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# Prediction of atmospheric air pollution near a coal stack in adverse weather conditions

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**Abstract.** Coal piles on the territory of enterprises are long-term sources of dust pollution of atmospheric air. Forecasting the level of dust pollution of the air for such objects is carried out, as a rule, for convection conditions. But during inversion, very high concentrations of dust can occur on industrial sites. The task of assessing the level of dust pollution of atmospheric air at an industrial site during dust emission in conditions of inversion from a coal stack is considered. A three-dimensional equation of convective-diffusion dispersion of contamination in atmospheric air, compatible with the approach of Prof. Berliand M. on determining the value of the vertical diffusion coefficient in the surface layer of the atmosphere for the case of inversion, to model dispersion of dust from a coal stack under inversion conditions is used. Numerical integration of the modeling equation of convective-diffusion transport of contamination is carried out on the basis of the splitting method compatible with the use of a locally one-dimensional finite-difference scheme. The results of a computational experiment to determine dust pollution zones at the Prydniprovsk thermal power station are presented.

## 1. Introduction

Coal piles are significant and long-term sources of dust pollution of atmospheric air at industrial sites. Prediction of dust concentrations in work areas near stacks is an important task in the field of environmental protection. Such prediction makes it possible to determine negative impact of the stack and is the basis for developing a strategy for reducing dust pollution by using various means. But in practice, predicting of dust pollution zones of atmospheric air is carried out for convection conditions. It is also important to note that the methods of calculating the concentration fields of impurities used in practice are developed specifically for such weather conditions - for example, the Gaussian model or the OND-86 model [1, 2, 7-10]. But it is known that in adverse weather conditions - during



inversion, the surface layer of the atmosphere have the highest concentrations of impurities [1]. This is due to the fact, that during the inversion in the surface layer of the atmosphere, layers with different intensity of impurity scattering are formed. This leads to the formation of areas of pollution with a very significant concentration of impurities on the territory of the enterprise. The formation of inversion layers in the atmospheric air may be because, for example, if thermal power station (TPS) using coal is located near a large reservoir (figure 1), then cold air from the surface of the reservoir moves in the direction of the territory of the TPS and creates a layer of low air temperature above the ground, and above this layer there is a layer of heated air. In this way, a local inversion is formed, that is, negative conditions are created for dust dispersion from coal stacks.



**Figure 1.** Prydniprovskaya TPS: 1 – a pile of coal (Google Image, 2022).

Therefore, for practice, it is very important to have methods of operational assessment of the level of atmospheric air pollution during inversion.

The purpose of this work is to develop a kinematic numerical model that allows quickly obtain a predictive assessment of the level of atmospheric air pollution in the presence of emission from coal stacks under inversion conditions.

## 2. Methods

Assessment of the level of air pollution at the industrial site under conditions of inversion and during the emission of dust from the coal stack is carried out numerically. To solve the modeling mass transfer equation, the finite difference method is used in conjunction with the splitting method. Splitting is carried out in the way to consider dispersion of dust in stages only in one coordinate direction. For each one-dimensional differential equation, a locally one-dimensional difference scheme is constructed.

### 2.1. Theoretical part

To predict the level of atmospheric air pollution during the emission of dust from coal stacks in inversion conditions, the equation of contamination dispersion in the atmosphere is used [1-3, 5]:

$$\begin{aligned} & \frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial (w-w_s)C}{\partial z} = \\ & = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_z \frac{\partial C}{\partial z} \right) + \\ & + \sum_i Q_i \delta(x-x_i) \delta(y-y_i) \delta(z-z_i), \end{aligned} \quad (1)$$

where  $C$  – dust concentration in the air,  $\text{mg}/\text{m}^3$ ;  $\mu_x, \mu_y, \mu_z$  – atmospheric diffusion coefficients,  $\text{m}^2/\text{s}$  (the specific value of these coefficients corresponds to the inversion conditions [1]);  $w_s$  – rate of gravitational sedimentation of heavy dust particles,  $\text{m}/\text{s}$ ;  $Q_i$  – intensity of dust emission of the  $i$ -th source from the stack surface,  $\text{mg}/\text{s}$ ;  $\delta(x-x_i), \delta(y-y_i), \delta(z-z_i)$  – the Dirac delta function;  $x_i, y_i, z_i$  – Cartesian coordinates of the dust emission source,  $\text{m}$ ;  $t$  – time,  $\text{s}$ .

The emission surface is modeled by a set of point sources located on this surface.

Initial and boundary conditions for the equation of dust dispersion in atmospheric air are considered in [3, 5].

To model the dispersion of coal dust for inversion conditions, the approach of Prof. Berliand M. E. to determine the vertical diffusion coefficient is used. According to this approach, the following dependence is used to determine the vertical diffusion coefficient [1]:

$$\mu_z = \mu_i \cdot \left(1 - \frac{z - z_i}{L_i}\right)^2, \quad (2)$$

where  $\mu_i$  – the lower limit of the inversion,  $\text{m}^2/\text{s}$ ,  $L_i$  – a special function that takes into account the energy of turbulence,  $\text{m}$  [1],  $z$  – the current value of the height above the ground,  $\text{m}$ . Thus, changing the value of the parameter  $z_i$  it is possible to simulate atmospheric air pollution at different sizes of the inversion layer.

Dependence (2) allows to take into account changing value of the vertical diffusion coefficient with height. To determine the value of other diffusion coefficients following dependences are used:

$$\mu_x = ku, \quad \mu_y = kv,$$

where  $u, v$  – components of the wind speed vector in projections on the axis  $x, y$  in accordance,  $k$  – empirical parameter [1-3].

The wind speed profile is determined by the following dependence [1]:

$$u = u_1 \left(\frac{z}{z_1}\right)^{n_1},$$

where  $u_1$  – wind speed,  $\text{m}/\text{s}$ , at height  $z_1 = 1 \text{ m}$ ;  $n_1 = 0.16$ .

Thus, in order to model dust concentration fields at an industrial site under inversion conditions, it is necessary to solve the three-dimensional equation of the distribution of a heavy impurity with the corresponding dependencies for the velocity profile and atmospheric diffusion coefficients. The solution of this problem can be obtained only numerically.

## 2.2. Numerical model

For the numerical solution of equation (1), the finite-difference method of numerical integration is used [3-5]. The basic equation (1) is split into a sequence of equations describing only one direction of dust dispersion in atmospheric air (equations 3-5):

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial C}{\partial x} \right); \quad (3)$$

$$\frac{\partial C}{\partial t} + \frac{\partial vC}{\partial y} = \frac{\partial}{\partial y} \left( \mu_y \frac{\partial C}{\partial y} \right); \quad (4)$$

$$\frac{\partial C}{\partial t} + \frac{\partial (w - w_g)C}{\partial z} = \frac{\partial}{\partial z} \left( \mu_z \frac{\partial C}{\partial z} \right); \quad (5)$$

$$\frac{\partial C}{\partial t} = \sum_i Q_i(t) \delta(x - x_i)(y - y_i)(z - z_i). \quad (6)$$

Equation (6) takes into account changing of dust concentration due to its emission from the stack surface.

For the numerical solution of equation (3), the following two-step splitting scheme is used:

– the first step [5]:

$$C_{i,j,k}^{n+\frac{1}{2}} = C_{i,j,k}^n - \Delta t \frac{u_{i+1,j,k}^+ C_{i,j,k}^{n+\frac{1}{2}} - u_{i,j}^+ C_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta x} + \Delta t \mu_x \frac{-C_{i,j,k}^{n+\frac{1}{2}} + C_{i-1,j,k}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t \mu_x \frac{-C_{i,j,k}^n + C_{i+1,j,k}^n}{2\Delta x^2},$$

– the second step [5]:

$$C_{i,j,k}^{n+1} = C_{i,j,k}^{n+\frac{1}{2}} - \Delta t \frac{u_{i+1,j,k}^- C_{i+1,j,k}^{n+1} - u_{i,j,k}^- C_{i,j,k}^{n+1}}{\Delta x} + \Delta t \mu_x \frac{-C_{i,j,k}^{n+\frac{1}{2}} + C_{i-1,j,k}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t \mu_x \frac{-C_{i,j,k}^{n+1} + C_{i+1,j,k}^{n+1}}{2\Delta x^2},$$

where  $u^+ = \frac{u + |u|}{2}$ ,  $u^- = \frac{u - |u|}{2}$ .

For the numerical solution of equation (4), the following two-step local one-dimensional splitting scheme is used:

– the first step [5]:

$$C_{i,j,k}^{n+\frac{1}{2}} = C_{i,j,k}^n - \Delta t \frac{v_{i,j+1}^+ C_{i,j,k}^{n+\frac{1}{2}} - v_{i,j,k}^+ C_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y} + \Delta t \mu_y \frac{-C_{i,j,k}^{n+\frac{1}{2}} + C_{i,j-1,k}^{n+\frac{1}{2}}}{2\Delta y^2} + \Delta t \mu_y \frac{-C_{i,j,k}^n + C_{i,j+1,k}^n}{2\Delta y^2},$$

– the second step [5]:

$$C_{i,j,k}^{n+1} = C_{i,j,k}^{n+\frac{1}{2}} - \Delta t \frac{v_{i,j+1}^- C_{i,j+1,k}^{n+1} - v_{i,j}^- C_{i,j,k}^{n+1}}{\Delta y} + \Delta t \mu_y \frac{-C_{i,j,k}^{n+\frac{1}{2}} + C_{i,j-1,k}^{n+\frac{1}{2}}}{2\Delta y^2} + \Delta t \mu_y \frac{-C_{i,j,k}^{n+1} + C_{i,j+1,k}^{n+1}}{2\Delta y^2},$$

where  $v^+ = \frac{v+|v|}{2}$ ,  $v^- = \frac{v-|v|}{2}$ .

Similarly, a locally one-dimensional difference scheme for equation (5) is constructed. The Euler method [4] is used for the numerical integration of equation (6). The calculated dependence has the form:

$$C_{ijk}^{n+1} = C_{ijk}^n + \Delta t \sum Q_i \delta(x - x_i) \delta(y - y_i) \delta(z - z_i).$$

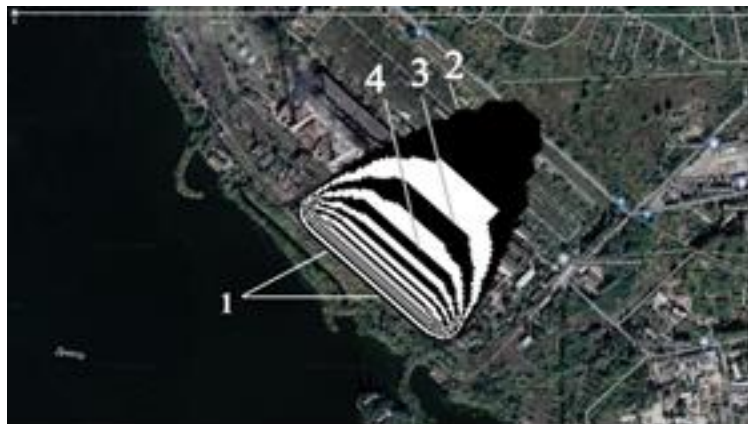
Thus, to calculate contamination concentration fields, the given difference equations are solved sequentially.

Based on the developed numerical model, the "PILE-C2" code is developed in the FORTRAN programming language.

### 3. Results and discussion

The results of solving the problem of determining the level of dust pollution of the air at the industrial site of the Prydniprovskaya TPS during inversion are presented. Dust emission occurs from the surface of the stack (figure 1). Data for predicting: wind speed  $u_1 = 3$  m/s;  $z_1 = 1.5$  m,  $L_i = 100$  m [1];  $\mu_1 = 0.05$  m/s;  $k = 0.1$ ; dimensions of the calculation area  $1800 \text{ m} \times 1000 \text{ m} \times 250 \text{ m}$ . The emission rate of finely dispersed dust from the surface of the stack is calculated on the basis of empirical dependence [6]; it is assumed that the rate of gravitational settling of dust particles  $w_s = 0.0001$  m/s.

The predicted zone of dust pollution of the industrial site with a south-westerly wind direction is shown on the level  $z = 1.8$  m (figure 2).



**Figure 2.** The area of dust pollution at the industrial site during inversion: 1 – stack location area; 2 –  $C=9.01 \text{ mg/m}^3$ ; 3 –  $C=20.6 \text{ mg/m}^3$ ; 4 –  $C=30.9 \text{ mg/m}^3$  (Google Image, 2022).

As can be seen from figure 2, the pollution area covers a large part of the industrial site. The shape of the pollution area has the form of "waves" leaving the source of pollution - a stack, that is, this area is similar to the area of pollution formed from a linear source of pollution. The area of pollution with a significant dust concentration gradient corresponds to the position of the coal stack. The value of dust concentration at the industrial site exceeds the Maximum Permissible Concentration (MPC)  $\text{MPC}=6 \text{ mg/m}^3$ . This is because the inversion layer does not allow impurities to disperse well in the air.

Change in dust concentration at altitude 1.8 m and along the line that corresponds to the middle of the pollution source and is directed in the direction of the wind, as well as how many times the concentration exceeds the MPC, shown in the table 1.

As can be seen from the table 1, during the inversion, there is intense pollution at the industrial site

and the dust concentration significantly exceeds the MPC near the coal stack.

**Table 1.** Change in dust concentration at the industrial site during inversion.

Length x, m	Dust concentration / exceeding the MPC
40 m	71.4 mg/m <sup>3</sup> / 11.9
50 m	65.1 mg/m <sup>3</sup> / 10.8
60 m	59.2 mg/m <sup>3</sup> / 9.8

Note that the calculation time using the developed numerical model is 4 s.

#### 4. Conclusions

A numerical model and an express assessment of the level of pollution of the territory of industrial sites in the conditions of man-made emissions during calm and inversion are given. The calculation based on the developed numerical model takes a few seconds, which makes it possible to use it widely when carrying out serial calculations for the purpose of determining the size of zones of dangerous air pollution.

1. The proposed mathematical model, which allows assess the shape and size of air dust pollution zones in the case of dust emission from a coal stack under adverse weather conditions – an inversion.

2. The proposed numerical model belongs to the group of kinematic models and makes it possible to determine pollution zones very quickly on low- and medium-power computers.

3. The proposed numerical model can be useful in assessing the level of danger on the territory of enterprises in case of the appearance of additional piles of coal at the industrial site.

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