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Conjugated mathematical model for optimal location of industrial objects

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Abstract. The urgent problem related to solving the problems of monitoring and predicting the ecological state of the air basin in industrial regions is considered in the paper. It provides a brief review of scientific publications devoted to these problems. A mathematical model has been developed to study, predict and monitor the concentration of harmful substances in the atmosphere. The model takes into account weather and climate conditions, soil erosion, physicomechanical properties of aerosol particles, and other factors affecting the process under consideration as a whole; it is designed for optimal location of newly constructed production facilities.

1. Introduction

The rapid pace of development of the Republic's economy requires the construction and location of powerful industrial facilities and complexes in cities and districts, depending on the raw material potentials and labor power. These facilities are built in densely populated areas or in their vicinity. This circumstance imposes special restrictions on the location of facilities that release harmful substances into the atmosphere that violate the ecological state in the region. Therefore, the problem of rational or optimal location of objects is a complex and, at the same time, an urgent problem.

Based on the foregoing, new industrial facilities near settlements, recreation areas and other environmentally significant zones should be located so that their total annual pollution from harmful industrial emissions does not exceed permissible sanitary standards; and the overall environmental load on the entire region due to it pollution should be as minimal as possible.

Despite this, as a result of growth in the number of industrial facilities, the emission of harmful substances and aerosol impurities into the environment increases and that directly affects the ecological condition of the territories.

The issue of environment, atmosphere, soil, groundwater and underground water protection from techno-genic factors and the problems of mathematical modeling of the abovementioned tasks were studied and solved by many researchers; a number of schools were created under the guidance of famous scientists; theoretical and applied results were obtained.

In particular, in [1-2], mathematical models and numerical algorithms and software were developed for predicting and monitoring the multicomponent air motion and the pollutants transport in the atmosphere; the problem of multicomponent air motion in the atmosphere was solved with account for vaporization and condensation.

The studies in [3] were devoted to the active aerosol particles transport and diffusion in the atmosphere, taking into account chemical transformations in the air. Chemical reactions with aerosol particles in the atmosphere were presented.

In [4], the processes of substance transformation under transfer and diffusion of harmful substances in the air over long and medium distances were studied. The paper also addressed the trajectory and evolutionary models of the propagation of aerosol particles in the atmosphere; the results of calculations were compared with field measurements.

[5] is devoted to the development of a mathematical model of the dynamics and kinetics of gas and aerosol impurities transport and diffusion in the atmosphere. The paper presents a model of multicomponent impurity transfer taking into account photochemical transformation and aerosol formation in the troposphere of the northern hemisphere, with account for the kinetic processes of nucleation, condensation, and coagulation.

Mathematical support for the process of fire hazardous objects location and their optimization with account for the topography and spatial form is given in [6].

In [7], a computer model was developed for the study, forecasting and monitoring of harmful substances emission into the environment by vehicles. A numerical computer implementation of a model was presented using the control volume method based on the developed distributed computer calculation algorithm.

Modeling of wind currents field with the Navier-Stokes system of equations considering compressibility and turbulence of the air, lay of land was proposed in [8], and the SIMPLE algorithm was used as a numerical method.

The studies in [9] present the basic approaches to creating computer models of atmospheric phenomena. A review of modern models of substance spread in the atmosphere, and dust and plant pollen filters is made, and the advantage of the SILAM model developed in the Finnish Meteorological Institute is shown.

In [10], significant factors affecting the process of harmful substances transport and diffusion are shown: the atmosphere circulation mode, its thermal stability; atmospheric pressure, air humidity, temperature; temperature inversions, their repeatability and duration; wind speed, repeatability of air and light winds (speed lower than 1 m/s) stagnation; duration of fogs; lay of land, geological structure and hydrogeology of the area; soil and plant conditions (soil type, water permeability, porosity, granulometric composition of soils, state of vegetation, composition of rocks, age, growth class); background values of pollution indices of atmospheric natural components; state of the animal world.

In [11], analytical studies of the processes of harmful emissions spread in the atmosphere from industrial enterprises were carried out. Carbon dioxide (CO2) is considered as the main atmospheric pollutant. The Green function is given for the problem of a single instantaneous release of harmful impurities in a standard surface layer of the atmosphere at a given wind field; an expression is obtained for the impurities concentration in a stationary case and under continuously acting pollution source.

Sukhinov A.I. and Khachunts D.S. in [12] considered the problem of multicomponent air motion with account for vaporization and condensation. The authors noted that one of the pressing problems of modern atmosphere physics is mathematical modeling of the variability of gas and aerosol composition of the atmosphere, and an assessment of atmospheric impurities effect on the environment.

In another paper, Sukhinov A.I. et al. [13] presented the development of a mathematical model of multicomponent air motion, taking into account the pollutants and heat transport, phase transfers, as well as the effect of vegetation (tree planting) on the harmful substances spread in the atmosphere.

To study the air pollutants transport by turbulent diffusion and advection by the wind, Stockie J.M. used a Gaussian model [14]. He considered the assumptions underlying the model, the model derivation from advection-diffusion equation, and the key properties of the trail model solution. Then the results were used to solve the inverse problem, in which the emission source rate was determined from a given set of measurements of pollutants concentration on the underlying surface.

The paper by Yerramilli A. and his coauthors [15] is focused on determining the location of emission sources and trends in harmful substances transfer. The simulation is based on the joint use of the HYSPLIT model (integrated Lagrange model of single particles trajectory) and WRF model (numerical model of weather forecast); these models allow calculating the direct and reverse trajectories and air pollutants concentrations.

The studies showed that in order to develop an adequate mathematical model of the process it is necessary: firstly, to take into account soil erosion, which, under unstable stratification of the air mass, significantly changes the harmful substances concentration in the atmosphere; secondly, to take into account the speeds of atmospheric air mass flow in three directions over time; thirdly, to consider a change in diffusion coefficient and the coefficient of turbulent mixing vertically under stable and unstable stratification; fourthly, to account for the changes in wind direction over time and due to the orography of the area; fifthly, to account for the changes in interaction coefficient, which depends on the characteristics of the underlying surface and the orography of the area.

2. Problem Statement

To monitor and forecast the ecological state of industrial regions and make specific managerial decisions, we assume that industrial facilities emit harmful aerosol particles with an intensity of Q, which is then transported and spread by the air mass in the atmosphere, per a unit of time to a height of $z=h$. The aims of mathematical modeling of the process of harmful substances transport and diffusion in the atmosphere are: monitoring and predicting the aerosol particles concentration in the region, investigating the key parameters and weather-climate factors affecting the process as a whole, determining the location and amount of substances emitted into the atmosphere, at which the sanitary pollution standards are met in some areas and in the whole region and accounting the number of polluting sources.

The solution of the problems of industrial facilities optimal location (which meets the sanitary standards) in the region, is obviously associated with the multiple integration of the direct task to choose various options for the location of harmful substances emission sources. However, the same goals can be achieved if a conjugated problem is solved. The task is to choose a site to locate production facilities in which global and local sanitary standards on pollution will be met for the entire region and for specially selected zones of this region.

The conjugate problem with respect to the basic one has the following form [16-20]:

$$-\frac{\partial\theta^*(x,y,z,t)}{\partial t}-u\frac{\partial\theta^*(x,y,z,t)}{\partial x}-v\frac{\partial\theta^*(x,y,z,t)}{\partial y}-w\frac{\partial\theta(x,y,z,t)^*}{\partial z}+\sigma\theta^*=$$
$$=\frac{\partial}{\partial z}(\kappa\frac{\partial\theta^*(x,y,z,t)}{\partial z})+\mu\left(\frac{\partial^2\theta^*(x,y,z,t)}{\partial x^2}+\frac{\partial^2\theta(x,y,z,t)^*}{\partial y^2}\right)+P(x,y,z,t); \quad (1)$$

$$-\mu\frac{\partial\theta^*}{\partial x}\bigg|_{x=0}=\gamma\left(\theta_t-\theta^*\right);\ \ \mu\frac{\partial\theta^*}{\partial x}\bigg|_{x=L_x}=\gamma\left(\theta_t-\theta^*\right); \quad (2)$$

$$-\mu\frac{\partial\theta^*}{\partial y}\bigg|_{y=0}=\gamma\left(\theta_t-\theta^*\right);\ \ \mu\frac{\partial\theta^*}{\partial y}\bigg|_{y=L_y}=\lambda\left(\theta_t-\theta^*\right); \quad (3)$$

$$\kappa\frac{\partial\theta^*}{\partial z}\bigg|_{z=0}=\beta\cdot\theta^*-F_0\left(x,\mathrm{y},z\right);\ \ \kappa\frac{\partial\theta^*}{\partial z}\bigg|_{z=H_z}=\gamma\left(\theta_t-\theta^*\right); \quad (4)$$

$$\theta^*(x,y,z,T) = \theta^*(x,y,z,0)\,. \tag{5}$$

Here θ^* is the amount of propagating substance, t - time, x,y,z - coordinates, u,ϑ,w - components of the wind speed in the x, y, z directions, respectively, w_g - particle deposition rate, κ - turbulent mixing coefficient, μ - diffusion coefficient, σ - absorption coefficient, β - coefficient of interaction with the underlying surface, $P(x,y,z,t)$ - capacity of harmful substances emission into the atmosphere from stationary sources; $F_0(x,\mathrm{y},z)$ - the amount of salts and aerosol particles emission from the earth surface; θ_b - the concentration of suspended solids transferred through the boundaries of the problem solution region.

So, a conjugate model (6) - (10) was obtained for solving the problem of the aerosol particles distribution in the atmosphere, considering potential sources of harmful substances in the atmosphere and soil erosion.

To determine the turbulence coefficient, consider the following functional dependencies:

1. $\kappa = const$, u,v,w - $const$;
2. $\kappa = \begin{cases} v + \kappa_1 \dfrac{z}{z_1}, & z \le h, \\ v + \kappa_1 \dfrac{h}{z_1}, & z > h, \end{cases}$
3. $\kappa = \kappa(z),\ v = v(z),\ w = w(z),\quad v = |v|\, z^n;$

where h is the height of the surface layer, v is the turbulent viscosity.

The value of F_0 is a function of $x,\ y,\ z,\ t$ and the surface source can be written as

$$F_0 = f(u,w), \tag{6}$$

where F_0 is the volume flow rate of particles entrained by atmospheric front, m^3/s.

To determine the form of function (6), proceed to the analysis of the acting forces causing soil destruction and resisting this destruction. Destructive forces are denoted by F . They are opposed by resistance forces R , which include moisture content and other physical and mechanical properties of soil.

When the force F exceeds the force R , the process of soil erosion and entrainment of harmful particles from the earth's surface begins. To obtain the theoretical dependence, consider the equilibrium process. In dynamic equilibrium, the difference in forces F and R must be equal to zero:

$$F - R = 0\,. \tag{7}$$

Then the relationship between the volume flow rate F_0 of the entrained particles and the flow rate takes the form

$$F = \frac{\partial F_0}{\partial u}\chi, \tag{8}$$

where χ is the shear stress, kg/m^2.

For the resistance force R , by analogy with F , the following expression is taken:

$$R = c_0 \frac{\mu_c}{l}\frac{\partial F_0}{\partial \zeta}, \tag{9}$$

where μ_c is the viscosity of the mixture (air + soil), kg*f/m^2; l is the distance between individual particles, m; c_0 is the soil constant.

Substituting (8) and (9) into (7), we have

$$\frac{\partial F_0}{\partial u} - c_0 \frac{\mu_c}{l\chi}\frac{\partial F_0}{\partial \zeta} = 0.$$

And finally we get

$$\frac{\partial F_0}{\partial u} - k_p \zeta \frac{\partial F_0}{\partial \zeta} = 0. \qquad (10)$$

So, an equation is obtained for determining the volume of particles entrained from the surface, depending on wind speed and soil moisture content. According to the results of the calculated value of F_0 - the volume flow rate of particles entrained by the atmospheric front - one can solve the problem of the process of harmful substances transfer and diffusion in the atmosphere using the first equation of the boundary condition (4).

From the statement of the problem, it is seen that, in contrast to Marchuk G.I. [20] here, firstly, a three-dimensional statement of the problem of harmful aerosol particles propagation in the atmosphere is considered taking into account the substance inflow and outflow through the boundaries of the considered solution region, secondly, industrial production facilities are taken as a main source of harmful substances emission; under unstable wind stratification the underlying surface is considered as an additional source generator of emissions of harmful substances due to soil erosion.

3. Method of Solution

For solving the conjugate problem (1) - (5) in principle do not differ from the solution of the major task, however, there time countdown begins. The initial point of time starts from $t = T$ and continues in the direction of decreasing t. Problem (1) - (5) can be reduced to the form characteristic of the basic equations by replacing the independent variable t by $t' = T - t$ and $u' = -u, v' = -v, w' = -w$, then it takes the following form

$$\frac{\partial \theta^*(x,y,z,t)}{\partial t'} + u'\frac{\partial \theta^*(x,y,z,t)}{\partial x} + v'\frac{\partial \theta^*(x,y,z,t)}{\partial y} + w'\frac{\partial \theta^*(x,y,z,t)}{\partial z} + \sigma\theta^*(x,y,z,t) =$$
$$= \frac{\partial}{\partial z}\left(\kappa \frac{\partial \theta^*(x,y,z,t)}{\partial z} \right) + \mu\left(\frac{\partial^2 \theta^*(x,y,z,t)}{\partial x^2} + \frac{\partial^2 \theta^*(x,y,z,t)}{\partial y^2} \right) + P(x,y,z,t); \qquad (11)$$

$$\theta^*(x,y,z,t') = g^*(x,y,z,0); \text{ at } t' = 0; \qquad (12)$$

$$-\mu \frac{\partial \theta^*}{\partial x}\bigg|_{x=0} = \gamma\left(\theta_t - \theta^*\right); \; \mu \frac{\partial \theta^*}{\partial x}\bigg|_{x=L_x} = \gamma\left(\theta_t - \theta^*\right); \qquad (13)$$

$$-\mu \frac{\partial \theta^*}{\partial y}\bigg|_{y=0} = \gamma\left(\theta_t - \theta^*\right); \; \mu \frac{\partial \theta^*}{\partial y}\bigg|_{y=L_y} = \gamma\left(\theta_t - \theta^*\right); \qquad (14)$$

$$-\kappa \frac{\partial \theta^*}{\partial z}\bigg|_{z=0} = (\beta\cdot\theta^* - F_0(x,y,z)); \; \kappa \frac{\partial \theta^*}{\partial z}\bigg|_{z=H_z} = \gamma\left(\theta_t - \theta^*\right). \qquad (15)$$

Since the posed problem (11) - (15) is also described using partial differential equations, it is difficult to obtain analytical solutions. To solve the problem, the finite-difference method is used, that is, in domain D=(0<x<a, 0<y<b, 0<z<H) continuous change in the sought for, predicted variables is substituted into a grid along x; a uniform grid - along y and an uneven grid along z.

To solve problem (11) - (15), the finite-difference method is used; replacing differential operators (11) - (15) with difference ones, we obtain a system of three-diagonal algebraic equations for the sought for variables. Based on the solution obtained $\theta^*(x,y,z,t)$, it is possible to calculate the total amount of substances in suspension in domain D over a period of time (O, T):

$$Y_D(\vec{r}) = Q\int_0^T \theta^*(\vec{r},t)dt\ ,$$

where $\vec{r}$ =(x,y,z) is the vector.

Introduce an auxiliary function

$$Y_D^* = Q\int_0^T \theta^*(r_0,t)dt\ ,$$

which parametrically depends on the location $r_0 \in D$ of an industrial facility in the region in question.

Auxiliary function $Y_D^*(\bar{r})$ is used to find r_0 from condition

$$Y^*(r) = \min_{\vec{r}\in D}.$$

The point of minimizing $Y^*(\bar{r})$ is $\bar{r}^0$. It is necessary to construct a function field, $Y_P^*(x,y,h)$, where *h* is the release height. As a result, on the plane (x, y) the field of changes is obtained

$$Y^*(x,y,h) = const$$

and domain *D* is determined where sanitary pollution standards are met.

According to the developed model and the corresponding algorithm, a set of programs was developed that made it possible to calculate the functional $Y_P^*, Y(x,y,h)$, thereby determining the location of a new industrial facility with minimal pollution.

4. Conclusion

For monitoring and predicting the environmental conditions of air basin in industrial regions and the optimal location of production facilities, a conjugated mathematical model of the object under research has been developed.

One of the principal factors of atmospheric basin pollution in the considered region is soil erosion of the underlying surface. A differential equation is obtained, its solution makes possible to calculate the amount of harmful substances emissions depending on weather and climatic factors.

In order to ensure sanitary standards in the selected zones of the region, an optimization problem is posed; its solution is used to determine the coordinates of harmful substances sources depending on their capacity and weather and climatic factors.

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