Mathematical modeling and numerical methods of atmospheric processes determining pollutants transfer at emergency emissions

Aydosov A.A., Zaurbekov N.S., Absamatova K.A.

Almaty Technological University, Almaty, Kazakhstan

Aydosov G.A., Zaurbekova G.N.

Al-Farabi Kazakh National University, Almaty, Kazakhstan

Zaurbekov I.S.

Academy of the National Security Committee of Kazakhstan, Almaty, Kazakhstan
e-mail: *agu_nurgali@mail.ru*

Abstract
According to actual data, the developed mathematical models and computational schemes of pollutants transfer give the opportunity to speak about rather realistic forecasts of trajectories of impurity transfer in the specified regions as well as about values of impurity concentration in the atmosphere. Program of model implementation and the initial data organization make it possible to modify easily model settings, to select any region, number of points of integration grid, number of levels, coordinates of emissions sources, etc. The developed software tools can be used for numerical forecasting experiments when modeling impurity transfer in the atmosphere from the field of sources with various intensity and density of polluting substances.
Keywords: MATHEMATICAL MODEL, GRAVITY SEDIMENTATION, APPROXIMATION, MODEL

It is known that distribution of polluting substances in the atmosphere is described by the three-dimensional equation of mass conservation [1-5]:

$$\frac{\partial q}{\partial t}+\frac{\partial(uq)}{\partial x}+\frac{\partial(vq)}{\partial y}+\frac{\partial((w+v_g)q)}{\partial z}= \\ =K_S\left(\frac{\partial^2 q}{\partial x^2}+\frac{\partial^2 q}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial(uq)}{\partial x}\right)+IS, \quad (1)$$

where q – volume concentration of impurity; u, v, w – wind speed components variables in space and time; v_g – gravity sedimentation rate; K_S, K_z – coefficients of horizontal and vertical diffusion; IS – the field of sources (instant or continuous) emissions performing the function of spaces and time.

Horizontal components of wind speed u, v were input parameters of model and were defined by the objective analysis. The vertical component of wind speed w was determined from the continuity equation:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0. \quad (2)$$

Rate of gravity sedimentation was described by Stocks' law and was determined for particles with radius r of 10 microns as follows:

$$v_g=1{,}26*10^{-5}*\rho*r^2, \quad (3)$$

where ρ – density of polluting substances; r – particles radius.

The equation (1) was solved under the following initial and boundary conditions:

$$q(x, y, z, 0)=q_b(x, y, z), \quad (4)$$

where $q_b(x, y, z)$ – background value of volume concentration of impurity for the first days of calculation:

$$q(x, y, z, 0)=q_0(x, y, z), \quad (5)$$

where $q_0(x, y, z)$ – the volume concentration of impurity formed during the previous day.

In the upper boundary of field (N = 5 km) zero concentration is set:

$$q(x, y, z, H)=0 \quad (6)$$

In the lower boundary (underlying surface), conditions of full absorption at the previous step of time are set and full (turbulent and advective) impurity stream to the underlying surface at the estimated step of time is calculated:

$$q(x, y, 0, t-\Delta t)=0;$$

$$\frac{\partial q(x,y,0,t)}{\partial x}=\frac{\partial}{\partial z}\left(K_z\frac{\partial q}{\partial z}\right)-(w+v_g)\frac{\partial q}{\partial z}. \quad (7)$$

Also statement of boundary conditions of the third kind is considered:

$$K_z\frac{\partial q}{\partial z}-\beta q=0, \quad (8)$$

where β – empirical constant determining absorption of impurity of underlying surface.

Condition (7) is for heavy impurity with higher speed gravitational subsidence, condition (8) is for light impurity.

Moreover, it takes into account turbulent raising of impurity that allows considering underlying surface as the field of secondary sources and calculating secondary transfer of pollutant. Side boundary conditions were of the following form:

- in the field of inward flow: $q=0$;
- in the field of flowing out

$$\frac{\partial q}{\partial t}=-\frac{\partial(uq)}{\partial x}-\frac{\partial(vq)}{\partial y}-\frac{\partial\left((w+v_g)q\right)}{\partial z}. \quad (9)$$

Distribution of impurity under the conditions of complex relief and plain surface will significantly differ because of deformation of stream with hindrances. In the case of relief, the system (1)-(9) should be solved in the field with curved boundary. The concrete form of field in case of rigid horizontal wall at height N will be determined by the function describing relief form $Z_S(x, y)$. In order to avoid the difficulties connected with numerical integration in curvilinear field, usually it is necessary to pass to new coordinates where the computational region becomes rectilinear. The transformation meeting the following conditions was selected: transformation is reversible; identical at $Z_S=0$ and $Z_S=H$; has continuous second derivatives; keeps error of approximation of the order as in Cartesian coordinate system that is reached by proximity of its determinant to 1.

Boundary and initial conditions for the solution of this equation are selected identical as for model above uniform surface.

In the model convective motions are estimated; they are caused by unevenness of heating of underlying surface (heat sink temperature) and unevenness of temperature in surface layer (heat island above heat sink):

$$w_{conv}=\left(\alpha\left|g\left(T_v-\overline{T_v}\right)/T_v\right|\Delta Z\right)^{1/2},\ T_v>\overline{T_v},\ \frac{\partial T_v}{\partial Z}>\gamma_{MA};$$

$$w_{conv}=0,\ T_v\le\overline{T_v},\ \frac{\partial T_v}{\partial Z}\le\gamma_{MA}, \quad (10)$$

where α – empirical constant; T_v – virtual temperature; $\overline{T_v}$ – average virtual temperature by the area; γ_{MA} – moist-adiabatic gradient of temperature; ΔZ – layer thickness.

In the suggested model, the finite-difference method well-proven in many numerical models of impurity transfer [6-9] has been selected for the numerical solution of equations system (1)-(9). At that, differential equations describing an initial task were approximated by the finite-difference scheme:

$$\prod_{S=1}^{p}\left(E-\frac{\Delta t}{2}L_S\right)\left(\varphi_i^{n+1}+\varphi_i^{n}\right)=\sum_{S=1}^{p}\Delta t L_S\left(\varphi_i\right)^n+\Delta t S_i^{n+1/2}, \quad (11)$$

where $L_S(\varphi_i)=\frac{\partial(v_S\varphi)}{\partial x_S}+\frac{\partial}{\partial x_S}\left(K_S\frac{\partial\varphi}{\partial x_S}\right)$, ($S$=1, 2, 3),

S_i – the members of the equation describing sources;

Δt – step of time.

The scheme (11) is the two-layer differential scheme with the splitting operator and has the second order of accuracy of time and is absolutely steady.

At implementation of the differential scheme (11), the solution was found not for the function φ at the step g+1, but for its transformation for step of time $\varepsilon_{ијl}^{+1}=\varphi_{ијl}^{+1}-\varphi_{ијl}$. This method of implementation has allowed getting rid of approximation of mixed derivatives. The implementation of the scheme in each spatial direction was performed by double-sweep method.

Approximation of advective operators of transfer equation is the main difficulty which appears at formulation of differential task. Problem is that in case of solution of the equation for positive definite functions, the finite-difference scheme must meet the following basic requirements:

- to possess small countable viscosity, that is to have an approximation order of time and space, which is not below the second one;
- to be monotonous, that is not to generate non-physical and negative values;
- to be conservative, that is to satisfy the equation of mass preservation in the specified volume;
- to have a small phase error, that is to transfer the maximum values of function and its gradients with the specified speed.

The program is implemented by the computer.

As it was already mentioned, tests results of the numerical scheme used for approximation of the differential equation of impurity transfer and boundary conditions for this equation are stated in the second section in detail. In this section, test experiments, which have been conducted for correctness proof of model, will be described.

From the data file of synoptic and aerological observations, pressure, temperature, dew points and components of wind speed were selected and then interpolated into points of the set grid (U, V). The calculation area was 30x30 km, with a step of grid $\Delta x=\Delta y$=1 km in horizontal direction and 5 km with variable step in vertical direction. Then, the vertical speed component W was calculated from the equation of continuity. Five continuous sources discharging the polluting substances were set. Coordinates of sources corresponded to the following points of grid:

- first source: i=4, j=4, k=3;
- second source: i=8, j=4, k=2;
- third source: i=6, j=16, k=2;
- fourth source: i=16, j=6, k=2;
- fifth source: i=10, j=10, k=3.

Amount of the discharged impurity is 0.5; 1.0; 1.0; 0.5; 1.0 g/s respectively. Effective height of emissions was 100 m that corresponded to the third level of model (k=3). On the sixtieth step of time (in 6 hours) on the fifth source, an abnormal emission emerged when for one step of time (360 sec) 10^4 g of the polluting substances were discharged. Effective height of abnormal emission was190 m; that corresponded to the fourth level of model (k=4). Further, under the influence of wind field, horizontal and vertical diffusion, the polluting substances were distributed and discharged to the underlying surface generally due to their gravitational and turbulent subsidence.

Every other day, the fields were printed out:

- impurity (g) dropped out to the underlying surface;
- impurity (g) which has remained in air at 40, 100, 190, 350 m respectively.

The field of impurity was given also in the form of isolines for demonstrativeness and conveniences of analysis. Also for control the following values were given: sums of discharger pollutants (g); sums of impurity (g) dropped out to the underlying surface; sums of the substances (g) which have remained in the atmosphere and the ratio of dropped out to discharged sources of polluting substances in percentage terms.

In Figures 1 and 2, isolines of density (μg/m^2 *day) of dropping out aerosol impurity with a density of ρ=1 g/sm^3 and with radius of 1 micron from five sources described above in a day are presented.

According to actual data, results of numerical experiments on the computer with model of pollutants transfer give the opportunity to speak about rather realistic forecasts of trajectories of impurity transfer in the specified regions as well as about values of impurity concentration in the atmosphere.

Program of model implementation and the initial data organization make it possible to modify easily model settings, to select any region in the territory of the Northern hemisphere, number of points of integration grid, number of levels, coordinates of emissions sources, etc. The developed software tools can be used for numerical forecasting experiments when

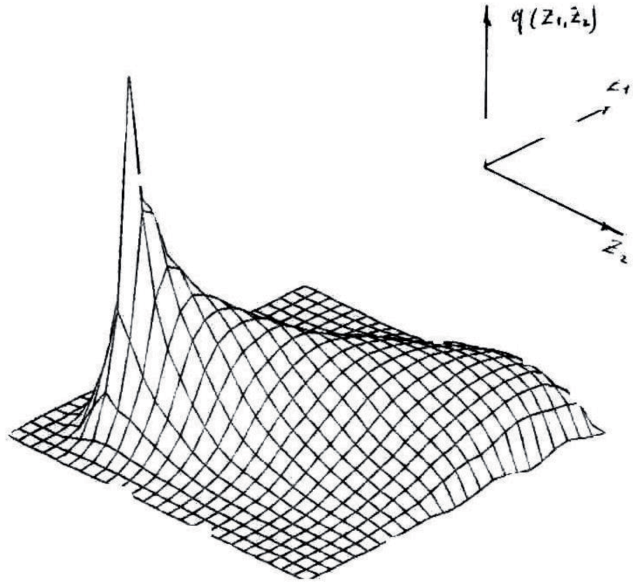

Figure 1. Distribution of impurity of one source

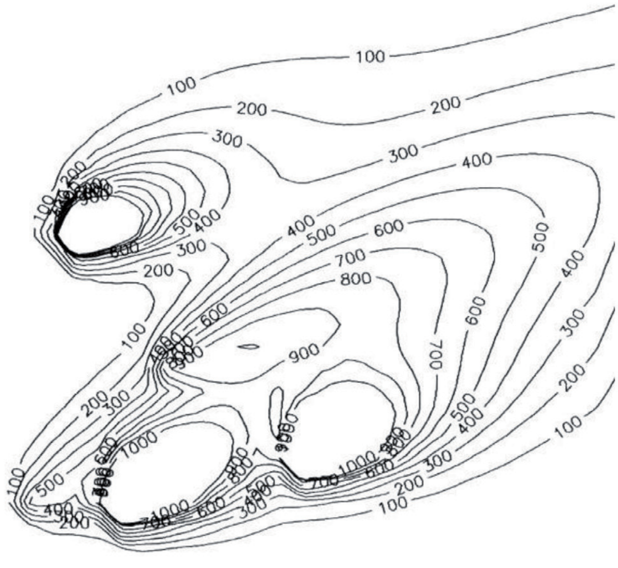

Figure 2. Isolines of density of dropping out (μg/m^2 *day)

modeling impurity transfer in the atmosphere from the field of sources with various intensity and density of polluting substances.

References

1. Aydosov A.A., Aydosov G.A., Zaurbekov N.S. *Model'naya otsenka ekologicheskoy obstanovki okruzhayushchey sredy pri avariynykh situatsiyakh*. [Model assessment of ecological situation of environment in case of emergencies]. Almaty, 2010. 414 p.
2. Aydosov A.A., Aydosov G.A., Zaurbekov N.S. *Modeli ekologicheskoy obstanovki okruzhayushchey sredy pri real'nykh atmosfernykh protsessakh*. [Models of ecological situation of environment in case of real atmospheric processes]. Almaty, 2010. 368 p.
3. Bakirbaev B., Kerimkul Zh. (2001) Numerical model of turbulent diffusion of impurity in atmosphere interface. *Prirodopol'zovanie i problemy antroposfery*. *Journal of M.KH. Dulati Taraz State University*. No 4, p.p.123-130.
4. Perminov V. (2003) Mathematical modeling of crown forest fire initiation. *Lecture Notes in Computer Science*. Vol. 2667, p.p. 549-557.
5. Berlyand M.E. (1963) Theory of turbulent diffusion. *Proceedings of the Main Geophysical Observatory*. No138, p.p.31-37.
6. Miyakoda K., Rosati A. (1977) One-way nested grid models: The interface condition and the numerical accuracy. *Mon. Weather Review*. Vol. 105, p.p. 1092–1107.
7. Aydosov A.A., Zaurbekov N.S. *Teoreticheskie osnovy prognozirovaniya atmosfernykh protsessov, ekologicheskoy obstanovki okruzhayushchey sredy i postroenie geoekologicheskoy karty na primere KNGKM*. [Theoretical bases of forecasting of atmospheric processes, ecological situation of environment and creation of the geoecological map drawing on the example of Karachaganak oil-gas condensate field]. Almaty, Қазақ университеті (Kazakh University), 2000, 219 p.
8. Aydosov A.A., Aydosov G.A., Zaurbekov N.S., Azhieva G.I. *Model'naya otsenka tekhnogennoy nagruzki komponentov prirodnoy sredy neftegazodobyvayushchego regiona*. [Model assessment of technogenic burden of components of oil and gas extraction region environment]. Almaty, 2015, 160 p.
9. Aidosov A.A., Aidosov G.A., Zaurbekov N.S., Baibolova L.K., Admaeva A.M., Zaurbekova N.Dzh. (2015) The Estimation of Height of the Mouth of the River of Sources and Influence of Building of Industrial Facilities at the Modelling of Pollution of the Atmosphere by the Emissions. *Research Journal of Applied Sciences*. No 10 (2), p.p. 54-58, ISSN: 1815-932X © Medwell Journals