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ALGORITHM OF ATMOSPHERE CONTAMINATION NONLINEAR MODEL NUMERICAL REALIZATION

The article presents the algorithm for solving nonlinear partial differential equations, that describe the process of air contamination. The algorithm is based on an appropriate modification of the grid method. Boundary conditions and border values are considered, and a difference scheme construction method is proposed. As a result, problem is degenerated in two-dimensional one, and reliable algorithms for its solution are developed and approved.

Key words: *atmosphere contamination, nonlinear model, grid method.*

Computing experiment in contamination modeling. Revealing tendencies of environmental contamination and determination of antropogeneous influence on it are extremely actual problems. The research of natural and chemical processes and defining the given problem are not allowed be conducted as the location experiment in most cases. Therefore, important issues acquire the possibility of realization of a computing experiment, for which the construction of mathematical models adequate to the natural processes researched and realized on modem computer facilities is necessary.

The problem of calculation of contamination concentration $q(x, y, z, t)$ in: he atmosphere owing to their ejection and transposition can be represented as following [1]:

$$\frac{\partial q}{\partial t}+\sum_{i=1}^{3} u_i \frac{\partial q}{\partial x_i}+aq=\sum_{i=1}^{3} \frac{\partial}{\partial x_i} k_i \frac{\partial q}{\partial x_i}+v_s \frac{\partial q}{\partial z}+f\ , \qquad (1)$$

here $(x_1, x_2, x_3) = (x, y, z)$ — cartesian coordinates, whose plan XOY corresponds to a terrestrial surface, t — temporary coordinate, (u_1, u_2, u_3) — components of the wind field, a — factor of disintegration of substance taken as a boundary value for the equation.

Taking into account chemical transformation of substance and washing the partials away by settlings ki — factors of turbulent transposition, vs — the settled velocity of the gravitational settling of partials of substance, $f = f(x, y, z, t)$ is the known function circumscribing the density function of contamination sources.

The solution of the equation (1) is discovered for want of certain initial and boundary conditions. The entry conditions are usually formulated as known concentration of substance in researched area for want of $t = 0$:

$$Q(x,y,z,0)=q_0(x,y,z)\,. \tag{2}$$

The boundary conditions, at first, should correctly reflect the process researched, and secondly ensure correctness of the delivered problem. If the researched area is infinite on a horizon, it is natural to assume, that the concentration decreases up to zero for the want of rushing x, y to infinity. However, while applying numerical methods for the solution of the considered problem, the research area should be limited, that is to have, for example, some kind of a parallelepiped:

$$D=\left\{(x,y,z): a_1\le x\le b_1, a_2\le y\le b_2, z_0\le z\le H\right\}.$$

On the boundaries side it is possible to put

$$\left.\frac{\partial q}{\partial n}\right|_{\substack{a_1\le x\le b_1\\ a_2\le y\le b_2}}=0\,.$$

On the upper boundary of the area the modeling of various processes is possible:

- The concentration of substance equal to zero:

$$q\big|_{z=H}=0\,;$$

- Absence of diffusion transposition provided that vertical component of the velocity of wind is equal to zero:

$$\left.\frac{\partial q}{\partial z}\right|_{z=H}=0\,; \tag{3}$$

- Availability of the substance stream through the upper bound:

$$-k_3(z)\frac{\partial q}{\partial z}+v_s q\Big|_{z=H}=0\,. \tag{4}$$

It is possible to simulate processes taking place on a spreading surface, also by various images. For example, in [2; 3] it is considered that impurities poorly interact with the surface of the ground usually and, hitting on it, are not accumulated, and are again carried away in the atmosphere with turbulent curls. As such curls at the surface are insignificant, it is possible to put:

$$k_3\left.\frac{\partial q}{\partial z}\right|_{z=z_0}=0\,. \tag{5}$$

However, while modeling such processes as shaping of spots of increased concentration of impurity on the spreading surface, secondary rise and sedimentation of partials, the condition (5) becomes unsatisfactory. In such condition on the spreading surface it is offered:

$$k_3(z)\frac{\partial q}{\partial z}+v_s q\Big|_{z=z_0}=\left.\frac{\partial Q}{\partial z}\right|_{z=z_0}\,, \tag{6}$$

where $Q(x,\ y,\ t)$ — the concentration of the ground field of impurity, $Z_0=z^*+\partial z$, z^* — level of roughness, ∂z — the thickness of the saltation stratum. As this concentration can vary in time, the condition (6) is supplemented by the ratio

$$\frac{\partial Q}{\partial t} = j = v_d q(x, y, z_0, t) - \gamma Q(x, y, t) , \tag{7}$$

where v_d — the velocity of the dry settling of impurity; γ — the intensity of wind rise. The use of conditions (6), (7) requires, in turn, the giving of initial concentration of impurity on the surface:

$$Q(x, y, 0) = Q_0(x, y) . \tag{8}$$

If the spreading surface represents a mirror of water space, that, assuming the water to swallow all impurities, we receive a boundary condition

$$q\Big|_{z=z_0} = 0 .$$

Boundary value problem in contamination process mathematical modeling. The correctness of statement of boundary value problems for the equations of type (1) is proved with certain restrictions superimposed on diffuseness and convection and for some combinations of boundary conditions.

It is natural that the most adequately considered processes describe three-dimensional boundary value problems. The difficulties accompanying realization of such mathematical models are also obvious. The problems of choosing the solution method and correctness of the appropriate difference problem (when apply the different methods of solution), maintenance of practical computing stability of algorithm, the necessity of work with large scale arrays of data concern them. Many scientists try to solve these problems by simplification of the model, more often at the expense of diminution of dimensionality of the problem. In this work the method of solution of a three-dimensional boundary value problem is stated, which statement is indicated.

Let us consider a problem about evolution of the ground field of impurities $Q(x, y, t)$ and field of impurities of near-the-land stratum of an atmosphere $q(x, y, z, t)$. The given problem is described by the equation (1) $q = 0, f(x, y, z, t)=$ $= 0$ with the given initial concentration of fields of impurity (2), (8) and boundary conditions (3), (4), (6). The last boundary condition is supplemented by ratio (7). With allowance for the last parity (ratio), the problem of impurity transposition with the availability of wind rise and dry sedimentation is essentially non-stationary, and the dynamic equilibrium between the concentration of impurity on the surface and in near-the-surface stratum arises in time ($t_0 \sim \gamma^{-1}$), as γ is rather a small number according to [4].

With allowance for (7) let us copy boundary condition (6) as:

$$k_3 \frac{\partial q}{\partial z} + v_s q = v_d q(x, y, z_0, t) - \gamma Q(x_1, y, t),$$

or

$$k_3 \frac{\partial q}{\partial z} + vq = -\gamma Q(x, y, t), x_3 = z_0, v = v_s - v_d .$$

By designating $\bar{u}_3 = u_3 - v_s$, let us copy the equation (1) in the developed way:

$$\frac{\partial q}{\partial t}+u_1\frac{\partial q}{\partial x}+u_2\frac{\partial q}{\partial y}+\bar{u}_3\frac{\partial q}{\partial z}=\frac{\partial}{\partial x}k_1\frac{\partial q}{\partial x}+\frac{\partial}{\partial y}k_2\frac{\partial q}{\partial y}+\frac{\partial}{\partial z}k_3\frac{\partial q}{\partial z}. \qquad (1`)$$

For the solution of the problem (1'), (2)–(4), (8), (9) we shall use the difference method offered in [5]. For it in area $\Omega = D[0, T]$

$$D=\{(x,y,z),a_1\le x\le b_1,a_2\le y\le b_2,z_0\le z\le H\},$$

we shall enter a grid

$$\omega_x=\left\{x_i : x_i=a_1+ih_x, i=\overline{0,n}, h_x=(b_1-a_1)/n\right\},$$

$$\omega_y=\left\{y_j : y_j=a_2+jh_y, j=\overline{0,m}, h_y=(b_2-a_2)/m\right\},$$

$$\omega_z=\left\{z_k : z_k=z_0+kh_z, k=\overline{0,l}, h_z=(H-z_0)/l\right\},$$

$$\omega_\tau=\{t_v : t_v=v\tau, \tau=T/\mu\},$$

here in after we shall deal with the grid area

$$\Omega_{h_z}=D_h\omega_\tau, D_h=\omega_x+\omega_y+\omega_z.$$

In the grid area Ω_{h_τ} (problem (1 '), (2)–(4), (8), (9) we shall put in the orrespondence the difference scheme of the second order of approximation on space variables:

$$\frac{w_{ijk}^{v+1}-w_{ijk}^{v}}{\tau}=$$
$$=\eta_1((d_x w_{\bar{x}}^{v+1})_x)_{ijk}-r_1^-(w_x^{v+1})_{ijk}-r_1^+(w_{\bar{x}}^{v+1})_{ijk}+\eta_2((d_y w_{\bar{y}})_y^{v+1})_{ijk}- \qquad (11)$$
$$-r_2^-(w_y)_{ijk}^{v+1}-r_2^+(w_{\bar{y}})_{ijk}^{v+1}+\eta_3((d_z w_{\bar{z}}^{v+1})_z)_{ijk}-r_3^-(w_z^{v+1})_{ijk}-r_3^+(w_{\bar{z}})_{ijk}^{v+1},$$

$$i=\overline{1,n-1}, j=\overline{1,m-1}, k=\overline{1,l-1}, v=0,1,2...$$

Here is designated: $w_{ijk} = w(x_i, y_j, z_k)$ — the grid function, approximating function $q(x, y, z, t)$ in knots of grid (10),

$$\eta_1=(1+R_1)^{-1}, R_1=0,5h_x|u_1|, r_1^+=0,5(|u_1|+u_1), r_1^-=0,5(u_1-|u_1|),$$

$$(d_x)_{ijk}=K_1(x_{i-0,5}, y_j, z_k),$$

$$\eta_2=(1+R_2)^{-1}, R_2=0,5h_y|u_2|, r_2^+=0,5(|u_2|+u_2), r_2^-=0,5(u_2-|u_2|),$$

$$(d_y)_{ijk}=K_2(x_i, y_{j-y_2}, z_h),$$

$$\eta_3 = (1+R_3)^{-1}, R_3 = 0,5h_z\left|u_3\right|, r_3^+ = 0,5(\left|u_3\right|+u_3), r_3^- = 0,5(u_3-\left|u_3\right|),\quad (d_z)_{ijk} = K_3(x, y_j, z_{k-y_2}). \tag{12}$$

$$(d_z)_{ij1}(w_z^{v+1})_{ij0} + v_{ij0}w_{ij0}^{v+1} = -y_{ij}Q_{ij}^{v+1}, j=\overline{1,m-1}; v=0,1,...$$

$$(d_z)_{ijk} = (w_z^{v+1})_{ijk} + (v_s)_{ij}w_{ijk}^{v+1} = 0, i=\overline{1,n-1}; j=\overline{1,m-1}; v=0,1,...$$

$$w_{1jk}^{v+1} = w_{0jk}^{v+1}, j=\overline{1,m-1}; k=\overline{1,l-1}; v=0,1,... \tag{14}$$

$$w_{h-1,jk}^{v+1} = w_{njk}^{v+1},\ j=\overline{1,m-1}; k=\overline{1,l-1}; v=0,1,... \tag{15}$$

$$w_{i1k}^{v+1} = w_{i0k}^{v+1}, i=\overline{1,n-1}; k=\overline{1,l-1}; v=0,1,... \tag{16}$$

$$w_{in-1k}^{v+1} = w_{ink}^{v+1},\ i=\overline{1,n-1}; k=\overline{1,l-1}; v=0,1,... \tag{17}$$

Difference scheme construction. The conventional designations in theory of different schemes [6] are used here. Thus, the constructed difference scheme is monotonous. That is why the grid of a maximum principle without restrictions on pitches of a grid on space variables is executed.

The difference analogue of conditions (9), (8) looks as following:

$$\frac{v_{ij}^{v+1}-v_{ij}^{v}}{\tau} = (v_d)_{ij}w_{ij0}^{v+1} - \gamma_{ij}v_{ij}^{v+1}, i=\overline{0,n}; j=\overline{0,n}; v=0,1,... \tag{18}$$

$$v_{ij}^0 = Q_{0ij},\ i=\overline{0,n}; j=\overline{0,n}, \tag{19}$$

where $v^v_{ij} = v(x_j, y, t_v)$ — grid function, approximating function $Q(x, y, t)$.

Let us copy a difference scheme (11)–(19) as:

$$w_{ijk}^{v+1} = [A_{ijk}w_{ijk}^{v} + B_{ijk}w_{i-1jk}^{v+1} + C_{ijk}w_{i+1jkw}^{v+1} + D_{ijk}w_{ij-1k}^{v+1} + E_{ijk}w_{ij+1k}^{v+1} + F_{ijk}w_{ijk-1}^{v+1} +$$

$$+G_{ijk}w_{ijk+1}^{v+1}], i=\overline{1,n-1}; j=\overline{1,m-1}; k=\overline{1,l-1}; v=0,1,...,$$

where $A_{ijk}^{-1} = 1+\tau(B_{ijk}+C_{ijk}+D_{ijk}+E_{ijk}+F_{ijk}+G_{ijk})$,

$$B_{ijk} = \tau\left(\frac{(\eta_1)_{ijk}}{h_1^2}(d_x)_{ijk} + \frac{(r_1^+)_{ijk}}{h_1}\right), C_{ijk} = \tau\left(\frac{(\eta_1)_{ijk}}{h_1^2}(d_x)_{i+1jk} - \frac{(r_1^-)_{ijk}}{h_1}\right),$$

$$D_{ijk} = \tau\left(\frac{(\eta_2)_{ijk}}{h_2^2}(d_y)_{ijk} + \frac{(r_2^+)_{ijk}}{h_2}\right), E_{ijk} = \tau\left(\frac{(\eta_2)_{ijk}}{h_2^2}(d_y)_{ij+1k} - \frac{(r_2^-)_{ijk}}{h_2}\right),$$

$$F_{ijk} = \tau\left(\frac{(\eta_3)_{ijk}}{h_3^2}(d_z)_{ijk} + \frac{(r_3^+)_{ijk}}{h_3}\right), G_{ijk} = \tau\left(\frac{(\eta_3)_{ijk}}{h_3^2}(d_z)_{ijk+1} - \frac{(r_3^-)_{ijk}}{h_3}\right),$$

$$w_{ij0}^{v+1} = a_{ij}[h_3\gamma_{ij}v_{ij}^{v+1} + (d_z)_{ij1} w_{ij1}^{v+1}], i = \overline{1, n-1}; j = \overline{1, m-1}; v = 0,1,... \quad (20)$$

Where

$$a_{ij} = ((d_z)_{ij1} - v_{ij0}h_3)^{-1}, w_{ij1}^{v+1} = b_{ij} w_{ijl-1}^{v+1}, i = \overline{1, n-1}; j = \overline{1, m-1}; \; v = 0,1,... \quad (21)$$

Where $b_{ij} = ((d_z)_{ijk} + h_3(v_s)_{ij})^{-1}(d_z)_{ijk}$,

$$v_{ij}^{v+1} = C_{ij}[\tau(v_d)_{ij} w_{ij0}^{v+1} + v_{ij}^{v}], i = \overline{1, n-1}; j = \overline{1, m-1}; v = 0,1,... \quad (22)$$

Where $c_{ij} = (1 + \tau\gamma_{ij})^{-1}$.

We shall discover an approximate solution of the difference problem using :he relaxation method [7]. The settlement formulas look as follow:

$$\begin{gathered} {}^{s+1}w_{ijk}^{v+1} = (1-\omega)^{s} w_{ijk}^{v+1} + \omega \; A_{ijk}(w_{ijk}^{v} + B_{ijk}^{s+1} w_{i-1jk}^{v+1} + C_{ijk}^{s} w_{i+1jk}^{v+1} + \\ + D_{ijk}^{s+1} w_{ij-1k}^{v+1} + E_{ijk}^{s} w_{ij+1k}^{v+1} + F_{ijk}^{s+1} w_{ijk-1}^{v+1} + G_{ijk}^{s} w_{ijk+1}^{v+1}), \\ i = \overline{1, n-1}; j = \overline{1, m-1}; k = \overline{1, l-1}; v = 0,1,...; s = 0,1,... \end{gathered} \quad (23)$$

$$\begin{gathered} {}^{s+1}w_{ijk}^{v+1} = (1-\omega)^{s} w_{ijk}^{v+1} + \omega \; a_{ijk}[h_3\gamma_{ijk} + (d_z)_{ijk}^{s} w_{ijk}^{v+1}], \\ i = 1, n-1; j = 1, m-1; v = 0,1,...; s = 0,1,... \end{gathered} \quad (24)$$

$$\begin{gathered} {}^{s+1}w_{0jk}^{v+1} = (1-\omega)^{s} w_{0jk}^{v+1} + \omega^{s} w_{1jk}^{v+1}, \\ j = \overline{1, m-1}; k = \overline{1, l-1}; v = 0,1,..; s = 0,1,.. \\ {}^{s+1}w_{njk}^{v+1} = (1-\omega)^{s} w_{njk}^{v+1} + \omega^{s} w_{n-1jk}^{v+1}, \\ j = \overline{1, m-1}; k = \overline{1, l-1}; v = 0,1,..; s = 0,1,.. \\ {}^{s=1}w_{i0k}^{v+1} = (1-\omega)^{s} w_{i0k}^{v+1} + \omega^{s} w_{i0k}^{v+1}, \\ j = \overline{1, m-1}; k = \overline{1, l-1}; v = 0,1,..; s = 0,1,.. \end{gathered} \quad (25)$$

$$\begin{gathered} {}^{s+1}w_{ink}^{v+1} = (1-\omega)^{s} w_{ink}^{v+1} + \omega^{s} w_{in-1k}^{v+1}, \\ j = \overline{1, m-1}; k = \overline{1, l-1}; v = 0,1,..; s = 0,1,.. \end{gathered} \quad (26)$$

$${}^{s+1}w_{ijl}^{v+1} = (1-\omega)^{s} w_{ijl}^{v=1} + \omega^{s} w_{ijl-1}^{v+1}, \quad i = \overline{1, n-1}; j = \overline{1, m-1}; \quad (27)$$

$$\begin{gathered} {}^{s+1}v_{ij}^{v+1} = (1-\omega)^{s} v_{ij}^{v+1} + \omega c_{_{ij}}[\tau(v_d)_{ij} \; {}^{s}w_{ij0}^{v+1} + v_{ij}^{v}], \\ i = \overline{1, n-1}; j = \overline{1, m-1}; v = 0,1,...; s = 0,1,... \end{gathered} \quad (28)$$

Here s — the number of iteration, ω — parameter of a relaxation. As an initial approximation on (v + 1)-e the temporary stratum the significance of the solution obtained on the previous temporary stratum is selected. The criterion of completion of iteration process:

$$\max_{i,j,k} \left| {}^{s+1}w_{ijk}^{v+1} - {}^{s}w_{ijk}^{v+1} \right| \le \varepsilon_A + \varepsilon_R \left| {}^{s+1}w_{ijk}^{v+1} \right|$$

$$\max_{i,j}\left|{}^{s+1}v_{ij}^{v+1} - {}^{s}v_{ij}^{v+1}\right| \le \varepsilon_A + \varepsilon_R \left|{}^{s+1}v_{ijk}^{v+1}\right|.$$

unites monitoring absolute ε_A and relative ε_R errors.

Devised solution description. One of the features of the considered problem is the absence of model examples permitting to be convinced in a regularity work of the computing algorithm. As one of the schemes of check it is possible to offer the following. Let's assume that the transposition of impurity along one of the coordinate axis, for example, along the axis *OY* is absent, that is $k_2 \equiv 0$, $u_2 \equiv 0$. Then, our problem is degenerated in two-dimensional one, and reliable algorithms for its solution are developed and approved. Conducting calculation on these algorithms and on offered algorithm of calculation of the three-dimensional problem and comparing outcomes, with their concurrence to the exactitude required it is possible to consider the offered algorithm as acceptable.

The program realization of circumscribed algorithm in language PASCAL allows to solve problems on the Pentium type COMPUTER with volume of the main memory 1 in the protect mode on a grid by a size up to 100x100x70 knots.

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У роботі розглянутий алгоритм розв'язання нелінійного рівняння з частинними похідними, який описує процес забруднення атмосфери. Алгоритм оснований на відповідній модифікації сіткового методу.

Ключові слова: *забруднення атмосфери, нелінійна модель, сітковий метод.*

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