}^{k+1/3}}{2\Delta x} - \nu_{m,n,j}^{k+1/2}\frac{C_{m+1,n,j}^{k+1/3} - 2C_{m,n,j}^{k+1/3} + C_{m-1,n,j}^{k+1/3}}{(\Delta x)^2} + \frac{\sigma_{m,n,j}^{k+1/2}}{3}C_{m,n,j}^{k+1/3} \quad (19)$$

$$\Omega_2^{k+1/2}C^{k+2/3} = a_2^{k+1/2}\frac{C_{m,n+1,j}^{k+2/3} - C_{m,n-1,j}^{k+2/3}}{2\Delta y} - \nu_{m,n,j}^{k+1/2}\frac{C_{m,n+1,j}^{k+2/3} - 2C_{m,n,j}^{k+2/3} + C_{m,n-1,j}^{k+2/3}}{(\Delta y)^2} + \frac{\sigma_{m,n,j}^{k+1/2}}{3}C_{m,n,j}^{k+2/3} \quad (20)$$

$$\Omega_3^{k+1/2}C^{k+1} = a_3^{k+1/2}\frac{C_{m,n,j+1}^{k+1} - C_{m,n,j-1}^{k+1}}{2\Delta z} - \mu_{m,n,j}^{k+1/2}\frac{C_{m,n,j+1}^{k+1} - 2C_{m,n,j}^{k+1} + C_{m,n,j-1}^{k+1}}{(\Delta z)^2} + \frac{\sigma_{m,n,j}^{k+1/2}}{3}C_{m,n,j}^{k+1} \quad (21)$$

$$\Omega^{k+1/2}C^k = \Omega_1^{k+1/2}C^k + \Omega_2^{k+1/2}C^k + \Omega_3^{k+1/2}C^k. \quad (22)$$

Putting (19), (20), (21), (22) in (8), (9), (10), we have:

$$\alpha_m^x C_{m-1,n,j}^{k+1/3} + \beta_m^x C_{m,n,j}^{k+1/3} + \gamma_m^x C_{m+1,n,j}^{k+1/3} = \delta_m^x, \quad (23)$$

where $\alpha_m^x = -\frac{\tau\theta(a_1)_{m,n,j}^{k+1/2}}{2\Delta x} - \frac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta x)^2}$;

$\beta_m^x = 1 + \frac{2\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta x)^2} + \frac{\tau\theta\sigma_{m,n,j}^{k+1/2}}{3}$;

$\gamma_m^x = \frac{\tau\theta(a_1)_{m,n,j}^{k+1/2}}{2\Delta x} - \frac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta x)^2}$;

$\delta_m^x = \tau f_{m,n,j}^{k+1/2} + C_{m,n,j}^k - \tau(1-\theta)\Omega^{k+1/2}C_{m,n,j}^k$.

$$\alpha_n^y C_{m,n-1,j}^{k+2/3} + \beta_n^y C_{m,n,j}^{k+2/3} + \gamma_n^y C_{m,n+1,j}^{k+2/3} = \delta_n^y, \quad (24)$$

where $\alpha_n^y = -\frac{\tau\theta(a_2)_{m,n,j}^{k+1/2}}{2\Delta y} - \frac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta y)^2}$;

$\beta_n^y = 1 + \frac{2\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta y)^2} + \frac{\tau\theta\sigma_{m,n,j}^{k+1/2}}{3}$;

$$\gamma_n^y = \frac{\tau\theta(a_2)_{m,n,j}^{k+1/2}}{2\Delta y} - \frac{\tau\theta\nu_{m,n,j}^{k+1/2}}{(\Delta y)^2};$$

$$\delta_n^y = C_{m,n,j}^{k+1/3}.$$

$$\alpha_j^z C_{m,n,j-1}^{k+1} + \beta_j^z C_{m,n,j}^{k+1} + \gamma_j^z C_{m,n,j+1}^{k+1} = \delta_j^z, \tag{25}$$

where $\alpha_j^z = -\dfrac{\tau\theta(a_3)_{m,n,j}^{k+1/2}}{2\Delta z} - \dfrac{\tau\theta\mu_{m,n,j}^{k+1/2}}{(\Delta z)^2};$

$$\beta_j^z = 1 + \frac{2\tau\theta\mu_{m,n,j}^{k+1/2}}{(\Delta z)^2} + \frac{\tau\theta\sigma_{m,n,j}^{k+1/2}}{3};$$

$$\gamma_j^z = \frac{\tau\theta(a_3)_{m,n,j}^{k+1/2}}{2\Delta z} - \frac{\tau\theta\mu_{m,n,j}^{k+1/2}}{(\Delta z)^2};$$

$$\delta_j^z = C_{m,n,j}^{k+2/3}.$$

To prove the condition (18), it is necessary to choose

$$\Delta x < \min_{m,n,j,k}\left(\frac{2\nu}{|a_1|}\right)_{m,n,j}^k; \Delta y < \min_{m,n,j,k}\left(\frac{2\nu}{|a_2|}\right)_{m,n,j}^k; \Delta z < \min_{m,n,j,k}\left(\frac{2\mu}{|a_3|}\right)_{m,n,j}^k \tag{26}$$

The equations (23), (24), (25) approximate (1) or (2) or (3) with the order $O(\tau^2 + h^2)$ if $\theta = 1/2$ and with the one $O(\tau + h^2)$ if $\theta \neq 1/2$.

Remark:

If the coefficients σ, ν, μ depend on C, then the equations (1) or (2) or (3) is nonlinear. For solve this equations, it is necessary to linearise the one, so difference equation can approximate (1) or (2) or (3) with the order $O(\tau + h)$ or $O(\tau + h^2)$.

The boundary condition is approximated as follows

a) If the boundary condition is a given function φ, we take

$$C_{q_m,n,j}^p = \varphi_{q_m,n,j}^p, C_{m,q_n,j}^p = \varphi_{m,q_n,j}^p, C_{m,n,q_j}^p = \varphi_{m,n,q_j}^p, \tag{27}$$

where q_m is equals to 0 or M, q_n is equals to 0 or N, q_j is equals to 0 or J, and p is equals to $k+1/3; k+2/3; k+1$.

b) If the boundary conditions are as follows

$$\left.\frac{\partial C}{\partial n}\right|_{\Sigma} = 0;\ \left.\frac{\partial C}{\partial n}\right|_{\Sigma_H} = 0 \text{ and } \left.\frac{\partial C}{\partial n}\right|_{\Sigma_0} = \alpha C, \alpha \geqslant 0$$

then the following approximations will be used

$$\begin{gathered} C_{0,n,j}^p = C_{1,n,j}^p + O(\Delta x^2); C_{M,n,j}^p = C_{M-1,n,j}^p + O(\Delta x^2); \\ C_{m,0,j}^p = C_{m,1,j}^p + O(\Delta y^2); C_{m,N,j}^p = C_{m,N-1,j}^p + O(\Delta y^2); \\ C_{m,n,J}^p = C_{m,n,J-1}^p + O(\Delta z^2); C_{m,n,0}^p = \frac{C_{m,n,1}^p}{1+\alpha\Delta z} + O(\Delta z^2); \end{gathered} \tag{28}$$

From (18) we obtain that the equations (15), (16), (17), (23), (24), (25) have unique solution. These equations can be solved by the double sweep method

$$C^{k+1/3}_{m,n,j} = L^x_m C^{k+1/3}_{m-1,n,j} + K^x_m, \tag{29}$$

$$C^{k+2/3}_{m,n,j} = L^y_n C^{k+2/3}_{m,n-1,j} + K^y_n, \tag{30}$$

$$C^{k+1}_{m,n,j} = L^z_j C^{k+1}_{m,n,j-1} + K^z_j, \tag{31}$$

where

$$L_i = \frac{-\alpha_i}{\beta_i + \gamma_i L_{i+1}}; \quad K_i = \frac{\delta_i - \gamma_i K_{i+1}}{\beta_i + \gamma_i L_{i+1}}; \quad (i = m, n, j).$$

with $\zeta_i = \zeta^x_m$ or ζ^y_n or ζ^z_j and ζ may be $L, K, \alpha, \beta, \gamma, \delta$.

Numerical error of the double sweep methods (29), (30), (31) with the coefficients satisfying (18) is not accumulated (see [8]).

The coefficients $L_M, K_M, L_N, K_N, L_J, K_J$ and the values $C^{k+1/3}_{0,n,j}$, $C^{k+2/3}_{m,0,j}$, $C^{k+1}_{m,n,0}$ are defined by the boundary conditions.

3. STABILITY OF DIFFERENCE SCHEMES (see [5, 9])

Let G be the rectangular cylinder.

Theorem 1. *The difference scheme (8) - (10) with respect to time and (11) - (14) with respect to space with the boundary conditions (27), (28) is unconditionally stable if* $\theta = 1$, *and is stable if* $\theta \neq 1$ *and*

$$\tau < \frac{1}{(1-\theta)(\lambda^x_2 + \lambda^y_2 + \lambda^z_2)}, \quad \forall\ k, m, n, j, \tag{32}$$

where $\lambda^x_2 = \left(\dfrac{|a_1|}{\Delta x} + \dfrac{2\nu}{(\Delta x)^2} + \dfrac{\sigma}{3}\right)^{k+1/2}_{m,n,j}; \lambda^y_2 = \left(\dfrac{|a_2|}{\Delta y} + \dfrac{2\nu}{(\Delta y)^2} + \dfrac{\sigma}{3}\right)^{k+1/2}_{m,n,j};$

$$\lambda^z_2 = \left(\frac{|\omega|}{\Delta z} + \frac{\sigma}{3}\right)^{k+1/2}_{m,n,j} + \frac{\mu^{k+1/2}_{m,n,j+1/2} + \mu^{k+1/2}_{m,n,j-1/2}}{(\Delta z)^2}$$

Proof. Suppose that at the step $t_{k+1/3}$, we have

$$\left|C^{k+1/3}_{m_0,n_0,j_0}\right| = \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^{k+1/3}_{m,n,j}\right|.$$

From the equation (15) or (23) ue have

$$\begin{aligned}&\left|\alpha_{m_0} C^{k+1/3}_{m_0-1,n_0,j_0} + \beta_{m_0} C^{k+1/3}_{m_0,n_0,j_0} + \gamma_{m_0} C^{k+1/3}_{m_0+1,n_0,j_0}\right| \\ &= \left|C^k_{m_0,n_0,j_0} - \tau(1-\theta)\Omega C^k_{m_0,n_0,j_0} + \tau f^k_{m_0,n_0,j_0}\right|.\end{aligned} \tag{33}$$

so

$$
\begin{aligned}
&\left|\alpha_{m_0} C^{k+1/3}_{m_0-1,n_0,j_0} + \beta_{m_0} C^{k+1/3}_{m_0,n_0,j_0} + \gamma_{m_0} C^{k+1/3}_{m_0+1,n_0,j_0}\right| \\
&\geq |\beta_{m_0}| \cdot \left|C^{k+1/3}_{m_0,n_0,j_0}\right| - |\alpha_{m_0}| \cdot \left|C^{k+1/3}_{m_0-1,n_0,j_0}\right| - |\gamma_{m_0}| \cdot \left|C^{k+1/3}_{m_0+1,n_0,j_0}\right| \\
&\geqslant (|\beta_{m_0}| - |\alpha_{m_0}| - |\gamma_{m_0}|) \left|C^{k+1/3}_{m_0,n_0,j_0}\right| \\
&\geqslant \delta \left|C^{k+1/3}_{m_0,n_0,j_0}\right|.
\end{aligned} \tag{34}
$$

From (33), (34) and $\delta \geqslant 1$ it follows that

$$
\left|C^{k+1/3}_{m_0,n_0,j_0}\right| \leqslant \left|C^{k}_{m_0,n_0,j_0} - \tau(1-\theta)\Omega C^{k}_{m_0,n_0,j_0}\right| + \tau \left|f^{k}_{m_0,n_0,j_0}\right|. \tag{35}
$$

Differencing $\Omega^{k+1/2}$ we get

$$
\begin{aligned}
\Omega_1^{k+1/2} C^{k}_{m_0,n_0,j_0} = &\left(\frac{a_1+|a_1|}{2}\right)^{k+1/2}_{m_0,n_0,j_0} \frac{C^{k}_{m_0,n_0,j_0} - C^{k}_{m_0-1,n_0,j_0}}{\Delta x} \\
&+ \left(\frac{a_1-|a_1|}{2}\right)^{k+1/2}_{m_0,n_0,j_0} \frac{C^{k}_{m_0+1,n_0,j_0} - C^{k}_{m_0,n_0,j_0}}{\Delta x} \\
&- \nu^{k+1/2}_{m_0,n_0,j_0} \frac{C^{k}_{m_0+1,n_0,j_0} - 2C^{k}_{m_0,n_0,j_0} + C^{k}_{m_0-1,n_0,j_0}}{(\Delta x)^2} \\
= &\lambda_1^x C^{k}_{m_0-1,n_0,j_0} + \lambda_2^x C^{k}_{m_0,n_0,j_0} + \lambda_3^x C^{k}_{m_0+1,n_0,j_0},
\end{aligned}
$$

where, $\lambda_1^x = -\left(\dfrac{a_1+|a_1|}{2\Delta x} + \dfrac{\nu}{(\Delta x)^2}\right)^{k+1/2}_{m_0,n_0,j_0} < 0;$

$$\lambda_2^x = \left(\frac{|a_1|}{\Delta x} + \frac{2\nu}{(\Delta x)^2} + \frac{\sigma}{3}\right)^{k+1/2}_{m_0,n_0,j_0} > 0;$$

$$\lambda_3^x = -\left(\frac{|a_1|-a_1}{2\Delta x} + \frac{\nu}{(\Delta x)^2}\right)^{k+1/2}_{m_0,n_0,j_0} < 0,$$

and

$$
\lambda_2^x = |\lambda_1^x| + |\lambda_3^x| + \frac{\sigma}{3} \tag{36}
$$

Similarly, we obtain

$$
\Omega_2^{k+1/2} C^{k}_{m_0,n_0,j_0} = \lambda_1^y C^{k}_{m_0,n_0-1,j_0} + \lambda_2^y C^{k}_{m_0,n_0,j_0} + \lambda_3^y C^{k}_{m_0,n_0+1,j_0}, \tag{37}
$$

where $\lambda_1^y < 0; \lambda_3^y < 0$ and $\lambda_2^y = |\lambda_1^y| + |\lambda_3^y| + \dfrac{\sigma}{3}.$

$$
\Omega_3^{k+1/2} C^{k}_{m_0,n_0,j_0} = \lambda_1^z C^{k}_{m_0,n_0,j_0-1} + \lambda_2^z C^{k}_{m_0,n_0,j_0} + \lambda_3^z C^{k}_{m_0,n_0,j_0+1}, \tag{38}
$$

where $\lambda_1^z < 0; \lambda_3^z < 0$ and $\lambda_2^z = |\lambda_1^z| + |\lambda_3^z| + \dfrac{\sigma}{3}.$

Therefore,

$$\begin{aligned}
&C^k_{m_0,n_0,j_0} - \tau(1-\theta)\Omega^{k+1/2}C^k_{m_0,n_0,j_0} \\
&= \left[1-\tau(1-\theta)(\lambda^x_2+\lambda^y_2+\lambda^z_2)\right]C^k_{m_0,n_0,j_0} + \tau(1-\theta)\Big[|\lambda^x_1|C^k_{m_0-1,n_0,j_0} \\
&\quad + |\lambda^x_3|C^k_{m_0+1,n_0,j_0} + |\lambda^y_1|C^k_{m_0,n_0-1,j_0} + |\lambda^y_3|C^k_{m_0,n_0+1,j_0} \\
&\quad + |\lambda^z_1|C^k_{m_0,n_0,j_0-1} + |\lambda^z_3|C^k_{m_0,n_0,j_0+1}\Big]. \qquad (39)
\end{aligned}$$

If $\theta = 1$, from (35) we have

$$|C^{k+1/3}_{m_0,n_0,j_0}| \leqslant |C^k_{m_0,n_0,j_0}| + \tau|f^k_{m_0,n_0,j_0}|. \qquad (40)$$

For $\theta \neq 1$, and τ satisfy condition (32) we obtain that

$$1-\tau(1-\theta)(\lambda^x_2+\lambda^y_2+\lambda^z_2) > 0. \qquad (41)$$

Combining (36) - (39) and (41) yields

$$\begin{aligned}
&|C^k_{m_0,n_0,j_0} - \tau(1-\theta)\Omega^{k+1/2}C^k_{m_0,n_0,j_0}| \leqslant \Big[1-\tau(1-\theta)(\lambda^x_2+\lambda^y_2+\lambda^z_2)+ \\
&\quad \tau(1-\theta)(|\lambda^x_1|+|\lambda^x_3|+|\lambda^y_1|+|\lambda^y_3|+|\lambda^z_1|+|\lambda^z_3|)\Big] \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} |C^k_{m,n,j}| = \\
&\quad (1-\tau(1-\theta)\sigma^{k+1/2}_{m_0,n_0,j_0}) \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} |C^k_{m,n,j}| \leqslant \\
&\quad \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} |C^k_{m,n,j}|. \qquad (42)
\end{aligned}$$

From (35), (40) and (42) we have

$$\begin{aligned}
&\sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^{k+1/3}_{m,n,j}\right| \\
&\leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^k_{m,n,j}\right| + \tau\sup_k \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|f^k_{m,n,j}\right|. \quad (43)
\end{aligned}$$

Similarly, (16), (17) or (24), (25) it follows that

$$\sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^{k+2/3}_{m,n,j}\right| \leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^{k+1/3}_{m,n,j}\right|; \qquad (44)$$

$$\sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^{k+1}_{m,n,j}\right| \leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1} \left|C^{k+2/3}_{m,n,j}\right|. \qquad (45)$$

Combining (43), (44), (45) gives that

$$\sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{k+1}_{m,n,j}\right|\leqslant$$
$$\sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{k}_{m,n,j}\right| + \ \tau\sup_k\ \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|f^{k}_{m,n,j}\right|\leqslant$$
$$\sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{0}_{m,n,j}\right| + \tau(k+1)\sup_k\ \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|f^{k}_{m,n,j}\right|\leqslant$$
$$\sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant n\leqslant N}\ \sup_{0\leqslant j\leqslant J}\left|C^{0}_{m,n,j}\right| + T\sup_k\ \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|f^{k}_{m,n,j}\right|, \tag{46}$$

where $\mathrm{T} = K.\tau$ is given.

At the boundaries

i) If the boundary condition is a given function $\varphi(x, y, z, t)$, then we have

$$\sup_{0\leqslant n\leqslant N}\ \sup_{0\leqslant j\leqslant J}\left|C^{k+1}_{q_m,n,j}\right|\leqslant \sup_k\ \sup_{0\leqslant n\leqslant N}\ \sup_{0\leqslant j\leqslant J}\left|\varphi(x_{q_m}, y_n, z_j, t_k)\right|, \tag{47}$$

where q_m may be 0 or M.

Similarly,
$$\sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant j\leqslant J}\left|C^{k+1}_{m,q_n,j}\right|\leqslant \sup_k\ \sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant j\leqslant J}\left|\varphi(x_m, y_{q_n}, z_j, t_k)\right|, \tag{48}$$

$$\sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant n\leqslant N}\left|C^{k+1}_{m,n,q_j}\right|\leqslant \sup_k\ \sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant n\leqslant N}\left|\varphi(x_m, y_n, z_{q_j}, t_k)\right|, \tag{49}$$

where q_n is equal to 0 or N and q_j is equal to 0 or J.

ii) If the boundary condition is $\dfrac{\partial C}{\partial n} = 0$, by (28) we get

$$C^{k+1}_{0,n,j} = C^{k+1}_{1,n,j} \text{ or } C^{k+1}_{M,n,j} = C^{k+1}_{M-1,n,j};\ C^{k+1}_{m,0,j} = C^{k+1}_{m,1,j} \text{ or } C^{k+1}_{m,N,j} = C^{k+1}_{m,N-1,j},$$

$$C^{k+1}_{m,n,J} = C^{k+1}_{m,n,J-1};\ C^{k+1}_{m,n,0} = \frac{C^{k+1}_{m,n,1}}{(1+\alpha\Delta z)} < C^{k+1}_{m,n,1}.$$

The values $C^{k+1}_{q_m,q_n,j}, C^{k+1}_{q_m,n,q_j}, C^{k+1}_{m,q_n,q_j}, C^{k+1}_{q_m,q_n,q_j}$ are taken by C^{k+1} at the nearest node of the interior grid points.

It is easy to verify that

$$\sup_{0\leqslant n\leqslant N}\ \sup_{0\leqslant j\leqslant J}\left|C^{k+1}_{0,n,j}\right|\leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{k+1}_{m,n,j}\right|, \tag{50}$$

$$\sup_{0\leqslant n\leqslant N}\ \sup_{0\leqslant j\leqslant J}\left|C^{k+1}_{M,n,j}\right|\leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{k+1}_{m,n,j}\right|, \tag{51}$$

$$\sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant j\leqslant J}\left|C^{k+1}_{m,q_n,j}\right|\leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{k+1}_{m,n,j}\right|, \tag{52}$$

$$\sup_{0\leqslant m\leqslant M}\ \sup_{0\leqslant n\leqslant N}\left|C^{k+1}_{m,n,q_j}\right|\leqslant \sup_{1\leqslant m\leqslant M-1}\ \sup_{1\leqslant n\leqslant N-1}\ \sup_{1\leqslant j\leqslant J-1}\left|C^{k+1}_{m,n,j}\right|. \tag{53}$$

Let us define norms by

$$\| C^{k+1} \| = \sup_{0\leqslant m\leqslant M} \sup_{0\leqslant n\leqslant N} \sup_{0\leqslant j\leqslant J} \left| C^{k+1}_{m,n,j} \right| = \sup_m \sup_n \sup_j \left| C^{k+1}_{m,n,j} \right|,$$

$$\| C^0 \| = \sup_m \sup_n \sup_j \left| C^0_{m,n,j} \right|,$$

$$\| f \| = \sup_k \sup_{1\leqslant m\leqslant M-1} \sup_{1\leqslant n\leqslant N-1} \sup_{1\leqslant j\leqslant J-1} \left| f^k_{m,n,j} \right|, \tag{54}$$

$$\| \varphi \| = \max\Big\{ \sup_k \sup_n \sup_j \left| \varphi^k_{0,n,j} \right|, \sup_k \sup_n \sup_j \left| \varphi^k_{M,n,j} \right|, \sup_k \sup_m \sup_j \left| \varphi^k_{m,0,j} \right|,$$
$$\sup_k \sup_m \sup_j \left| \varphi^k_{m,N,j} \right|, \sup_k \sup_m \sup_n \left| \varphi^k_{m,n,0} \right|, \sup_k \sup_m \sup_n \left| \varphi^k_{m,n,J} \right| \Big\}.$$

From (46) and (54) it follows that

$$\sup_{1\leqslant m\leqslant M-1} \sup_{1\leqslant n\leqslant N-1} \sup_{1\leqslant j\leqslant J-1} \left| C^{k+1}_{m,n,j} \right| \leqslant \| C^0 \| + T \| f \| . \tag{55}$$

On the other hand, by (47) - (55) we have

$$\sup_n \sup_j \left| C^{k+1}_{q_m,n,j} \right| \leqslant$$
$$\max\Big\{ \sup_k \sup_n \sup_j \left| \varphi^k_{q_m,n,j} \right|, \sup_{1\leqslant m\leqslant M-1} \sup_{1\leqslant n\leqslant N-1} \sup_{1\leqslant j\leqslant J-1} \left| C^{k+1}_{m,n,j} \right| \Big\} \leqslant$$
$$\max\Big\{ \| \varphi \|, \| C^0 \| + T \| f \| \Big\}. \tag{56}$$

Similarly,

$$\sup_m \sup_j \left| C^{k+1}_{m,q_n,j} \right| \leqslant \max\{\| \varphi \|, \| C^0 \| + T \| f \|\}, \tag{57}$$

$$\sup_m \sup_n \left| C^{k+1}_{m,n,q_j} \right| \leqslant \max\{\| \varphi \|, \| C^0 \| + T \| f \|\}. \tag{58}$$

Therefore,

$$\| C^k \| = \sup_m \sup_n \sup_j \left| C^k_{m,n,j} \right| = \max\Big\{ \sup_{1\leqslant m\leqslant M-1} \sup_{1\leqslant n\leqslant N-1} \sup_{1\leqslant j\leqslant J-1} \left| C^k_{m,n,j} \right|,$$
$$\sup_n \sup_j \left| C^k_{q_m,n,j} \right|, \sup_m \sup_j \left| C^k_{m,q_n,j} \right|, \sup_m \sup_n \left| C^k_{m,n,q_j} \right| \Big\}, \tag{59}$$

where q_m is equal to 0 or to M, q_n is equal to 0 or to N, q_j is equal to 0 or to J.

Substituting (55) - (58) in (59) yields that

$$\| C^k \| \leqslant \max\{\| C^0 \| + T \| f \|, \| \varphi \|\}.$$

Therefore

$$\| C^k \| \leqslant \| C^0 \| + T \| f \| + \| \varphi \| .$$

i.e, the above mentioned difference scheme is unconditionally stable if $\theta = 1$ and stable with the condition (32) if $\theta \neq 1$.

Theorem 2. *The difference scheme (8) - (10) in time and (19) - (22) in space with boundary conditions (27), (28) is stable with condition (26) if* $\theta = 1$*, and if* $\theta \neq 1$*, it is stable with condition (26) and*

$$\tau < \frac{1}{(1-\theta)(\overline{\lambda}_2^x + \overline{\lambda}_2^y + \overline{\lambda}_2^z)}, \quad \forall \;\; k, m, n, j \tag{60}$$

where

$$\overline{\lambda}_2^x = \left(\frac{2\nu}{(\Delta x)^2} + \frac{\sigma}{3}\right)_{m,n,j}^{k+1/2}; \overline{\lambda}_2^y = \left(\frac{2\nu}{(\Delta y)^2} + \frac{\sigma}{3}\right)_{m,n,j}^{k+1/2}; \overline{\lambda}_2^z = \left(\frac{2\mu}{(\Delta z)^2} + \frac{\sigma}{3}\right)_{m,n,j}^{k+1/2};$$

The proof is as analogous as one of Theorem 1.

4. THE NONNEGATIVE PROPERTY OF NUMERICAL SOLUTION (see [9])

Let the initial and boundary conditions be nonnegative and $f \geqslant 0$.

Theorem 3. *The solution of the difference equations (8) - (10) with upwind scheme (11) - (14) in space and boundary conditions (27), (28) is nonnegative when* $\theta = 1$*. In case* $\theta \neq 1$*, the solution is nonnegative if time step satisfies the condition (32).*

Proof. Assume that at the time step t_k the values $C_{m,n,j}^k$ be nonnegative. The equations (15), (23) are solved by the following double sweep method

$$C_{m,n,j}^{k+1/3} = L_m^x C_{m-1,n,j}^{k+1/3} + K_m^x, \tag{61}$$

where

$$L_m^x = \frac{-\alpha_m^x}{\beta_m^x + \gamma_m^x L_{m+1}^x}, \;\; K_m^x = \frac{\delta_m^x - \gamma_m^x K_{m+1}^x}{\beta_m^x + \gamma_m^x L_{m+1}^x}.$$

Applying the mathematical induction, we obtain

$$0 \leqslant L_m^x < 1 \text{ and } K_m^x \geqslant 0, \;\; (m = 1, 2, ..., M-1). \tag{62}$$

Indeed, assume that $0 \leqslant L_{m+1}^x \leqslant 1$ and $0 \leqslant K_{m+1}^x$.

From (15) or (23) we have

$\delta_m^x = (C_{m,n,j}^k - \tau(1-\theta)\Omega^{k+1/2} C_{m,n,j}^k) + \tau f_{m,n,j}^{k+1/2} = C_{m,n,j}^k - \tau(1-\theta)[\lambda_1^x C_{m-1,n,j}^k + \lambda_2^x C_{m,n,j}^k + \lambda_3^x C_{m+1,n,j}^k + \lambda_1^y C_{m,n-1,j}^k + \lambda_2^y C_{m,n,j}^k + \lambda_3^y C_{m,n+1,j}^k + \lambda_1^z C_{m,n,j-1}^k + \lambda_2^z C_{m,n,j}^k + \lambda_3^z C_{m,n,j+1}^k] + \tau f_{m,n,j}^{k+1/2} = [1 - \tau(1-\theta)(\lambda_2^x + \lambda_2^y + \lambda_2^z)] C_{m,n,j}^k + \tau(1-\theta)(|\lambda_1^x| C_{m-1,n,j}^k + |\lambda_3^x| C_{m+1,n,j}^k + |\lambda_1^y| C_{m,n-1,j}^k + |\lambda_3^y| C_{m,n+1,j}^k + |\lambda_1^z| C_{m,n,j-1}^k + |\lambda_3^z| C_{m,n,j+1}^k) + \tau |f_{m,n,j}^{k+1/2}|$.

If $\theta = 1$ then $\delta_m^x = C_{m,n,j}^k + \tau f_{m,n,j}^{k+1/2} \geqslant 0$.

If $\theta \neq 1$ and τ satisfies the condition (32) then

$$\delta_m^x = C_{m,n,j}^k - \tau(1-\theta)\Omega^{k+1/2} C_{m,n,j}^k + \tau f_{m,n,j}^{k+1/2} \geqslant 0.$$

Moreover,

$$\beta_m^x + \gamma_m^x L_{m+1}^x = \beta_m^x - |\alpha_m^x| - |\gamma_m^x| + |\alpha_m^x| + |\gamma_m^x| - |\gamma_m^x| L_{m+1}^x \geqslant$$
$$\delta + |\alpha_m^x| + |\gamma_m^x|(1 - L_{m+1}^x) > |\alpha_m^x|,$$

$$0 \leqslant L_m^x = \frac{-\alpha_m^x}{\beta_m^x + \gamma_m^x L_{m+1}^x} = \frac{|\alpha_m^x|}{\beta_m^x + \gamma_m^x L_{m+1}^x} < \frac{|\alpha_m^x|}{|\alpha_m^x|} = 1,$$

$$K_m^x = \frac{\delta_m^x - \gamma_m^x K_{m+1}^x}{\beta_m^x + \gamma_m^x L_{m+1}^x} = \frac{\delta_m^x + |\gamma_m^x| K_{m+1}^x}{\beta_m^x + \gamma_m^x L_{m+1}^x} \geqslant 0.$$

From (61), (62) and the nonnegative boundary condition we have

$$C_{m,n,j}^{k+1/3} = L_m^x C_{m-1,n,j}^{k+1/3} + K_m^x \geqslant 0.$$

Similarly, it is easy to verify that $C_{m,n,j}^{k+2/3} \geqslant 0$, $C_{m,n,j}^{k+1} \geqslant 0$.

So the numerical solution is nonnegative.

Theorem 4. *The solution of the difference equations (8) - (10) with the central difference scheme (19) - (22) in space and boundary conditions (27), (28) are nonnegative for $\theta = 1$ if the time step satisfies the condition (26), and for $\theta \neq 1$ if it satisfies two conditions (26) and (60) hold.*

The proof is similar to that used for the proof of Theorem 3.

5. NUMERICAL EXPERIMENTS

The above algorithm is applied in solving the following problems.

a) In comparison with analytical solution

The matter propagation equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + \sigma C - \nu \Delta C = Q\delta(r - r_0)\delta(t - t_0); \tag{63}$$

$C|_{t=0} = 0, C(r) \to 0$ with $|r| \to \infty$, $r = (x, y)$ with the assumption $u = \text{const} > 0, v = \text{const} > 0, \sigma = \text{const}, \nu = \text{const}$, we have the following analytical solution (see [1, 4])

$$C(x, y, t) = \begin{cases} \dfrac{Q}{4\pi\nu(t - t_0)} \exp\{-\alpha(r - r_0, t - t_0)\}, & t \in (t_0, T] \\ 0, & t \in [0, t_0]; \end{cases} \tag{64}$$

where, $\alpha(r, t) = \sigma t + \dfrac{(x - ut)^2 + (y - vt)^2}{4\nu t}$.

From the above algorithm, we can find C in a large enough region G contains source point r_0 so that at the boundaries Σ, we can take $C = 0$, and $w = 0, \mu = 0, \alpha = 0$.

Consider the following two cases

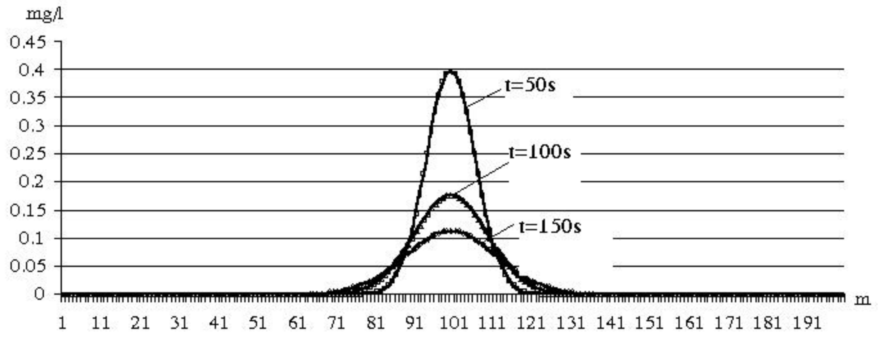
i) *Diffusion case* ($u = 0, v = 0$)

The input parameters are $\nu = 0.5m^2/s$, $\sigma = 0.01s^{-1}, Q = 100mg/l.s, t_0 = 10s, r_0 = (100, 100, 0), \Delta x = \Delta y = \Delta z = 1m, \tau = 1s$.

If $f = Q\delta(r - r_0)\delta(t - t_0)$ then the equation for differencing is of the form

$$\frac{\partial C}{\partial t} + \Omega C = \begin{cases} \dfrac{Q}{\tau.\Delta x \Delta y \Delta z}, & \text{if } r = r_0, t = t_0 \quad \text{where} \quad r = (x, y, 0) \\ 0, & \text{if } (r, t) \neq (r_0, t_0). \end{cases}$$

The computational results and analytical solutions (64) are given in Fig.1.



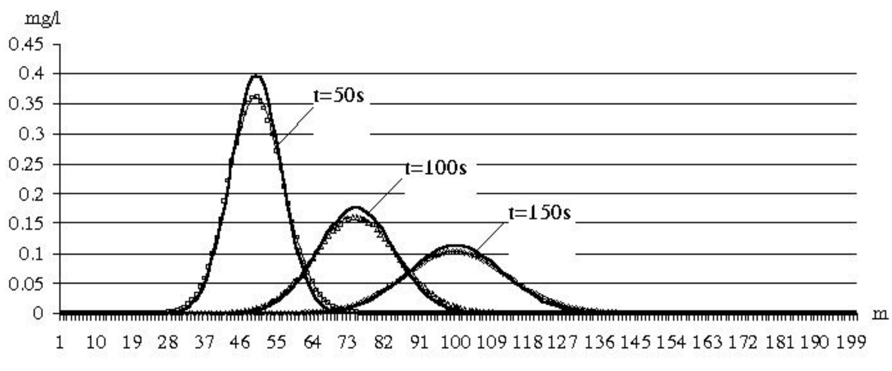
——- analytical solution, - - - computational solution

Fig.1

Concentration distribution along a ray passing the source point r_0 and parallel to the axis Ox, at $t = 50$s, $t = 100$s and $t = 150$s.

ii) *Transport and diffusion case*

The parameters are taken the same as above, except for $u = 0.5m/s, v = 0, r_0 = (30, 100, 0), \tau = 1.0s$. The computational and analytical solutions are give in Fig.2



——- analytical solution - - - computational solution

Fig.2

Concentration distribution along a ray passing the source point r_0 and parallel to the direction Ox, at $t = 50s, t = 100s$ and $t = 150s$.

b) *Three dimensional matter propogation problems*

The matter transport and diffusion in a region with $10000m$ in length, $10000m$ wide and $50m$ in height, the parameters are $\Delta x = \Delta y = 100m, \Delta z = 5m, \tau = 20s, \nu = 2m^2/s, \mu = 0.05m^2/s, u = 0.2m/s, v = w = 0, \sigma = 0$, and the initial condition $C(x, y, z, 0) = 0$. Two cases of the pollution propagation are considered.

i) *Case 1*

In G there is a source point $r_0 = (300, 5000, 25)$. The function $f = Q\delta(r - r_0), Q = 5000g/ls$ is given.

The numerical results are presented in Fig.3. They are isoconcentration C lines at the plane $z = 0$, after 2 hours.

ii) *Case 2*

In G there are three source points: $r_1 = (300, 5000, 25); r_2 = (900, 5500, 25); r_3 = (900, 4500, 25)$. At these source points r_i, we have $f_i = Q\delta(r - r_i);\ i = 1, 2, 3;\ Q = 5000g/ls$.

The numerical results are presented in Fig.4. They are isoconcentration C lines at the plane $z = 0$, after 2 hours.

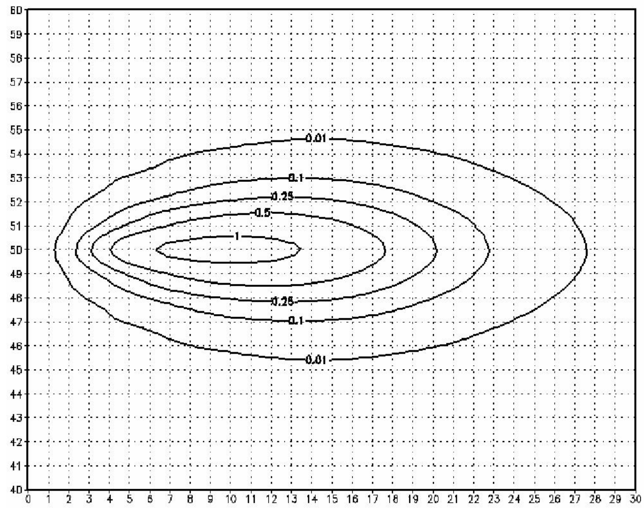


Fig.3

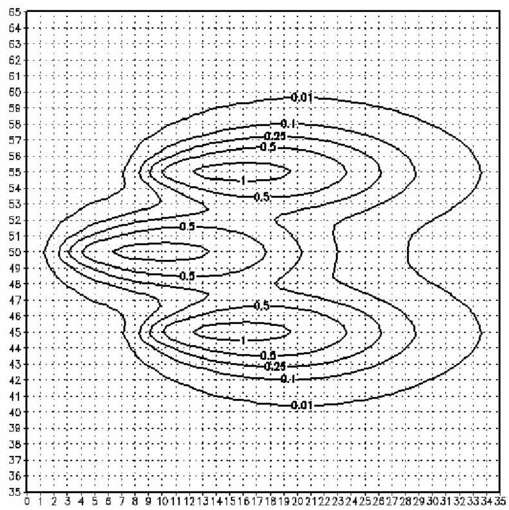


Fig.4

c) *Environmental pollution problem in Cau river*

Let us determine the $BOD5$ pollution on one part of Cau river, which is $10km$ long, and starts $200m$ from Hoang Van Thu paper factory at the upstream side. The $BOD5$ concentration at this factory is $200mg/l$.

The parameters of problem are $\nu = 0.1m^2/s, \mu = 0.005m^2/s, \sigma_{BOD5} = 4.88 \cdot 10^{-4}/s$.

The discharge Q in the dry season is $11m^3/s$, and Q in the rainy season is $1850m^3/s$, $\Delta x = 50m, \Delta y = 3m, J = 10, \tau = 1s$.

The $BOD5$ concentration at the distance $500m$ from Hoang Van Thu paper factory on the downstream side is $0.6mg/l$.

The numerical results are the distribution of isoconcentration lines in the dry season (see Fig.5) and in the rainy season (see Fig.6).

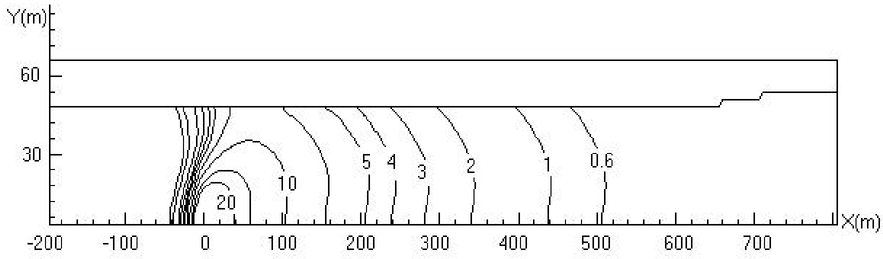


Fig.5

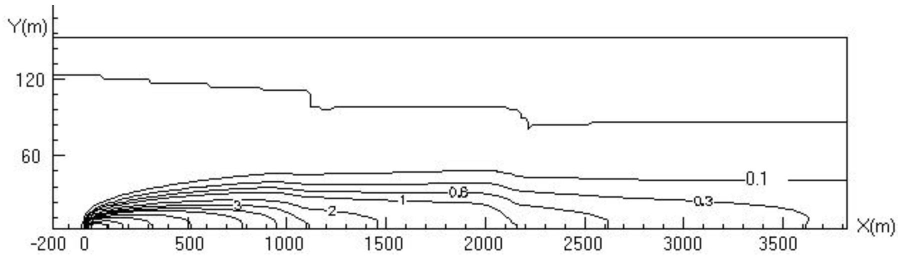


Fig.6

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