High-performance calculations for modeling of processes of transfer of pollution in an atmospheric boundary layer from superficial sources

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Abstract

The quasi-two-dimensional model of impurity propagation from a man-made source is devised on the basis of a three-dimensional model of hydrothermodynamics of mesoscale processes in the lower atmosphere with account for the thermal nonuniformity of the underlying surface in the environs of a large industrial city. The boundary conditions and the model coefficients are determined using the parametrization method. The results of numerical calculations are presented. The calculations are performed using parallel algorithms on a cluster supercomputer of the Vyatka State University. They show that, due to the action of an inhomogeneous horizontal temperature gradient in the lower atmosphere, vortex flows can be formed above populated areas. The disturbed wind flow has a considerable effect on the impurity propagation pattern in the neighborhood of the sources. This model is used for a research of processes of aerosol pollution transfer from solid waste landfill.

1 Introduction

The aim of this work is to consider developed mathematical models of an aerosol impurity propagation and the computer program complexes created on their basis that are implemented into analysis by various conditions of the atmospheric streams passed over the pollution sources which are the solid waste landfills in the territory of the Kirov region.

About 3,5 million tons of garbage are formed in the neighborhood of a city with a million population annually. A deposition (accumulation) is a traditional way of disposal of municipal solid waste. At this approach waste collects out on dumps. The structure of grounds with municipal solid waste is the same in modern cities of various countries. The main components (parts) of municipal solid waste are paper, fossils, glass, plastic, wood, fabrics and leather. These components are combustible and capable to decomposition. Microorganisms emit

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methane during accumulation and decomposition of this garbage. Burying garbage of solid waste becomes a source of formation of the harmful substances polluting ground waters, poisoning the soil and the atmosphere.

In this work the mathematical model for assessment of transfer of aerosol pollution from solid waste landfill is considered. Deterioration in an ecological situation results in need rather precisely to predict and make operational decisions on definition of consequences of pollution that it demands creation of special mathematical tools, models which reflect the occurring phenomena. Models of mesoscale atmospheric processes are widely used in studying local daily weather phenomena, convective processes, and impurity transport in the lower atmosphere. For this purpose, models of different types have been developed [Bel83, Pen85, Alo02]. The classical system of equations of mesoscale processes put forward by I.A. Kibel [Kib70] includes the equations of motion, continuity, heat conduction, and moisture transfer, together with the closing equations for determining the turbulent transfer coefficients. In modeling the atmospheric boundary layer this system is supplemented with boundary conditions which take into account the interaction of the underlying surface and the ground layer of the atmosphere. In studying the lower atmosphere it was found that a human-induced heat spot, named also a heat island [Vel79, Tar91], can arise above a city or a large populated area and the importance of the action of thermal nonuniformity of the underlying surface on mesoscale atmospheric processes was noted. In view of the intricacy of the modeling and the calculations, when using even modern computers, it makes sense to apply such two-dimensional models that retain the basic physical properties of the atmospheric processes under research. In this study, the quasi-two-dimensional model proposed describes three-dimensional convective processes in a thin rotating air layer in the presence of man-made heat and impurity sources. Its derivation is based on the well-known approach [Ari87, Ari88] successfully used in geophysical applications [Shv00, Shv09a].

2 Math Model of the Problem

We will consider the lower-atmosphere boundary layer restricting ourselves to mesoscale processes for which the layer height D and the horizontal scale L satisfy the relation is much less then 1. We will take the three-dimensional equations of the hydrothermodynamics of dry atmosphere in a rotating Cartesian coordinate system [Pen85] as the original equations

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}=-\frac{\partial \Phi}{\partial x}+lv+A_M\Delta u+\frac{\partial}{\partial z}k_M\frac{\partial u}{\partial z} \tag{1}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}=-\frac{\partial \Phi}{\partial y}-lu+A_M\Delta v+\frac{\partial}{\partial z}k_M\frac{\partial v}{\partial z} \tag{2}$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}=-\frac{\partial \Phi}{\partial z}+\beta\theta+A_M\Delta w+\frac{\partial}{\partial z}k_M\frac{\partial w}{\partial z} \tag{3}$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \tag{4}$$

$$\frac{\partial \theta}{\partial t}+u\frac{\partial \theta}{\partial x}+v\frac{\partial \theta}{\partial y}+w\frac{\partial \theta}{\partial z}=A_T\Delta\theta+\frac{\partial}{\partial z}k_T\frac{\partial \theta}{\partial z} \tag{5}$$

$$\frac{\partial \varphi}{\partial t}+u\frac{\partial \varphi}{\partial x}+v\frac{\partial \varphi}{\partial y}+w\frac{\partial \varphi}{\partial z}+\sigma\varphi=A_S\Delta\varphi+k_S\frac{\partial^2 \varphi}{\partial z^2} \tag{6}$$

The initial and boundary conditions are as follows:

$$u=-c_g\sin(dd),\quad v=-c_g\cos(dd),\quad \theta=\theta_S,\quad \varphi=0\qquad t=0 \tag{7}$$

$$\frac{\partial u}{\partial z}=\frac{\partial v}{\partial z}=w=0,\quad \frac{\partial \theta}{\partial z}=0,\quad \frac{\partial \varphi}{\partial z}=0\qquad z=D \tag{8}$$

$$u=v=w=0,\quad \frac{\partial \theta}{\partial z}=\gamma(\theta-\theta_S),\quad \frac{\partial \varphi}{\partial z}=\alpha\varphi-f_S\qquad z=0 \tag{9}$$

In Eqs. (1- 9) t is time, Δ is the Laplace operator, Ox, Oy, and Oz are the eastward, northward, and upward coordinate axes, (u, v, w) is the air flow velocity vector, $\Phi = RT_m p'/p$ is the geopotential fluctuation, where

R is the specific gas constant and T_m is the mean air temperature in the layer, p is the atmospheric pressure, $p = pp_0$, where p is the potential pressure dependent only on the altitude, l is the Coriolis parameter, $\beta = \frac{g}{\theta}$ is the buoyancy parameter, $\theta = T\frac{p_0}{p}^{\frac{R}{C_p}}$ is the potential temperature, where T is the air temperature, p_0 is the atmospheric pressure near the ground, and C_p is the specific heat at a constant pressure; φ is the impurity concentration, σ is the impurity absorption coefficient in the atmosphere, θ_S is the air temperature at the roughness level of the underlying surface, c_g is the geostrophic wind velocity [Gil82] at the upper free boundary of the atmospheric boundary layer, dd is the geostrophic wind azimuth, γ is the heat transfer coefficient, α is the coefficient of impurity absorption by the underlying surface, A_M,A_T, A_S, k_M, k_T, k_S are coefficients of gorizontal and vertical turbulent diffusion and $f_S = \sum_{i=1}^{m} f_i\delta(x - x_i)\delta(y - y_i)$ -intensivity of sources of impurity, x_i and y_i are coordinates of sources, m - number of sources. We will consider an LL area. The geostrophic wind velocity c_g above the atmospheric boundary layer and its direction, as well as the boundary layer height D, are assumed to be known. The horizontal wind velocity fields are calculated from the formulas [Gil82] $u = c_g \sin(dd)$ and $v = c_g \cos(dd)$, where $dd = 0$ corresponds to the north wind and $dd = \pi/2$ to the east wind. The wind can also be preassigned as the layer-average velocity field (mean across the layer). At the lateral boundaries it is assumed that

$$\frac{\partial \mathbf{v}}{\partial n} = 0, \quad \frac{\partial \theta}{\partial n} = 0, \quad \frac{\partial \varphi}{\partial n} = 0 \tag{10}$$

n is vector of external normal.

For to model mathematically the impurity transport from a ground source we will introduce a quasi-twodimensional model based on the locally-equilibrium approach. This technique was presented in [Shv00, Shv09a, Sch98, Shv06].

For the numerical solution of the task the explicit finite difference scheme [Sch98] is used. We will construct a grid, having entered discrete values of arguments:

$$x_i = ih, \quad i = 0, 1, \ldots, N; \qquad y_j = jh, \quad j = 0, 1, \ldots, N \qquad h = 1/N \tag{11}$$

n initial point of time

$$j^0_{i,j} = j(0, i, j); \quad y^0_{i,j} = y(0, i, j); \quad q^0_{i,j} = q(0, i, j) \tag{12}$$

On the following temporary layer the equation according to the explicit scheme pays off at:

$$\frac{q^{n+1}_{i,j} - q^n_{i,j}}{t} + \{y^n_{i,j}, q^n_{i,j}\} = \frac{1}{Pe_s}\Delta q^n_{i,j} - \bar{q}\Big(q^n_{i,j} - \bar{q}^n_{i,j}\Big|_s\Big) \tag{13}$$

$$\frac{j^{n+1}_{i,j} - j^n_{i,j}}{t} + \{y^n_{i,j}, j^n_{i,j}\} = \frac{1}{Pe_s}\Delta j^n_{i,j} - \bar{s} j^n_{i,j} + A\sum_{k=1}^{m} \bar{f}_k d(x_i - x_k) d(y_j - y_k) \tag{14}$$

For boundary conditions:

$$j^{n+1}_{0,j} = j^{n+1}_{1,j}; \quad j^{n+1}_{N,j} = j^{n+1}_{N-1,j}; \quad j^{n+1}_{i,0} = j^{n+1}_{i,1}; \quad j^{n+1}_{i,N} = j^{n+1}_{i,N-1} \tag{15}$$

$$q^{n+1}_{0,j} = q^{n+1}_{1,j}; \quad q^{n+1}_{N,j} = q^{n+1}_{N-1,j}; \quad q^{n+1}_{i,0} = q^{n+1}_{i,1}; \quad q^{n+1}_{i,N} = q^{n+1}_{i,N-1} \tag{16}$$

3 Creation of Algorithm for Solution of Problem

Calculations are carried out in three stages, in three various programs:

1 stage: classification of a land relief:

1) In the MapInfo program the territory within 20 km from solid waste landfill in the item Perekop (southern suburb of the city Kirovo-Chepetsk) is allocated. For this purpose the square with sizes of 20*20 km is under construction and the ground is located in the center of the set area (Fig. 1). Further the given card layer (with the allocated area) is transferred to the SIP program (Fig. 2);

2) For classification of a land relief raster images of May 25th, 2017 with an accuracy of 20 m at 1 pixel are used. These rasters are entered in the SIP program, the card layer from the MapInfo program is enclosed and further classification of the area by means of a method of classification ISODATA is made. The program classifies

the area by the following types: field; wood, bush; road, settlement; reservoir. This classification remains in the form of a vector layer for a possibility of the subsequent use in the MapInfo program.

2 stage: creation of a grid of squares.

1) In the MapInfo program by means of the utility of GRIDVIEW the chosen area (20 km in the neighborhood of the ground of the item Perekop) breaks into squares the sizes of 20*20 m.

2) For each of the received square is under construction centrodes where data are entered;

3) SQL inquiry which defines is created to what type of the area each of squares belongs. This definition happens to the help of SQL of inquiry which essence in the following: if centrodes of a square gets to a certain area, then and for all square the value of this area is appropriated. Further all results are entered in the table where a certain type of the area is appropriated to each square.

3 stage: calculation by itself.

1) Range of cages to which the pollution source gets is determined by a grid of squares;

2) Settlement data are entered in files of initial data, values of coefficients are entered;

3) The program built in Fortran is started.

4 Results of Modelling

The parallel computational algorithm was realized in the Intel Fortran 12 in Packet Intel Cluster Studio for Linux Open MP, installed on the Vyatka State University HPC Enigma X000 cluster supercomputer. The calculations were carried out on the basis of the system of equations (11- 16) with the initial and boundary conditions. The explicit difference scheme [Nau09] was used on a 1000×1000 grid. In accordance with the theory of Monin and Obukhov [Pen85, Alo02, Mon88], the coefficients of vertical and horizontal turbulent viscosity, thermal conductivity, and diffusion for mesoscale turbulent processes in the lower atmosphere were assumed the same, namely, $k_M, T, S = lD^2$, where $D = 400m$ and $A_M, T, S = 400m^2/s$.

In the reference frame chosen the westward wind was blowing from left to right. The wind velocity c_g was varied from 1 to 10 m/s. In most of calculations the velocity was 2 m/s; in this case, the temperature inhomogeneity effect on the wind flow in the vicinity of a heat source is most clearly expressed. The interaction between aerosol impurity and the underlying surface was taken into account on the basis of the information on the nonuniformities of the temperature and absorption coefficient distributions taken from the map of land utilization of the computation domain. The air temperature θ_S varied from 18° C outside populated areas to 23° C in the city of Kirov and Kirovo-Chepetsk. A minimum temperature was observable at the north boundary of the area. The coefficient of impurity absorption by the underlying surface was taken to be $\alpha = 0.0139m^{-1}$ outside populated areas and $\alpha = 0.00139m^{-1}$ on their territories. A point impurity source was located on the underlying surface, at the center of the region under consideration (within the city territory). In the calculations it was also taken that $l = 1.2410^{-4}s^{-1}$, $\sigma = 5.6710^{-8}s^{-1}$, $\gamma = 0.2510^{-3}m^{-1}$, $f_S = 0.999610^{-7}kg/m^4$, and $\varphi_{MPC} = 0.510^{-7}kg/m^3$.

In the calculations the layer-average fields of the impurity concentration, the air temperature, the stream function, and the stream function disturbances were obtained. It is shown that in the case of a relatively weak westward wind (with a velocity of 2 m/s) the horizontal temperature nonuniformity changes the wind flow direction (Fig. 3). The layer-average air temperature varies from 18.5° to 21.5° C. Under the action of a heat island a weak vortex motion arises over large populated areas (Fig. 4). This, in turn, changes the impurity propagation direction (Fig. 4).

5 Summary

Modeling of mesoscale atmospheric processes is developed in connection with the solution of problems of meteorology and monitoring of the environment now. On classification of Belov and another [Kut91] three classes of mesoscale processes are allocated: α- mesoscale (order of 200-2000 km), β- mesoscale (order of 20-200 km), γ- mesoscale (2-20 km).

The α synoptic, describes processes of formation of atmospheric fronts, cyclones. The β- scale describes orographical indignations, evolution of atmospheric processes over the industrial centers. The γ- scale describes processes of transfer of aerosols from local sources. In work [Kut91] by means of three-dimensional model in number investigates influence of thermal heterogeneity of the spreading surface on distribution of meteorological characteristics in a boundary atmospheric layer. Application of the two-dimensional models received by averaging across an interface is described in works [Ali80, Mat94]. In these works the mechanism of formation and development of synoptic whirlwinds in a barocline to the atmosphere under the influence of horizontal inhomogeneity of a stream without diffusion is investigated.

One of the most important problems of ecology is modeling of transfer and diffusion of impurity in the atmosphere. Systematic researches of atmospheric diffusion in relation to questions of air pollution have begun relatively recently. At school of sciences of G.I. Marchuk [Pen85, Alo02] three-dimensional models are developed for a research of conditions of formation of processes of air pollution of local, regional and global scales under the influence of natural and anthropogenic factors. The detailed review of works on this subject is provided in work [Shv15a].

The model of transfer, average across layer, and diffusion of aerosols is used rather seldom. The complexity of carrying out and interpretation of numerical experiments with three-dimensional models of hydrothermodynamics induces to creation of simpler models which keep the most characteristic features of real processes in mesolarge-scale atmospheric currents. One of such methods is use of quasi two-dimensional models [Ari87, Ari88, Shv00, Shv09a], [Sch98, Shv06, Ryc09, Shv09b, Nau09], [Shv15a, Sha11, Shv12, Shv15b]. Earlier this method was used by us for calculation of transfer of impurity from the dot and distributed sources of pollution in the neighborhood of the large industrial center. In the presented work this technique is applied to assessment of impact of aerosol emissions from solid waste landfills (the burning dumps). The studies in this formalization are very actual, relevant and analogous problems weren't earlier considered.

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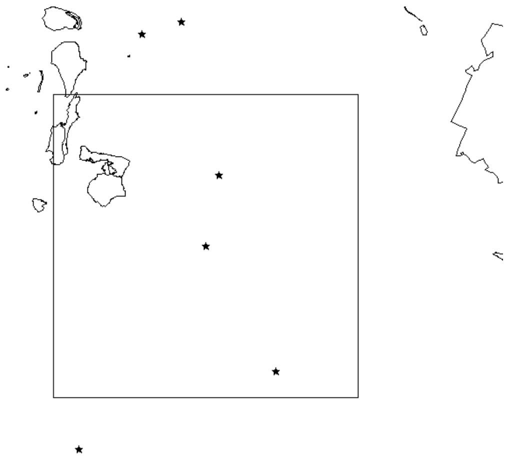

Figure 1: The 20-km zone around polygon in Perekop in MapInfo program

Figure 2: The 20-km zone around polygon in Perekop in SIP program

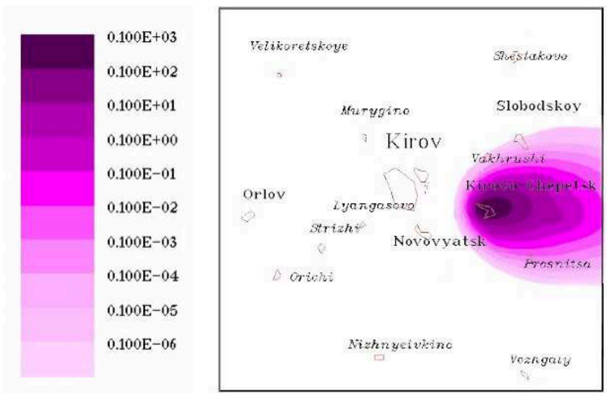

Figure 3: Distribution of contaminations by the wind from west

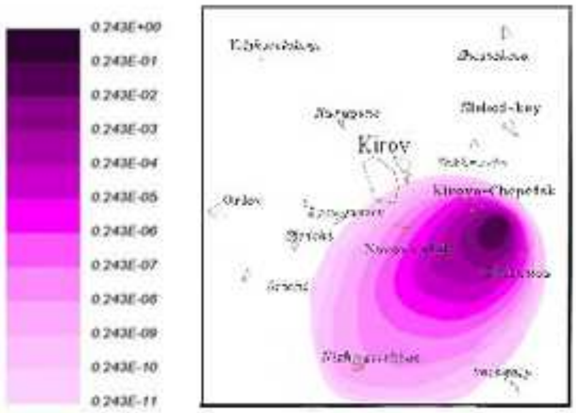

Figure 4: Distribution of contaminations by the wind from north-east