UDC 004.94

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ALGORITHMS OF SIMULATION OF THE POLUTIONS PROPAGATION PROCESSES IN ATMOSPHERE

In present paper the problem of the pollutions propagation processes in the atmosphere layer near the earth surface is considered. The problem formulation takes into account the wind rising of polluting particles. The numerical algorithms are based on two- and three-layer implicit schemes and Runge-Kutta method.

Key words: *pollution propagation, wind rising, finite difference methods, two- and three-layer implicit schemes.*

1. PROBLEM FORMULATION

The problem of protecting and restoring of the environment is one of the major tasks of the science. The heavy development of industry in the world has caused mankind emerging of an acute problem – the preservation of ecological systems historically generated on our planet. Per last decades these systems undergo significant influence of natural and, especially, man-caused factors, having undesirable trend. Therefore prognosis of ecological systems modifications due to the indicated reasons is the actual problem. The solving of the problem consists of two stages:

a) research of environment pollution process by ejection of scraps of industrial works and due to disastrous appearances of man-caused and natural origin;
b) evaluation of harmful contamination influence on ecosphere.

The evaluation of atmosphere and terrestrial surface pollution with passive and active pollutants is an important part of the problem. The pollution is called passive, if it does not undergo physics-chemical transformations. If it reacts with the steam and other components of the atmosphere in the course of spreading in the atmosphere and goes from one chemical state to another due to such reactions, thus changing its toxicity in relation to environment, then such pollution is called active.

The process of industrial ejections and disastrous appearances yields spreading in the atmosphere happens due to their advective transfer with air masses and due to diffusion which is caused by turbulent pulsation of air. If the pollution consists of the rough particles then being spreaded in the atmosphere these particles fall on the terrestrial surface by gravity with a constant speed according to the Stokes law. It is natural that nearly all particles settle out on the terrestrial surface in the end: heavy particles settle out by gravity and the light-weight particles — due to diffusion

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process. The gravitational stream of light-weight particles does not have any sufficient influence. It will be noted that most gaseous pollutions, such as oxides, are most dangerous for environment.

The problem under consideration is formulated as follows:

$$\rho \frac{\partial u}{\partial t} = Lu - f^*(x,t),\ x = (x_1, x_2) \in \bar{G},\ t_0 \le t \le T, \quad (1)$$

where

$$Lu \equiv \frac{\partial}{\partial x_1}(a^1 \frac{\partial u}{\partial x_1}) + \frac{\partial}{\partial x_2}(a^2 \frac{\partial u}{\partial x_2}) + b^1 \frac{\partial u}{\partial x_1} + b^2 \frac{\partial u}{\partial x_2} + au$$

is an elliptic type operator with variable coefficients:

$$c = c(x,t),\ c = \{\rho, a^1, a^2, b^1, b^2, a\},$$

$$\bar{G} = G \cup \Gamma = \{x = (x_1, x_2);\ x_0 \le x_1 \le l_1;\ \ y_0 \le x_2 \le l_2\}$$

is a rectangle in the plane Ox_1x_2 with the boundary Γ:

$$\Gamma = \bigcup_{\alpha} \gamma_{\pm\alpha}\ ,\ \ \alpha = 1,\ 2$$

are the rectangle $\bar{G}$ sides (Fig. 1);

$$\left(\frac{\partial u}{\partial N} + \partial u \right)\bigg|_{\Gamma} = \varphi\big(s,t\big),\ s \in \Gamma, \quad (2)$$

where

$$\frac{\partial u}{\partial N} = a^1 \frac{\partial u}{\partial x_1} \cos(\vec{n}, x_1) + a^2 \frac{\partial u}{\partial x_2} \cos(\vec{n}, x_2),$$

$\vec{n}$ is the outer normal to Γ, σ (*s, t*), φ (*s, t*) are functions given on Γ.

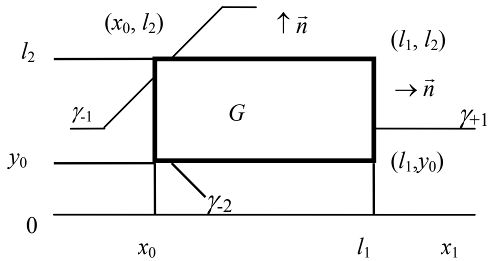

Fig. 1.

The expanded form of (2) can be written as

$$a^1 \frac{\partial u}{\partial x_1} - x_{-1} u = -g_{-1}, \quad x \in \gamma_{-1},$$

$$-a^1 \frac{\partial u}{\partial x_1} - x_{+1} u = -g_{+1}, \quad x \in \gamma_{+1},$$

$$-a^2 \frac{\partial u}{\partial x_2} - x_{+2} u = -g_{+2}, \quad x \in \gamma_{+2},$$
$$a^2 \frac{\partial u}{\partial x_2} - x_{-2} u = -g_{-2}, \quad x \in \gamma_{-2}. \tag{3}$$

The right hand side $g_{-2} = g_Q$ of boundary condition for the rectangle's lower side g_{-2} is obtained as a solution of the Cauchy problem [1]

$$\frac{\partial Q}{\partial t} = Vdu - \gamma Q, \tag{4}$$

where $Q = Q(N_1, t)$ corresponds to pollution concentration on the ground; V_d, V_s, g are the dry sedimentation speed of particles, the gravity settle out speed and the wind rise parameters.

At $r = 1$, $e = 0$, $f^* = 0$ the coefficients $a^{\alpha}, b^{\alpha}, x_{\pm\alpha}, \alpha = 1, 2$ are expressed in terms of diffusion coefficients, wind speed components V_1, V_2 and V_d, V_s.

The solution $u(x_1, x_2, t)$ of the problem (1), (3), (4) to be found corresponds to the polluting particles concentration in $\overline{G}$ (the atmosphere layer near the earth surface), the solution $Q(x_1, t)$ of the Cauchy problem (4) corresponds to polluting particles concentration on the earth surface $x_2 = 0$. The problem is solved when initial conditions

$$U(x_1, x_2, t_0) = u_0(x_1, x_2),$$
$$Q(x_1, t_0) = Q_0(x_1),$$

are satisfied.

Thus, the algorithm of the considered problem solution involves:

1) the assignment of the initial distributions u_0 and Q_0;
2) the simultaneous solution of the Cauchy problem (4) and the boundary value problem (1), (3) at instants of time $t_0 < t = t_k$, $k = 1, 2, 3, ...$

For solution of the Cauchy problem (4) the Runge-Kutta method of the 4th order is used. The boundary value problem (1), (3) is solved using finite difference two- and three-layer implicit schemes.

2. TWO-LAYER AND THREE-LAYER IMPLICIT SCHEMES

2.1. Two-layer implicit scheme of solving the problem (1), (3). The scheme for solving the problem (1), (3) is of the following form [2]:

$$\left[\frac{\rho(\overline{t})}{\tau} - \Lambda^h(\overline{t})\right]\hat{u} = \left[\frac{\rho(\overline{t})}{\tau}\right]u - f^*(\overline{t}), \tag{6}$$

where $\overline{t} = t_k + 0.5\tau$, $t_k = k\tau > 0$, τ is a fixed time step; $\hat{u} \equiv u^{(k+1)}$, $u \equiv u^{(k)}$, k is a number of the time layer.

Denote the operators $\Lambda^h(\overline{t})$ of discrete scheme corresponds to (1), (3) by

$$\Lambda_{\overline{\omega}}^{h}(\overline{t}) \equiv \begin{cases} \Lambda_{-1,-2}^{h,\tau} & \text{in the point} \quad P_1 = \gamma_{-1} \cap \gamma_{-2} \quad (i=0; j=0), \\ \Lambda_{-2}^{h,\tau}, & x \in \gamma_{-2}; \quad (i = \overline{1, N_1 - 1}; \quad j=0), \\ \Lambda_{+1,-2}^{h,\tau} & \text{in the point} \quad P_2 = \gamma_{+1} \cap \gamma_{-2} \quad (i = N_1; j=0), \\ \Lambda_{-1}^{h,\tau}, & x \in \gamma_{-1} \quad (i=0; j = \overline{1, N_2 - 1}), \\ \Lambda_{\omega}^{h,\tau}, & x \in \omega \quad (i = \overline{1, N_1 - 1}; \quad j = \overline{1, N_2 - 1}), \\ \Lambda_{+1}^{h,\tau}, & x \in \gamma_{+1} \quad (i = 1, N_1; \quad j = \overline{1, N_2 - 1}), \\ \Lambda_{-1,+2}^{h,\tau} & \text{in the point} \quad P_4 = \gamma_{-1} \cap \gamma_{+2} \quad (i=0; j=N_2), \\ \Lambda_{+2}^{h,\tau}, & x \in \gamma_{+2} \quad (i = \overline{1, N_1 - 1}; \quad i = N_2), \\ \Lambda_{+1,+2}^{h,\tau} & \text{in the point} \quad P_3 = \gamma_{+1} \cap \gamma_{+2}; \quad (i = N_1; j = N_2), \end{cases} \tag{7}$$

where

$$\overline{\omega} = \omega \cup \overline{\gamma} = \{ x \equiv (x_i, y_j); \quad x_i = x_0 + ih_1, y_j = y_0 + jh_2,$$
$$i = \overline{0, N_1}, \quad j = \overline{0, N_2};$$
$$h_1 = (l_1 - x_0)/N_1; \quad h_2 = (l_2 - y_0)/N_2 \},$$
$$l_1 \equiv x_{N_1} = x_0 + h_1 N_1; \;\; l_2 \equiv x_{N_2} = y_0 + h_2 N_2.$$

Noting the equation (6) as

$$A^{h,\tau} \widehat{u} = \Phi,$$

where

$$A^{h,\tau} = \frac{\rho(\overline{t})}{\tau} - \Lambda^h(\overline{t}), \; \Phi = \frac{\rho(\overline{t})}{\tau} u - f^*(\overline{t}),$$

we can find coefficients $S(\overline{t})$ of the discrete problem corresponded to the problem (1), (3).

We have

$$\begin{aligned} A_{0,0}^{h,\tau} \widehat{u} &\equiv \alpha_1(\overline{t}) \widehat{u}_{i+1,j} + \alpha_2(\overline{t}) \widehat{u}_{i,j+1} + \alpha_0(\overline{t}) \widehat{u}_{i,j} = \\ &= \frac{\rho(\overline{t})}{\tau} u_{i,j} - \left[f(\overline{t}) - \frac{2}{h_1} g_{-1}(\overline{t}) - \frac{2}{h_2} g_{-2}(\overline{t}) \right]_{i,j}, \end{aligned} \tag{8}$$

where

$$\alpha_1(\overline{t}) = -\frac{1}{h_1} \left[\frac{2}{h_1} \frac{a_{i,j}^1 + a_{i+1,j}^1}{2} + b_{i,j}^1 \right] (\overline{t});$$

$$\alpha_2(\overline{t}) = -\frac{1}{h_2} \left[\frac{2}{h_2} \frac{a_{i,j}^2 + a_{i+1,j}^2}{2} + b_{i,j}^2 \right] (\overline{t});$$

$$\alpha(\bar{t}) = \left(-\frac{2}{h_1} x_{-1} - \frac{2}{h_2} x_{-2} + a \right)_{i,j} (\bar{t});$$

$$\alpha_0(\bar{t}) = \left(\frac{\rho(\bar{t})}{\tau} - \alpha(\bar{t}) - \alpha_1(\bar{t}) - \alpha_2(\bar{t}) \right)_{i,j}.$$

The coefficients of the other eight operators $A_{-2}^{h,\tau},..., A_{+1,+2}^{h,\tau}$ (7) are determined similarly to (8). So for $A_{-2}^{h,\tau}$ and $A_{\omega}^{h,\tau}$ we have

$$A_{-2}^{h,\tau}\hat{u} \equiv \alpha_3 \hat{u}_{i-1,j} + \alpha_1 \hat{u}_{i+1,j} + \alpha_2 \hat{u}_{i,j+1} + \alpha_0 \hat{u}_{i,j} = \frac{\rho}{\tau} u_{i,j} - \left[f - \frac{2}{h_2} g_{-2} \right]_{i,j}, \quad (9)$$

where

$$\alpha_3 = -\frac{1}{h_1}\left(\frac{1}{h_1}\tilde{a}_-^1 - \frac{b_{i,j}^1}{2} \right); \ \alpha_1 = -\frac{1}{h_1}\left(\frac{1}{h_1}\tilde{a}_+^1 + \frac{b_{i,j}^1}{2} \right);$$

$$\alpha_2 = -\frac{1}{h_2}\left(\frac{2}{h_2}\tilde{a}_+^2 + b_{i,j}^2 \right); \ \alpha = \left(-\frac{2}{h_2} x_{-2} + a \right)_{i,j};$$

$$\alpha_0 = \left(\frac{\rho}{\tau} - \alpha - \alpha_1 - \alpha_2 - \alpha_3 \right)_{i,j}; \quad (i = 1, \overline{N_1 - 1}; \quad j = 0);$$

$$A_{\omega}^{h,\tau}\hat{u} \equiv \alpha_3 \hat{u}_{i-1,j} + \alpha_1 \hat{u}_{i+1,j} + \alpha_2 \hat{u}_{i,j+1} + \alpha_4 \hat{u}_{i,j-1} + $$
$$+ \alpha_0 \hat{u}_{i,j} = \frac{\rho}{\tau} u_{i,j} - f; \quad x \in \omega, \quad (10)$$

where

$$\alpha_3 = -\frac{1}{h_1}\left(\frac{1}{h_1}\tilde{a}_-^1 - \frac{b_{i,j}^1}{2} \right); \ \alpha_1 = -\frac{1}{h_1}\left(\frac{1}{h_1}\tilde{a}_+^1 + \frac{b_{i,j}^1}{2} \right);$$

$$\alpha_2 = -\frac{1}{h_2}\left(\frac{1}{h_2}\tilde{a}_+^2 + \frac{b_{i,j}^2}{2} \right); \ \alpha_4 = -\frac{1}{h_2}\left(-\frac{1}{h_2}\tilde{a}_-^2 - \frac{b_{i,j}^2}{2} \right);$$

$$\alpha_0 = \left(\frac{\rho}{\tau} - \alpha - \alpha_1 - \alpha_2 - \alpha_3 - \alpha_4 \right)_{i,j}; \quad (i = 1, \overline{N_1 - 1}; \quad j = 1, \overline{N_2 - 1}).$$

$\tilde{a}_-^1, \tilde{a}_+^1, \tilde{a}_-^2, \tilde{a}_+^2$ in (9), (10) are found according to the formulas

$$\tilde{a}_-^1 = \frac{1}{2}(a_{i,j}^1 + a_{i-1,j}^1); \ \tilde{a}_-^1 = \frac{1}{2}(a_{i,j}^2 + a_{i,j-1}^2),$$

$$\tilde{a}_-^1 = \frac{1}{2}(a_{i,j}^1 + a_{i-1,j}^1); \ \tilde{a}_-^1 = \frac{1}{2}(a_{i,j}^1 + a_{i-1,j}^1).$$

2.2. Three-layer implicit scheme for solving the problem (1), (3). Three-layer parametric implicit scheme [2] with $r(\bar{t}\,)$ can be written in the form:

$$\theta u_t + (1-\theta) u_{\bar{t}} = \Lambda^h(\bar{t}\,)\,\hat{u} - f^*(\bar{t}\,), \tag{11}$$

where q is the numerical parameter.

If $q = 1$ then we obtain a pure implicit two-layer scheme (6), and if $q = 3/2$ then it is a pure implicit three-layer scheme. The using of parametric scheme gives us the opportunity of additional checking of accuracy of the obtained numerical solution. This realization of the scheme (11) requires a solution of linear algebraic equations system $Ax = f$ with non-symmetric matrix for every time layer.

The calculating formulas of the algorithm which is used to solve the system look like [3]

$$\tilde{r} = f - Ax_0,\ r_0 = (\tilde{L}D\tilde{U})^{-1}\tilde{r},\ P_0 = r_0 = \left(\tilde{L}D\tilde{U}\right)^{-1} Ar_0, \alpha^{(s)} = \frac{\left(r^{(s)}, z^{(s)}\right)}{\left(z^{(s)}, z^{(s)}\right)}, \tag{12}$$

$$x(s+1) = x(s) + a(s)\,r(s),\ \ r(s+1) = r(s) - a(s)\,z(s),$$

$$t(s+1) = (\tilde{L}D\tilde{U})^{-1} Ar(s+1),\ \beta^{(s)} = \frac{\left(t^{(s+1)}, z^{(s)}\right)}{\left(z^{(s)}, z^{(s)}\right)},$$

$$r(s+1) = r(s+1)r + b(s)\,r(s),$$

$$z(s+1) = t(s+1)r + b(s)\,z(s)\ \ (j_0 = j(0);\ j = x;\ r;\ r;\ z),$$

where s is the iteration number; $s = 0, 1, 2, \ldots$; $\tilde{L}D\tilde{U}$ is the approximate Cholesky decomposition of the matrix A.

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У цій статті розглядається проблема поширення процесів забруднення атмосферного шару поблизу поверхні Землі. Постановка задачі враховує вітер, зростання забруднюючих частинок. Чисельні алгоритми грунтуються на двох- і тришарових схемах Рунге-Кутта.

Ключові слова: *забруднення поширення, вітер піднімається, методу кінцевих різниць, двох-і тришарові схеми.*

Отримано: 25.10.2012