

POLLUTANTS TRANSFER IN ENVIRONMENT WITH ONE NEW  
THREE-DIMENSIONAL NUMERICAL SCHEME

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Environmental protection is one of the main problems of the population. At present an investigation of this problem on the basis of mathematical modeling is widely used. Since the transference equation which describes pollutants migration and diffusion analytically is integrated only in the some special cases, therefore for its solving numerical methods are used. Imitational numerical models describing environmental pollution mainly are distinguished by physical and chemical characteristics and types of the sources ejecting harmful substances. With the purpose to reduce simulated problem to the classical problem of the mathematical physics it is necessary to stylize of the examine area and sources ejecting harmful substances.

For example to study pollutants migration and diffusion due to traffic in urban streets exhaust gases can be represented as linear sources and streets can be assumed as a box [1,2]. As regard to wind velocity it is possible to consider it as stationary in the limited time period [2]. Similar type of the problem we obtain when considering sewage waters protection from pollution [3]. For instance the problem of the rivers pollution from the drain-pipe in the urban areas. In this case it is possible to study pollutants migration and diffusion in the rectangular parallelepiped with the free surface. It is possible to suppose that velocity of flows is known and drain-pipes are represented as single (linear) sources.

In this paper we discuss one unconditionally stable difference economical scheme to solve the above mentioned environmental pollution problems.

Let us consider for the equation of parabolic type the following initial-boundary value problem:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} = k_1 \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + k_2 \frac{\partial^2 c}{\partial z^2} + Q(x, y, z, t) - \alpha c, \quad (1)$$

$$c(x, y, z, 0) = 0, C|_{\Gamma/\Gamma_i} = 0, \frac{\partial c}{\partial n} \Big|_{\Gamma_i} = 0,$$

where  $C$  is a concentration;  $u, v, w$  are the axial components of wind velocity along axis  $Ox, Oy, Oz$ ;  $k_1$  and  $k_2$  are the coefficients of turbulent diffusion;  $\alpha$  is the coefficient

that determines the velocity of substance concentration changes during the process of substance decomposition and transformation;  $Q(x, y, z, t)$  are internal sources.

$u = const_1, v = const_2, w = const_3$ , namely  $const_1 = 5; const_2 = 2; const_3 = 0.07$ .

$k_1 = 1, 2.10^3; k_1 = 10; \alpha = 0, 0001; Q = (0, 0, 2 + \Delta z, t) = 0, 01$ .

$(x, y, z, t) \in \overline{G_T} \times [0, T], (x, y, z) \in G, \overline{G} \in G \cup \Gamma$ ,

$\overline{G} = [0 \leq x \leq a_1, 0 \leq y \leq a_1, 0 \leq z \leq b_1]$  is a rectangular parallelepiped,  $\Gamma = \bigcup_{i=1}^6 \Gamma_i$  is a border of parallelepiped  $G$ , and  $\Gamma_i$ - is a right border.

$(a_1 = 4000\text{m}; b_1 = 2000\text{m};)$

The difference scheme for problem (1):

Let us use undimensional variables:

$x = x_1 a_1, y = y_1 a_1, z = z_1 b_1, t = t_1 \frac{a_1^2}{k_1}$

and rewrite the equation (1) equally in the following form:

$$\begin{aligned} \beta \frac{\partial c}{\partial t_1} + \frac{\partial^2 c}{\partial t_1^2} &= \left( \frac{\partial^2 c}{\partial t_1^2} + \beta \frac{\partial^2 c}{\partial x_1^2} \right) + \beta \frac{\partial^2 c}{\partial y_1^2} + \beta \frac{k_2}{k_1} \left( \frac{a_1}{b_1} \right)^2 \frac{\partial^2 c}{\partial z_1^2} - \\ &- \beta \frac{a_1}{k_1} \left( u \frac{\partial c}{\partial x_1} + v \frac{\partial c}{\partial y_1} \right) - \beta \frac{a_1^2}{l_2 k_1} w \frac{\partial c}{\partial z_1} - \beta \frac{a_1^2}{k_1} \alpha c + \beta \frac{a_1^2}{k_1} Q \end{aligned} \quad (2)$$

Let us consider for the equation (2) the following functional

$$\begin{aligned} I(c) &= \int_{t_0}^{t^n} \left\{ \int_G \left[ \beta c \frac{\partial c}{\partial t_1} - \left( \frac{\partial c}{\partial t_1} \right)^2 \right] + \left[ \left( \frac{\partial c}{\partial t_1} \right)^2 + \beta \left( \frac{\partial c}{\partial x_1} \right)^2 \right] + \right. \\ &+ \beta \left[ \left( \frac{\partial c}{\partial y_1} \right)^2 + \frac{k_2}{k_1} \left( \frac{a_1}{b_1} \right)^2 \left( \frac{\partial c}{\partial z_1} \right)^2 - \frac{a_1}{k_1} \left( u c \frac{\partial c}{\partial x_1} + v c \frac{\partial c}{\partial y_1} \right) - \right. \\ &\left. \left. - \frac{a_1^2}{b_1 k_1} w c \frac{\partial c}{\partial z_1} - \frac{a_1^2}{k_1} \alpha c^2 + 2 \frac{a_1^2}{k_1} v c \right] \right\} dx_1 dy_1 dz_1 \Bigg\} dt_1 \end{aligned}$$

If in the latter we replace the derivatives of function  $C$  by the directional derivatives, we obtain:

$$\begin{aligned} I(c) &= \int_{t_0}^{t^n} \left\{ \int_G \left[ \beta c \frac{\partial c}{\partial t_1} - \left( \frac{\partial c}{\partial t_1} \right)^2 \right] + \frac{1}{4} \sum_{i=1}^4 \left[ A_1^{(i)} \left( \frac{\partial c}{\partial l_i} \right)^2 + B_1^{(i)} \left( \frac{\partial c}{\partial l_{i+1}} \right)^2 + \right. \right. \\ &+ C_1^{(i)} \frac{\partial c}{\partial l_i} \frac{\partial c}{\partial l_{i+1}} \Bigg]_{(\delta_i)} + \beta \left[ \left( \frac{\partial c}{\partial y_1} \right)^2 + \frac{k_2}{k_1} \left( \frac{a_1}{b_1} \right)^2 \left( \frac{\partial c}{\partial z_1} \right)^2 \right] - \\ &\left. - \beta \frac{a_1}{k_1} c \left( u \frac{\partial c}{\partial x_1} + v \frac{\partial c}{\partial y_1} + \frac{a_1}{b_1} w + a_1 \alpha c \right) - 2 a_1 v \right\} dx_1 dy_1 dz_1 \Bigg\} dt_1, \end{aligned}$$

where the angles constructed of the directions  $l_i, (i = \overline{1, 4})$  with respect to axes  $ox_1$  in anti clockwise direction is denoted by  $\alpha_i$ , namely

$$(l_1, l_2, l_3, l_4) \doteq (\alpha, 180^\circ - \alpha, 180^\circ + \alpha, 360^\circ - \alpha)$$

see fig.1.

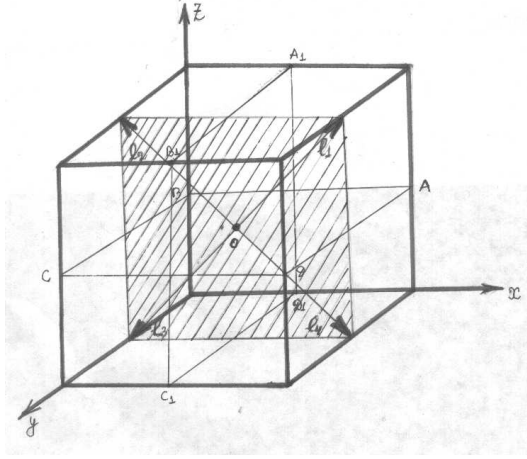


fig.1.

$$A_1^{(i)} = B_1^{(i)} = \frac{\cos^2 \alpha_{i+1} + \beta \sin_{i+1}^2}{\sin^2(\alpha_{i+1} - \alpha_i)}, C_1^{(i)} = \frac{-2(\cos \alpha_i \cos \alpha_{i+1} + \beta \sin_i \sin_{i+1})}{\sin^2(\alpha_{i+1} - \alpha_i)}$$

$(\delta_1)$  cross-section is hatched on the figure.

Let us divide the rectangular parallelepiped  $G$  in elemental cells by the planes parallel to coordinate planes  $xoy, xoz, xoy$ . After that we use the mean value formula and write out the difference functional corresponding to functional  $I(c)$  with respect to the main node of the elementary cell "0" ("0" node is a center of gravity of the cell), we obtain:

$$\begin{aligned} I_h(c_0) = & \left\{ \left[ \frac{\beta}{2} c(c_t + c_{\bar{t}}) + (c_t^2 + c_{\bar{t}}^2) \right]_{(0)} + \right. \\ & + \frac{1}{4} \sum_{i=1}^4 A_1^{(i)} c_i^2 + B_1^{(i)} c_{i+1}^2 + C_1^{(i)} c_i c_{i+1} \left. \right]_{(\delta_1)} - \\ & - \beta \left[ (c_{y_1}^2 + c_{\bar{y}_1}^2) + \frac{k_2}{k_1} \left( \frac{a_1}{b_1} \right)^2 (c_{z_1}^2 + c_{\bar{z}_1}^2) \right] + \\ & + \beta \frac{a_1 c_0}{k_1} (u c_{x_1}^0 + v c_{y_1}^0 + w c_{z_1}^0 + a_1 \alpha c_0 + 2a_1 Q) \left. \right\} v_0 \Lambda t \end{aligned}$$

According to the principle of Hamilton, we obtain the following three-layer difference scheme depending on the parameter  $\sigma$ :

$$\begin{aligned} (E + \sigma \tau^2 R)c = & c_{x_1 \bar{x}_1} + c_{y_1 \bar{y}_1} + \frac{k_2}{k_1} \left( \frac{a_1}{b_1} \right)^2 c_{z_1 \bar{z}_1} - \\ & - \frac{a_1}{k_1} (u c_{x_1}^0 + v c_{y_1}^0) - \frac{a_1^2}{b_1 k_1} w c_{z_1}^0 - \frac{a_1}{k_1} \alpha c_0 + \frac{a_1^2}{k_1} Q \end{aligned} \quad (3)$$

where

$$R = \frac{1}{2} L, L = -\Delta_{11}, -\Delta_{11} c = -c_{x_1 \bar{x}_1}, c_{x_1}^0 = \frac{1}{2} (c_{x_1} + c_{\bar{x}_1}).$$

The obtained scheme represents the generalization of the scheme considered in [4]. Let us write out the obtained scheme in the coordinates:

$$\begin{aligned}
& -\frac{\sigma}{2h_1^2}(C_{i+1,j,l}^{k+1} + C_{i-1,j,l}^{k+1}) + \left(\frac{\sigma}{h_1^2} + \frac{1}{2\tau}\right) C_{i,j,l}^{k+1} = \Phi_{ijl}, \\
& \Phi_{ijl} = 2 \left[ \frac{\sigma - 1}{h_1^2} - \frac{1}{h_2^2} - \frac{k_2}{k_1} \left(\frac{a_1}{b_1}\right)^2 \frac{1}{h_3^2} \right] C_{i,j,l}^k + \\
& \quad + (1 - \sigma) \frac{1}{h_1^2} (C_{i+1,j,l}^k + C_{i-1,j,l}^k) + \\
& \quad + \sigma \frac{1}{2h_1^2} (C_{i+1,j,l}^{k-1} - 2C_{i,j,l}^{k-1} + C_{i-1,j,l}^{k-1}) + \frac{1}{h_2^2} (C_{i,j+1,l}^k + C_{i,j-1,l}^k) + \\
& \quad + \frac{k_2}{k_1} \left(\frac{a_1}{b_1}\right)^2 \frac{1}{h_3^2} (C_{i,j,l+1}^k + C_{i,j,l-1}^k) + \frac{1}{2\tau} C_{i,j,l}^k - \\
& \quad - \frac{a_1}{k_1} u \frac{1}{2h_1} (C_{i+1,j,l}^k - C_{i-1,j,l}^k) - \frac{a_1}{k_1} v \frac{1}{2h_2} (C_{i,j+1,l}^k - C_{i,j-1,l}^k) - \\
& \quad - \frac{a_1^2}{b_1 k_1} w \frac{1}{2h_3} (C_{i,j,l+1}^k - C_{i,j,l-1}^k) - \frac{a_1^2}{k_1} \alpha C_{i,j,l}^k + \frac{a_1^2}{k_1} Q_{ijl}
\end{aligned}$$

The scheme (3) is unconditionally stable and it approximates the problem (1) by the order  $O(h^2 + \tau^2)$ . ( $h_i, i = \overline{1,3}$  are steps with respect to spatial variables,  $\tau$  - with respect to time).

The graphs describe a distribution of function  $C$  in the medium planes  $ABCD$  and  $A_1B_1C_1D_1$  of parallelepiped  $G$  (see fig.1), when  $C(x, y, z, 0) = C(x, y, z, \tau) = 0.5, T = 40000, h_1 = h_2 = 200; h_3 = 100; \tau = 400$ .

In the new coordinates accordingly  $T_1 = 3, h_1 = h_2 = \frac{1}{20}; h_3 = \frac{1}{40}; \tau = 0.03$ .

Our aim is to study the unconditionally stable scheme (3) in conditions of realization of the problems of hydrothermodynamics. In view of this we have carried out a number of numerical calculations, which differed from each other by values of axe components of the wind velocity, turbulence coefficients, the intensity of outer polluting source and its geometrical placement and type (point sources, linear sources). On the figures 2 and 3 there are given the results of some characteristic numerical calculations. In order to show the possibilities of numerical scheme, we everywhere left unchanged the axe components of the wind velocity and turbulence coefficients, the values of which were taken in the frame of the mean values of real processes appear in the atmosphere, and the polluting sources, which in the conditionally stable schemes greatly define the stability of numerical schemes, differ from each other by their placement in the rectangular parallelepiped and their type. Namely, on the figures 2 and 3 there are given the results of numerical calculation, when the polluting source had a linear form and it was placed on line  $A_1B_1$  of rectangular parallelepiped, and on the figures 4 and 5 analogously are given the pictures of the distribution of the pollutant concentration, when the polluting source was presented as three point sources, placed uniformly on line  $A_1B_1$  of the parallelepiped. (On the figures 2 and 4 are given the pollutant concentration on perpendicular vertical plane of the parallelepiped, which goes on the

polluting source, and on the figures 3 and 5 are shown the results of the same numerical calculations on horizontal plane of the central part of parallelepiped). The figures 6 and 7 show the results of numerical calculations, when the polluting source was placed on edge, parallel to line  $A_1B_1$ . (On the figure 6 there are given the results of numerical calculations, which correspond to linear source, and on the figure 7 - to three point sources.) By the comparing of figures 2 and 4, as well as figures 3 and 5, figures 6 and 7 with each other, it can be obviously seen (where are shown the results of numerical calculations corresponding to physical time 18.00) that for unconditionally stable scheme the character of the polluting source intensity did not make important changes. However the distributions of concentrations in case of linear and point sources differed from each other. Thus, we can conclude that the scheme (3) can be used for the numerical integration of the parabolic type equations, where are included the medium polluting sources.

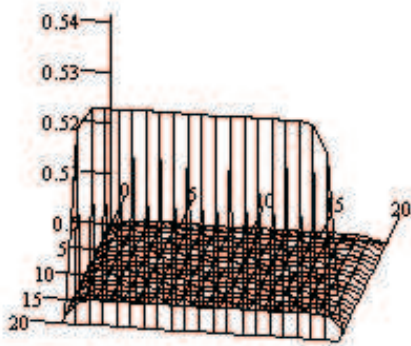


fig.2.

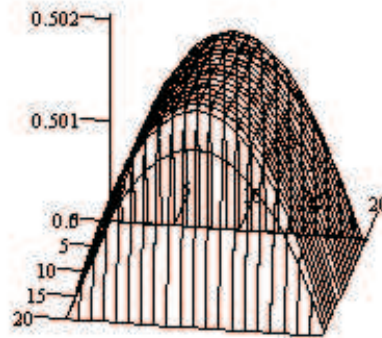


fig.3

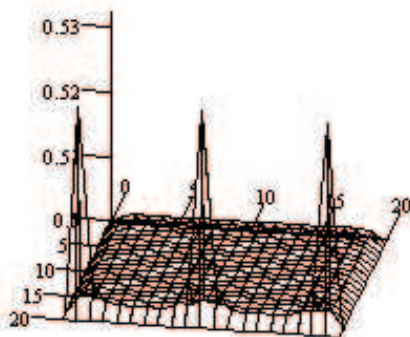


fig.4.

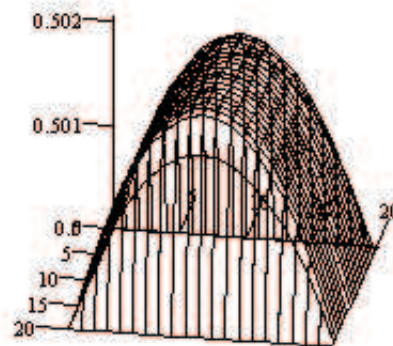


fig.5

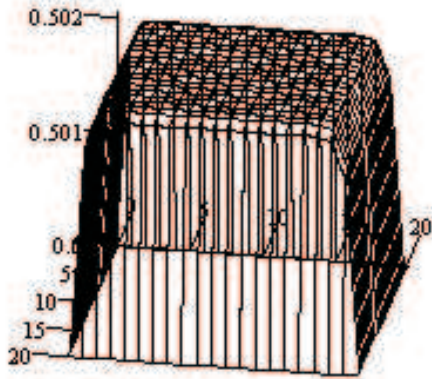


fig.6.

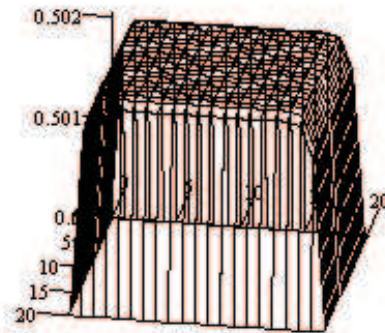


fig.7

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