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Numerical analysis of benzo[a]pyrene pollution data in the vicinity of power plant*

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Abstract. A model for reconstructing the surface concentration of a heavy non-homogeneous substance transferred into the atmosphere is proposed. The model is used to simulate the snow surface contamination by benzo[a]pyrene in the vicinity of Power Plant-3 in the city of Barnaul. The wind rotation effects in the atmospheric boundary layer on the field of a long-term aerosol substance are assessed.

Keywords: measurement, aerosol, reconstruction assessment, atmospheric boundary layer

Introduction

Designing the placement and operation modes of smoke stacks which can be several hundred meters high above the ground requires a more detailed consideration of the wind field vertical structure [1, 2]. This is due to the need for an adequate description of the atmospheric transport under conditions of the velocity vector alteration with height. The wind characteristics within the atmospheric boundary layer (ABL) can differ from a simple plane-parallel distribution, therefore the modeling with only surface values of the wind speed to calculate pollution fields may be incorrect [3, 4].

The Coriolis force determines deflection of the wind to the right with height. The deflection angle depends on many factors, and its theoretical value is about 30°. It is of particular interest to include this effect into the study of the migration of smoke aerosol emitted from a high-altitude source. When hot gases are emitted from a high-altitude stack, their additional ascent relative to the source occurs due to the buoyancy forces and dynamic momentum. The higher he height of emission and the temperature of mixture, the more significant the effect of the wind speed deflection.

Heavy particles caught by the atmospheric flow undergo a vertical shift, along with a horizontal drift, and therefore the direction of transfer changes in accord with a local direction of the velocity vector. This determines a complex three-dimensional structure of trajectories of a sedimentating admixture and specific features of the fallout trace which is expressed by a substantial difference between the trace axis and the prevailing surface wind

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direction. It should be noted that in the vicinity of low-located emission sources, where the wind deflection does not play a major role, a high correlation between the main transfer directrix and the plume axis is usually maintained.

The proposed mechanism of forming the field of fallout from high-altitude sources is extremely important for the description of the long-term (seasonal) pollution of areas from industrial stacks. The application of direct methods of mathematical modeling of aerosol transport into the atmosphere from high-altitude sources involves difficulties. Thus, there is uncertainty in prescription of the emitted substance size-consist characteristics, emission rate, and the source operation mode [5]. In addition, a detailed information about the actual meteorological conditions is required. This circumstance necessitates developing monitoring studies based on a trade-off approach assuming the setting of inverse problems of estimating the aerosol fallout parameters of sources and fields [6].

1. Experimental studies

The study subject having a practical importance is aerosol emission from the Power Plant-3 in the city of Barnaul. The outgoing gas-and-aerosol mixture is mainly emitted through the 230 m high stack. A snow sampling in the vicinity of the PP-3 was carried out in March, 2010, along two radial routes oriented in the north-eastern and eastern directions from the admixture source. Wind regime in the ABL for winter season was characterized based on climatological data from the upper-air station in the city of Novosibirsk [7], as it is shown in Figure 1.

Given the height of the stack and the frequency of wind directions, the aerosol deposition in the winter season is expected to prevail in the north-east and east directions.

Figure 2 shows a scheme of the en-route snow sampling. The sampling points were located denser on the routs in the vicinity of a stack, and with allowance for preliminary information on possible additional sources of benzo[a]pyrene (BaP) emissions, terrain conditions, road system, build-up

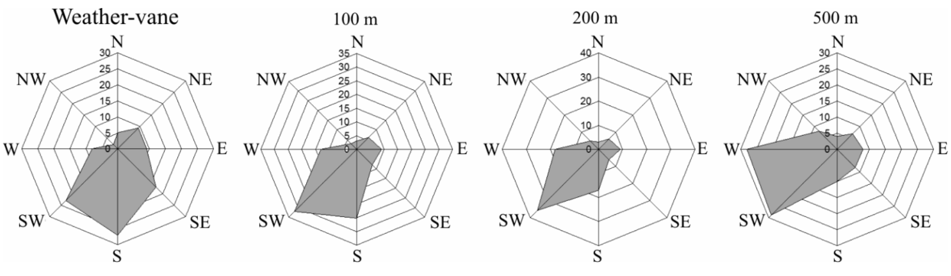

Figure 1. Winter wind pattern at a height of weather-vane, 100, 200, and 500 m

and forested areas distribution, snow cover conditions, etc. The results of field survey and chemical analysis of BaP content in the snow samples are shown in the table. A preliminary analysis of observational data, presented in the table, revealed that the most significant BaP fallout on the snow cover takes place in the nearest zone of 2–3 km. Taking into account a considerable height of the source, the major fallout of BaP in this region may be composed only of a large fraction of particles.

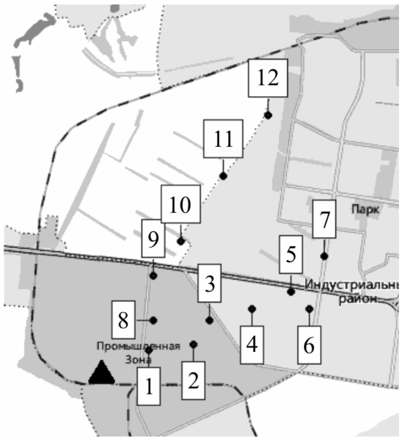

Figure 2. Scheme of en-route snow sampling in the vicinity of PP-3. Black triangle indicates the position of a high-altitude stack

Measured concentrations of benzo[a]pyrene (ng/kg) in snow samples to the east and north-east of the stack of PP-3

Direction of sampling route	East							North-east				
Point #	1	2	3	4	5	6	7	8	9	10	11	12
Distance, km	0.7	1.6	1.9	2.8	3.2	3.5	4.0	0.9	1.5	2.4	4.0	5.5
Concentration, ng/kg	114.2	84.2	97.4	28.1	41.4	34.5	9.0	73.7	54.5	22.7	16.4	14.7

2. Reconstruction of aerosol fallout fields

A preliminary analysis of observational data suggests that a kinematic scheme of the particles dispersion in the atmosphere is quite applicable to the models evaluating the BaP fallout field. In this case, the motion of particles in the wind field is represented by a drop at a constant velocity described by Stokes' law, and the admixture transport may be described by the following equation

$$u\frac{\partial q}{\partial r} - w\frac{\partial q}{\partial z} = 0 \tag{1}$$

with the boundary condition

$$q|_{r=0} = \psi(z) \equiv Q\,\delta(z - H), \tag{2}$$

where $q(r, z)$ is the admixture concentration in the plane (r, z), u is the average horizontal wind speed in the direction of r-axis, w is the sedimentation velocity of particles along z-axis, z-axis is directed vertically upward, Q and

H are the power and the effective height of the source, and δ is the Dirac delta function.

The admixture transport occurs according to characteristics of equation (1), and the solution of (1), (2) is represented as

$$q(r,z) = \psi(z + rw/u). \tag{3}$$

Description of the particle size spectrum $N(w)$ of a polydispersed admixture in the source with respect to sedimentation rate was performed using the following two-parameter function [5]:

$$N(w) = \frac{n^{n+1}}{w_k \Gamma(n+1)} \left[\frac{w}{w_k} \exp\left(-\frac{w}{w_k} \right) \right]^n. \tag{4}$$

Then, using (3), (4) and the properties of the delta function, the admixture fallout density in the radial direction away from the source may be represented as

$$\begin{aligned} \sigma(r,\vec{\theta}) &= \int_0^\infty w\, q|_{z=0} N(w)\, dw = \int_0^\infty w \frac{u}{r}\, \delta(w - Hu/r)\, N(w)\, dw \\ &= \frac{Hu^2}{r^2} N\left(\frac{Hu}{r} \right) = \theta_1 r^{-\theta_2} \exp\left(-\frac{\theta_3}{r} \right), \end{aligned} \tag{5}$$

where

$$\theta_1 = \frac{u}{\Gamma(n+1)} \left(\frac{nHu}{w_k} \right)^{n+1}, \quad \theta_2 = n+2, \quad \theta_3 = \frac{nHu}{w_k}.$$

The density field of the fallout of a heavy heterogenous admixture in the vicinity of the source is described by the relation

$$\Pi(r,\varphi,\vec{\theta}) = \sigma(r,\vec{\theta}) P(\varphi + 180^\circ). \tag{6}$$

Here $P(\varphi)$ is the wind direction frequency averaged over the sedimentation layer. An unknown vector of the parameters $\vec{\theta}$ in (5) may be estimated from the data of the surface sediment concentration using the method of least squares.

The validation of estimation model (5) was conducted on experimental data of BaP fallout in the vicinity of Power Plant-3 in the city of Barnaul. Fallouts of BaP in the considered directions were numerically reconstructed based on a very limited set of measurement points. The results of numerical reconstruction of BaP fallout fields along the sampling routes are presented in Figure 3. The eastward fallout fields were evaluated using BaP measurements only at points 1, 2, and 4 (reference points). When restoring a field in the north-east direction, the values of parameters θ_2, θ_3 were taken from the previous calculation. In this case, restoration of the dependence was per-

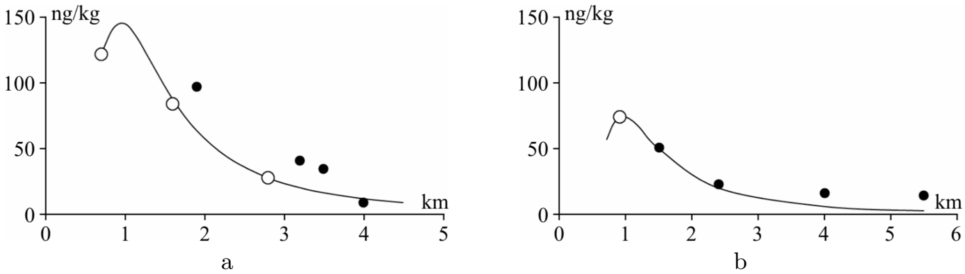

Figure 3. Reconstructed concentrations of benzo[a]pyrene (ng/kg) in the snow based on model (5) in the eastern (a) and north-east (b) directions away from the stack of PP-3 in the city of Barnaul: ○ reference points, • control points

formed using a single reference point 8. It should be noted that the BaP fallout density in the north-east direction is half as high as the fallout density in the east direction and consistent with the ratio of the winter frequency of the south and south-west winds at an altitude of 200 m (see Figure 1).

Figure 4 shows the reconstructed field of BaP concentration in the snow using dependence (6), the winter wind pattern at an altitude of 200 m, and the data from reference points 1, 2 and 4. The analysis of Figure 4 shows that a maximum BaP fallout is eastward from the stack at a distance of about 1 km, and the main drift of admixture occurs in the east direction.

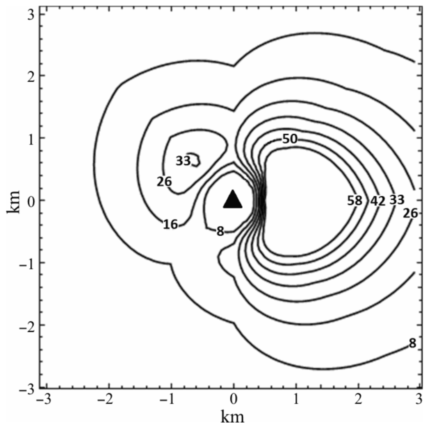

Figure 4. Reconstructed field of benzo[a]pyrene concentration (ng/kg) in snow for the winter season 2009/2010

3. The vertical structure of the wind field in the atmospheric boundary layer

Let us introduce a Cartesian coordinate system in which the axis x is horizontally directed parallel to the geostrophic velocity vector, the axis y is flatwise to it, and the axis z is vertically upwards. The origin is on line with the underlying surface. To describe the velocity fields, we will use the Ekman equations for ABL [2] approximating the balance of the Coriolis forces, the pressure gradient, and the turbulent viscosity

$$\frac{\partial u}{\partial t} = lv + \frac{\partial}{\partial z} K \frac{\partial u}{\partial z}, \qquad \frac{\partial v}{\partial t} = -l(u - u_g) + \frac{\partial}{\partial z} K \frac{\partial v}{\partial z}, \tag{7}$$

where t is time, u and v are velocity components along the axis x and y, u_g is geostrophic velocity, l is the Coriolis parameter, and K is the coefficient of the vertical turbulent exchange.

Let us define the boundary conditions for equations (7). At the lower boundary of the area, there is a conjugation of solution with velocity profiles in the surface layer of thickness h:

$$K\frac{\partial u}{\partial z}\Big|_{z=h} = c_u|\vec{u}|u, \qquad K\frac{\partial v}{\partial z}\Big|_{z=h} = c_u|\vec{u}|v, \tag{8}$$

where $|\vec{u}|$ is the velocity modulus, c_u is the drag coefficient calculated by the model of quasi-stationary sublayer. At the upper boundary $z = H$, we will accept the condition of decay of the boundary-layer disturbances

$$u|_{z=H} = u_g, \qquad v|_{z=H} = 0. \tag{9}$$

The description of the vertical turbulent exchange is based on applying the two-parameter model for the turbulent kinetic energy and its dissipation rate [8] in the implementation of [9]. The turbulence model assumes that the ABL is stably stratified with a standard value of static stability.

Equation system (7) with boundary conditions (8), (9) and the equations of turbulence closure was solved by the finite difference method using a grid which was non-uniform along the axis z with values of steps varying from $\Delta z = 2$ m at the lower boundary to $\Delta z = 6$ m at $z = H$. The implicit numerical scheme with a tridiagonal matrix algorithm was used, and the integration was carried out until the steady-state solution was obtained.

The stationary profiles u, v for the geostrophic wind $u_g = 5$ m/s are shown in Figure 5 (Curves 1 and 2).

The ABL height was determined by the level of damping of the turbulence coefficient, calculated with a two-parameter turbulence closure model. As is shown in Figure 5, the boundary layer height under given stratification conditions and the dynamic mode is 1400 m. The effect of a transverse velocity component occurs below the level $z = 1000$ m (Curve 2 in Figure 5), and its maximum is attained at an altitude of 250 m. Curve 3 in Figure 5 is built from Curves 1 and 2, and it shows the Ekman spiral in the hodograph plane (u, v). Points on the curve indicate to the heights z corresponding to the current wind direction. The above-mentioned velocity deflection is clearly visible.

In order to estimate the degree of the trace deflection due to velocity variations with height, let us analyze the trajectory of a heavy particle emitted from a stack at a height of 230 m, with the equations

$$\frac{dx_c}{dt} = u, \qquad \frac{dy_c}{dt} = v, \qquad \frac{dz_c}{dt} = w - w_g, \tag{10}$$

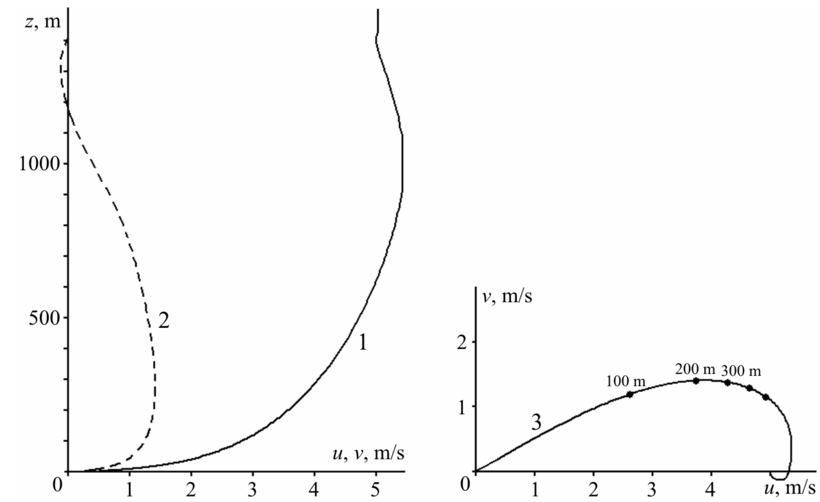

Figure 5. The calculated vertical structure of velocity components (Curves 1 and 2) and the Ekman spiral (Curve 3)

where (x_c, y_c, z_c) are the current positions of a particle, w is the own velocity of hot aerosol ascent, w_g is the gravitational sedimentation rate. Assuming that at the initial instant a particle has the coordinates $x_c = 0$, $y_c = 0$, and $z_c = 230$ m, and substituting the calculated velocities into (10), we will integrate system (10) until the particle reaches the underlying surface, i.e., when $z_c = 0$. Let us consider a coarsely dispersed aerosol with $w_g = 0.5$ m/s. The calculation shows that the particle falls after about 11 minutes, during which it covers a distance of 2100 m from the point of emission. The lateral displacement from the geostrophic flow line is 730 m. This value reflects the effect of the wind deflection at high altitudes and determines distortion of the trace geometry on the underlying surface.

Conclusion

The performed investigation using the data of snow cover pollution monitoring and model descriptions of wind field in the atmospheric boundary layer for a case of high-altitude stack of Power Plant-3 in the city of Barnaul has shown the need for incorporating the information about the frequency of wind directions throughout the layer where admixture propagates. In this case, information about the surface wind patterns is not sufficient for models of direct simulation and numerical reconstruction of the field of admixture concentration, since there is a significant disagreement between the model results and the field observations. It should also be noted that in the winter season the benzo[a]pyrene export is predominantly directed towards the city, thus indicating to a wrong location of the industrial site of PP-3, and eventually results in significant additional air pollution in the city of Barnaul.

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