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COMPUTATIONAL ALGORITHM OF SOLUTION OF THE THREE–DIMENSIONAL NON–STATIONARY TURBULENT DIFFUSION EQUATION ON THE BASE OF THE ALTERNATING DIRECTION METHOD

Abstract. *Solution of the 3D turbulent diffusion equation, based on the alternating direction method, is proposed. The advantage of this scheme is its physical validity and high stability. The numerical algorithm, developed, allows including the computing unit of air pollution dispersion in the 3D unsteady boundary layer of the atmosphere.*

Keywords: *turbulent diffusion equation, pollutant concentration, alternating direction method, modified Lax–Wendroff scheme.*

1 Problem statement

At some height a continuous point source creates “looping” pollutant plume. The plume moves in the downwind direction and in the calculation domain it creates the 2D air pollutants concentration fields (*x*, *y* and *y*, *z*), which are used as lateral boundary conditions for the turbulent diffusion equation during all calculation time. Under the action of wind and atmospheric turbulence the contaminants on lateral surfaces are transferred into the calculation domain and dispersed within it.

The problem is to calculate the spatial–temporal distribution of pollutant concentrations for a period of time T (till 6 hours), for which the meteorological conditions are possible to consider as constant.

2 Solution method

At some distance from a continuous point source the plume is conditionally broken on two subregions. In the near subregion the air pollutant distribution may be estimated by the Gaussian model, in distant subregion – the pollutant distribution is described by the turbulent diffusion equation (TDE).

The sizes of the near zone do not exceed a distance, at which the IAEA model is applicable. For the distant zone the TDE is solved.

According to the Gaussian plume model for a continuous point source, located at the height H above an underlying surface, the volumetric pollutant concentration $q(\eta,\zeta,z)$ is obtained from a formula:

$$q(\eta,\zeta,z)=\frac{M}{2\pi\sigma_y\sigma_z U}\exp\left(-\frac{(\zeta-\zeta_0)^2}{2\sigma_y^2}\right)\cdot\left(\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right), \quad (1)$$

where: η is the along–wind coordinate measured in wind direction, ζ is the cross–wind coordinate direction, z is the vertical coordinate measured from the ground, η_0, ζ_0 are the horizontal coordinates of a pollutant source, H is the source height, M is the mass emission rate, U is the velocity of pollutant transport in the direction of x–axe (m/s), σ_y, σ_z are the lateral and vertical dispersion parameters, respectively.

These diffusion parameters are power functions of the distance η from a source.

$$\sigma_j = \mathrm{P}_j \eta^{q_j}, \quad j = \zeta, z . \tag{2}$$

The factors P_j and q_j are defined as functions of the stability category and effective stack height.

In the near zone and, hence, in the distant three-dimensional area the pollutant concentrations is determined using the standard meteorological information and source parameters.

To calculate the pollutant concentrations in the distant zone the turbulent diffusion equation for pollutant is used:

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} + w\frac{\partial q}{\partial z} + \frac{\partial}{\partial x}K_x\frac{\partial q}{\partial x} + \frac{\partial}{\partial y}K_y\frac{\partial q}{\partial y} + \frac{\partial}{\partial z}K_z\frac{\partial q}{\partial z} - \beta q = 0, \tag{3}$$

where: x, y – arbitrary horizontal coordinates in the distant zone;
u, v, w – transport velocity in the direction of x–, y–, z–axes, respectively;
K_x, K_y, K_z – eddy diffusivities in the direction of x–, y–, z–axes, respectively;
β – coefficient of pollutant transformation in chemical reactions.

To choose K_x, K_y, K_z it is necessary to take into account scales of pollutant clouds, as their values is significantly depend on sizes of vortexes, participating in the pollutant dispersion. However we shall examine only such cases, under which the sizes of a pollutant cloud observed at a sufficiently long distance from the source, is great, and the eddy diffusivities for pollutant coincide with the eddy diffusivities for meteorological magnitudes:

$$K_x = K_y = k_L, \tag{4a}$$

$$K_z = k, \tag{4b}$$

where k_L, k are lateral and vertical eddy diffusivities for momentum, respectively.

Taking into account (4) the equation (3) can be written as:

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} + w\frac{\partial q}{\partial z} + \frac{\partial}{\partial x}k_L\frac{\partial q}{\partial x} + \frac{\partial}{\partial y}k_L\frac{\partial q}{\partial y} + \frac{\partial}{\partial z}k\frac{\partial q}{\partial z} - \beta q = 0. \tag{5}$$

To solve the equation (5) it is necessary to specify initial and boundary conditions. The initial conditions at $t = t_0$ is defined, assumed that at the upwind side of the calculation domain (the far zone) the pollutant concentrations, produced with the IAEA model for the near zone, are saved during all calculation time. In other points of the distant zone at the initial time the air is considered to be completely "pure" from pollutant. Thus, the pollutant concentrations instead of source parameters are used in the calculation domain, and it is rather significant for constructing of numerical solution algorithm.

The boundary conditions are determined from the following physical reasons. In increasing distance from the underlying surface, i.e. in approaching to the upper bound of the atmosphere boundary layer (ABL), the atmospheric turbulence gradually reduces, therefore it is naturally assumed that the vertical eddy pollutant flux becomes equal to zero at the upper bound of the ABL:

$$k\frac{\partial q}{\partial z} \to 0\,. \tag{6}$$

We shall specify the lower boundary condition as the following:

$$k\frac{\partial q}{\partial z} + W_g q = V_d q - \gamma q_0 \qquad \text{at} \qquad z = z_0\,, \tag{7}$$

where: W_g –gravitational settling velocity for particles (under influence of the gravity force particles deposit on the underlying surface) in ms^{-1};

V_d –dry deposition velocity of particles (ms^{-1});

γ –coefficient of particle rising, affected with the wind (m^{-1});

q_0 –initial areal pollutant concentration (gm^{-2}).

As the first approximation the effect of particle rising, affected with the wind, will be excluded. Then, rewrite the condition (7) in the following form:

$$k\frac{\partial q}{\partial z} + W_g q = V_d q\,, \qquad \text{at} \quad z = z_0 \tag{8}$$

By performing the sum of the turbulent $k\frac{\partial q}{\partial z}$ and gravitational $W_g q$ parts as the eddy fluxes of pollutant near the surface (S), (8) can be written as:

$$S = V_d q\left(x, y, z, t\right), \qquad \text{at} \qquad z = z_0 \tag{9}$$

At leeward lateral boundaries "radiation conditions", that is the open boundary conditions, are specified:

$$\frac{\partial q}{\partial t} + C_{ph}\frac{\partial q}{\partial n} = 0\,, \tag{10}$$

where C_{ph} – phase velocity of the sum wave in a solution at the boundary at the given time.

Thus, we described the problem of spatial–temporal distribution of pollutant concentrations in three-dimensional domain, assumed that leeward side concentrations, wind speed components, lateral and vertical eddy diffusivities, dry deposition velocity of particles and coefficient of pollutant transformation in chemical reactions, are specified,.

The computational algorithm is constructed on the base of the alternating directions method. This method is to calculate the function q at time $t = t_0 + \delta t$ with three successive fractional steps, provided that the field of q_0 is known at the instant $t = t_0$. At each fractional step, by–turn, calculation is carried out for half–time step and the whole time step by the modified Lax–Wendroff (LW) scheme. The primary equation is approximated at each half-time step: implicitly x–direction, and explicitly y-, z–directions for the first fractional step; implicitly y–direction, and explicitly x-, z-directions for the second fractional step; implicitly z–direction, and explicitly x-, y-directions for the third fractional step. The primary equation is approximated at each whole time step implicitly, and therefore it turns in a three–point one–dimensional equation, which is easily realized by the one–dimensional factorization method. The result is presented as $q^{1/3}$ in the x–axe direction at the first factorization stage, as $q^{2/3}$ in the y–axe direction at the second one and as q^{1} in the z–axe direction at the third one.

To realize numerical solution of the three-dimensional equation, it is necessary to construct a 3D mesh. It is necessary to note, that at the half–time step the additional nodes are located in the middle of grid element. It is a possibility to reduce calculation to one-dimensional factorization. So, the calculation mesh may be chosen as:

$$P = \{(x, y, z);\, x = i \cdot \delta x,\, y = j \cdot \delta y;\, z = k \cdot \delta z, \quad i = 1, I;\, j = 1, J;\, k = 1, K\}$$

where: δx, δy, δz – mesh spacing in the directions of x–, y–, z–axis , respectively;
i, j, k – grid node numbers in the direction of x–, y–, z–axes, respectively.

The mesh spacing in the x, y directions are constant; outward from the underlying surface in the z direction the spacing δz depends on the value H/k, where H – height of the boundary layer, k – number of nodes in the direction of z–axe.

Below numerical scheme of the turbulent diffusion equation solution, including quantitative evaluation of initial data, is presented. It consists of preparatory stage and realization stage. At the preparatory stage the input of source parameters, calculation of wind speed components and turbulent characteristics in the ABL model, determination of pollutant concentrations is fulfilled for the calculation domain. At the realization stage a solution of TDE is carried out with the following scheme:

Realization of the first fractional step:

- Calculation of intermediate values at the instant $t = t_0 + \dfrac{\delta t}{2}$;
- Determination of $q^{1/3}$ at time $t = t_0 + \delta t$;

Realization of the second fractional step:

- Calculation of intermediate values at the instant $t = t_0 + \dfrac{\delta t}{2}$;
- Determination of $q^{2/3}$ at time $t = t_0 + \delta t$;

Realization of the third fractional step:

- Calculation of intermediate values at the instant $t = t_0 + \dfrac{\delta t}{2}$;
- Determination of q^{1} at time $t = t_0 + \delta t$.

At a preparatory stage the input data (wind speed components, u, v, w; lateral and vertical eddy diffusivities, k_L and k) are specified with the ABL model.

To approximate the equations at each fractional step two finite difference operators are used:

Centered difference operator:

$$\delta_{x\alpha} q = \frac{1}{2\delta x_\alpha}\left[q\left(x_\alpha + \delta x_\alpha\right) - q\left(x_\alpha - \delta x_\alpha\right)\right], \tag{17}$$

Smoothing operator:

$$\bar{q}^{x} = \frac{1}{2}\left[q\left(x_\alpha + \delta x_\alpha\right) + q\left(x_\alpha - \delta x_\alpha\right)\right]. \tag{18}$$

We will write the whole time step equation for the first fractional step:

$$\begin{gathered} q^{1/3} - q^0 + r_1 \delta_x q_l' + r_2 \delta_y q_f^c + r_3 \delta_z q_{up}^0 - \tilde{\beta} q^0 = \\ = \delta t\left[\delta_x (K_S^{1/2} \delta_x q^{1/3}) + \delta_y (K_S^{1/2} \delta_y q^0) + \delta_Z (K^{1/2} \delta_Z q^0)\right], \end{gathered} \tag{19}$$

where $\tilde{\beta} = \beta \cdot \delta t; \quad r_i = \delta t \cdot u_i^{1/2} \quad i = 1,2,3$.

To transform (19) in the equation for $q^{1/3}$, three fields of q_l, q_f, q_{up} should be defined:

$$q_l = \overline{q^0}^{xyyzz} - \frac{1}{2}\left(r_1 \delta_x q^0 + r_2 \delta_y \overline{q^0}^{xyzz} + r_3 \delta_z \overline{q^0}^{xyyz}\right), \tag{20}$$

$$q_f = \overline{q^0}^{xxyzz} - \frac{1}{2}\left(r_1 \delta_x \overline{q^0}^{xyzz} + r_2 \delta_y q^0 + r_3 \delta_z \overline{q^0}^{xxyz}\right), \tag{21}$$

$$q_{up} = \overline{q^0}^{xxyyz} - \frac{1}{2}\left(r_1 \delta_x \overline{q^0}^{xyyz} + r_2 \delta_y \overline{q^0}^{xxyz} + r_3 \delta_z q^0\right). \tag{22}$$

In relation (20) q_l' differs from q_l in that implicit approximation is used for the term $u\frac{\partial q}{\partial x}$. Similarly, in (21) q_r' differs from q_r – implicit approximation for the term $v\frac{\partial q}{\partial y}$, in (22) q_{up}' from q_{up} – implicit approximation for the term $w\frac{\partial q}{\partial z}$.

Thus

$$q_l' - q_l = -\frac{r_1}{2}\left(\delta_x q^{1/3} - \delta_x q^0\right), \tag{23}$$

$$q'_f - q_f = -\frac{r_2}{2}\left(\delta_y q^{2/3} - \delta_y q^0\right), \tag{24}$$

$$q'_{up} - q_{up} = -\frac{r_3}{2}\left(\delta_z q^{3/3} - \delta_z q^0\right). \tag{25}$$

Taking into account (20)–(25) the equation (19) becomes:

$$\begin{gathered} q^{1/3} - q^0 + r_1\delta_x(q_l - \frac{r_1}{2}(\delta_x q^{1/3} - \delta_x q^0)) + r_2\delta_y q_r + r_3\delta_z q_{up} - \tilde{\beta} q^0 = \\ = \delta t(\delta_x(K_S^{1/2}\delta_x q^{1/3}) + \delta_y(K_S^{1/2}\delta_y q^0) + \delta_Z(K^{1/2}\delta_Z q^0) \end{gathered} \tag{26}$$

We shall note the whole time step equation for the second fractional step:

$$\begin{gathered} q^{2/3} - q^0 + r_1\delta_x q'_l + r_2\delta_y q'_r + r_3\delta_z q^0_{up} - \tilde{\beta} q^0 = \\ = \delta t\left[\delta_x(K_S^{1/2}\delta_x q^{1/3}) + \delta_y(K_S^{1/2}\delta_y q^{2/3}) + \delta_Z(K^{1/2}\delta_Z q^0)\right] \end{gathered} \tag{27}$$

Subtracting (27) from (19) and taking into account (21) and (24) we get the equation for $q^{2/3}$:

$$\begin{gathered} q^{2/3} - \frac{r_2}{2}\delta_y(r_2\delta_y q^{2/3}) - \delta t\cdot\delta_y(K_S^{1/2} q^{2/3}) = \\ q^{1/3} - \frac{r_2}{2}\delta_y(r_2\delta_y q^0) - \delta t\cdot\delta_y(K_S^{1/2}\delta_y q^0) \end{gathered} \tag{28}$$

For the third fractional step the whole time step equation may be written in the following form:

$$\begin{gathered} q^{3/3} - q^0 + r_1\delta_x q'_l + r_2\delta_y q'_r + r_3\delta_z q'_{up} - \tilde{\beta} q^0 = \\ = \delta t\left[\delta_x(K_S^{1/2}\delta_x q^{1/3}) + \delta_y(K_S^{1/2}\delta_y q^{2/3}) + \delta_Z(K^{1/2}\delta_Z q^{3/3})\right] \end{gathered} \tag{29}$$

Subtract (29) from (27) taking into account (22) and (25), the equation for q^1 is derived:

$$q^1 - \frac{r_3}{2}\delta_Z(r_3\delta_Z q^1) - \delta t\cdot\delta_Z(K^{1/2}\delta_Z q^1) = q^{2/3} - \frac{r_3}{2}\delta_Z(r_3\delta_Z q^0) - \delta t\cdot\delta_Z(K^{1/2}\delta_Z q^0). \tag{30}$$

Substitution of the finite difference operators (17), (18) in the equations (26), (28) and (30) yields:

$$a_i q^{1/3}_{i+1,j,k} + b_i q^{1/3}_{i,j,k} + c_i q^{1/3}_{i-1,j,k} = \left(F_q^{1/3}\right)_{i,j,k}, \tag{31a}$$

$$a_j q^{2/3}_{i,j+1,k} + b_j q^{2/3}_{i,j,k} + c_j q^{2/3}_{i,j-1,k} = \left(F^{2/3}_q\right)_{i,j,k}, \tag{31b}$$

$$a_k q^{1}_{i,j,k+1} + b_k q^{1}_{i,j,k} + c_k q^{1}_{i,j,k-1} = \left(F^{1}_q\right)_{i,j,k}, \tag{31c}$$

where all factors a_i, a_j, a_k and the right terms $\left(F_q\right)_{i,j,k}$ in these equations are expressed in terms of the variables u, v, w, k_L, k and q obtained at the previous instant. These equations are solved with the one–dimensional factorization method in the direction of $x-$, $y-$, z-axes. The field of q at time $t = t_0 + \delta t$ is derived at the last factorization stage. Then the obtained field q is used as the initial condition for calculation of the concentration field at the following instant $t = t_0 + 2\delta t$. Repeating such solution procedure, the pollutant concentration field may be derived at any time t.

At the preparatory stage the three-dimensional non-stationary ABL model, which is based the closed set of equations of the hydrothermodynamics, is used.

This model includes the evolutionary (momentum, heat, moisture transport) and diagnostic (statics, state and continuity) equations. The closure is realized with the turbulence kinetic energy (b) budget equation, dissipation (ε) equation and Kolmogorov relation, connecting the vertical eddy diffusivity k with b and ε. The description of horizontal turbulent mixing is based on undergrid lateral eddy diffusivity K_L, which is estimated with the Smagorinsky formula. We shall write the equations of the hydrothermodynamics in the Cartesian Coordinates.

<u>The equations</u>:

The momentum equations

$$\frac{\partial u}{\partial t} + A(u) = -\frac{1}{\rho}\frac{D_\varsigma(p)}{Dx} + fv + \frac{\partial}{\partial z}k\frac{\partial u}{\partial z} + \frac{D_\varsigma}{Dx}\left(k_L D_T\right) + \frac{D_\varsigma}{Dy}\left(k_L D_n\right), \tag{32}$$

$$\frac{\partial v}{\partial t} + A(v) = -\frac{1}{\rho}\frac{D_\varsigma(p)}{Dy} - fu + \frac{\partial}{\partial z}k\frac{\partial v}{\partial z} + \frac{D_\varsigma}{Dx}\left(k_L D_n\right) + \frac{D_\varsigma}{Dy}\left(k_L D_T\right), \tag{33}$$

The thermodynamic energy equation

$$\frac{\partial \theta}{\partial t} + A(\theta) = \alpha_\tau \frac{\partial}{\partial z}k\frac{\partial \theta}{\partial z} + \frac{D_\varsigma}{Dx}\left(k_L\frac{D_\varsigma(\theta)}{Dx}\right) + \frac{D_\varsigma}{Dy}\left(k_L\frac{D_\varsigma(\theta)}{Dy}\right) + \varepsilon_R + Lc, \tag{34}$$

The moisture budget equation

$$\frac{\partial m}{\partial t} + A(m) = \alpha_m \frac{\partial}{\partial z}k\frac{\partial m}{\partial z} + \frac{D_\varsigma}{Dx}\left(k_L\frac{D_\varsigma(m)}{Dx}\right) + \frac{D_\varsigma}{Dy}\left(k_L\frac{D_\varsigma(m)}{Dy}\right), \tag{35}$$

The turbulent kinetic energy budget equation

$$\frac{\partial b}{\partial t}+A(b)=k\left[\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial v}{\partial z}\right)^2\right]+k_L(D_S^2+D_T^2)-\alpha_T\frac{g}{\theta}k\frac{\partial\theta}{\partial z}+\alpha_b\frac{\partial}{\partial z}k\frac{\partial b}{\partial z}+$$
$$+\frac{D_\Gamma}{Dx}\left(k_L\frac{D_\Gamma(b)}{Dx}\right)+\frac{D_\Gamma}{Dy}\left(k_L\frac{D_\Gamma(b)}{Dy}\right)-\alpha_\varepsilon\frac{b^2}{k} \tag{36}$$

The dissipation equation

$$\frac{\partial\varepsilon}{\partial t}+A(\varepsilon)=\alpha_1\frac{\varepsilon}{b}\left\{k\left[\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial v}{\partial z}\right)^2\right]+k_L(D_S^2+D_T^2)\right\}-\alpha_4\frac{\varepsilon}{b}\frac{g}{\theta}k\frac{\partial\theta}{\partial z}+\alpha_2\frac{\partial}{\partial z}k\frac{\partial\varepsilon}{\partial z}+$$
$$+\frac{D_\Gamma}{Dx}\left(k_L\frac{D_\Gamma(\varepsilon)}{Dx}\right)+\frac{D_\Gamma}{Dy}\left(k_L\frac{D_\Gamma(\varepsilon)}{Dy}\right)-\alpha_3\frac{\varepsilon^2}{b} \tag{37}$$

The continuity equation:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0, \tag{38}$$

The hydrostatic equation

$$\frac{\partial p}{\partial z}=-\rho g, \tag{39}$$

The state equation

$$P=\rho RT. \tag{40}$$

<u>The relations:</u>

of Kolmogorov

$$k=\alpha_\varepsilon b^2/\varepsilon, \tag{41}$$

of Smagorinsky

$$k_L=\alpha_L\frac{\Delta s^2}{2}\left(D_T^2+D_S^2\right)^{1/2}. \tag{42}$$

of Poisson

$$\theta=T\left(\frac{1000}{P}\right)^{R/c_p}. \tag{43}$$

Boundary conditions in vertical direction

at $z = z_0$ $\quad u = 0,\ v = 0,\ w = 0,\ k\dfrac{\partial b}{\partial z} = 0,\ \varepsilon = \dfrac{V_*^3}{\kappa z_0},\ V_*^2 = k\left[\left(\dfrac{\partial u}{\partial z}\right)^2 + \left(\dfrac{\partial v}{\partial z}\right)^2\right]^{1/2};$

$z = z_\Gamma,\ p = p_\Gamma,\ T = T_\Gamma,\ m = m_\Gamma$, (subscript Γ indicates values at a level 2m above underlying surface).

$$\text{at } z = H \quad u = u_H,\ v = v_H,\ T = T_H,\ m = m_H,\ k\frac{\partial b}{\partial z} = 0,\ k\frac{\partial \varepsilon}{\partial z} = 0. \tag{44}$$

Here t is time; u, v, w are the velocities along $x-$, $y-$ axis, east– and northward directed along a parallel, meridian, respectively, and $z-$axe, vertical coordinate measured from the underlying surface $z = \tilde{z} - \Gamma(x, y)$, where $\tilde{z}$ is the vertical coordinate measured from the sea level; ρ is the density; p is the pressure; T is the temperature; θ is the potential temperature; ε_R is the radiative flux; m is the specific humidity; c – the specific heat, f is the Coriolis parameter; g is the gravitational acceleration; z_0 is the roughness parameter; H is the atmosphere boundary layer height; Δs is the lateral mesh spacing; $\Gamma = \Gamma(x, y)$ is the relief altitude above the sea ground; $G_1 = -\partial\Gamma/\partial x$, $G_2 = -\partial\Gamma/\partial y$ – the given functions of position, defining slope of the relief; α (with subscripts) is a universal constants.

– Operator of a scalar advection

$$A(f) = \frac{\partial(uf)}{\partial x} + \frac{\partial(vf)}{\partial y} + \frac{\partial(\tilde{w}f)}{\partial z}, \tag{45}$$

where $\tilde{w} = w + w_{\text{p}},\ w_{\text{p}} = G_1 u + G_2 v$. (46)

– Operators of spatial derivatives taking into account orographic effects,

$$\frac{D(f)}{Dx} = \frac{\partial f}{\partial x} + G_1\frac{\partial f}{\partial z},\ \frac{D(f)}{Dy} = \frac{\partial f}{\partial y} + G_2\frac{\partial f}{\partial z}; \tag{47}$$

– D_T, D_S – longitudinal and transversal stress taking into account orographic effects

$$D_T = \frac{Du}{Dx} - \frac{Dv}{Dy}, \tag{48}$$

$$D_S = \frac{Dv}{Dx} + \frac{Du}{Dy}. \tag{49}$$

In a horizontal plane a condition of the open boundaries as a condition of a radiation is put. It is realized with the help of approximations of the equation (10):

$$\frac{\partial \psi'}{\partial t} + c_{ph} \frac{\partial \psi'}{\partial n} = 0 , \tag{50}$$

where $\psi' = \psi - \psi_1$, ψ_1 – solution of an one–dimensional problem for required function ψ, n – exterior normal to the bound. The magnitude c_{ph} is estimated on known values ψ' In preceding instants $t - \Delta t$ and $t - 2\Delta t$ in two interior downwards knots of a regular grid.

At the initial instant $t = 0$ profiles of unknown quantities of magnitudes are given in all knots of calculated area on one–dimensional variant of the ABL model.

3 Discussion and conclusions

Thus, the computational method for calculation of 3D pollutant concentration fields is developed by means of physically grounded, high stable numerical scheme of alternating direction. Integration of both schemes – the IAEA and the alternating direction scheme – allows calculating concentration field in all 3D space surrounded a pollution source.

To calculate 3D distribution of transport velocity and turbulent parameters the model of the geophysical boundary layer (GBL) is used. Results of application of the GBL model to solution of the diffusion problem are presented in [3].

Figure 1 shows a calculated field of dust concentrations from a source with the following parameters: ventilating grill height is 70 m, grill diameter is 3.2 m, dust exit velocity is 5.5 m/s, dust temperature is 104^0C, emission rate is 363.4 g/s, at Kharkiv for 1400 UTC 17 October 1989.

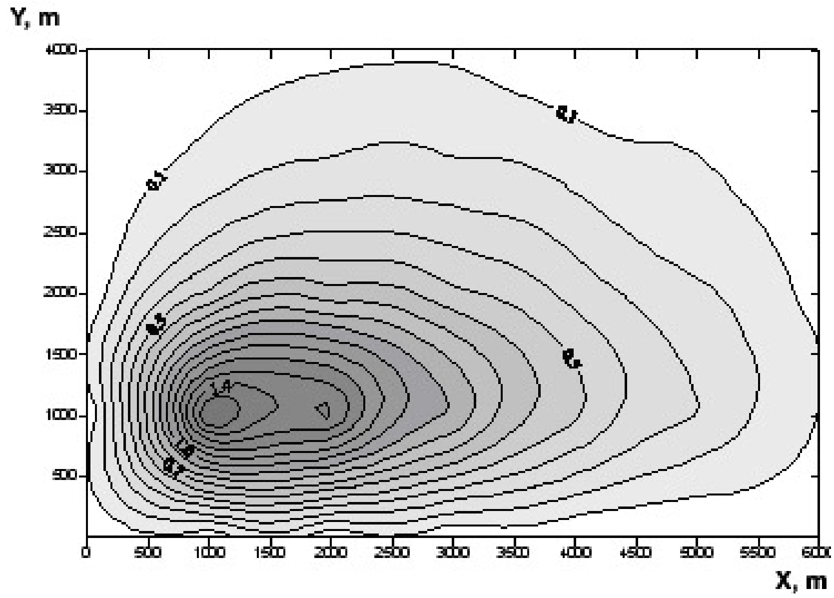

Fig. 1 – Pollutant concentration (g/m^3) distribution at the 2–m height at Kharkiv for 1400 UTC 17 October 1989

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Вычислительный алгоритм для решения трехмерного нестационарного уравнения турбулентной диффузии на основе метода переменных направлений

Аннотация. *Предлагается метод решения полуэмпирического трехмерного уравнения турбулентной диффузии на основе метода переменных направлений. Преимущество данной схемы заключается в её физической обоснованности и высокой устойчивости. Разработанный численный алгоритм позволяет включить блок расчета рассеивания примесей в модель трехмерного нестационарного пограничного слоя атмосферы.*

Ключевые слова: *уравнение турбулентной диффузии, концентрации примесей, метод переменных направлений, модифицированная схема Лакса-Вендорфа*