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Comprehensive Mathematical Model for Planning The Placement of Industrial Facilities

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Abstract:

The coupled problem of optimal placement of industrial facilities, taking into account global and local sanitary standards for pollution in regions and specific zones, is examined. The pollutant dispersion model incorporates soil erosion processes, physical and mechanical characteristics of emissions, and the region's weather and climatic conditions. An approach for integrating the coupled problem is proposed, which significantly reduces computational resource requirements and the number of calculation operations. A high-precision conservative numerical algorithm has been developed for integrating the problem with respect to time and spatial variables.

Keywords: Mathematical modeling, numerical methods, transport and diffusion of harmful substances, weather and climate factor

1. Introduction

Modern technological progress significantly simplifies life, but its downside is a negative impact on the environment. The Republic's economic growth necessitates the construction of industrial facilities, which are often located in densely populated areas, creating environmental risks.

The optimal placement of enterprises, minimizing harmful emissions and complying with sanitary standards, especially near residential areas and natural territories, is becoming a crucial task. However, industrial growth inevitably leads to increased environmental pollution.

Many scientists have addressed the issues of protecting the atmosphere, soil, and water resources from technogenic factors. Scientific schools have been established, and significant theoretical and practical results have been achieved. Thus, mathematical modeling is a key tool for studying pollution patterns and developing scientifically based environmental management strategies.

Sukhinov A.I. and Khachunets D.S. in their research [1] consider mathematical modeling of the motion of a multicomponent air medium, taking into account phase transitions such as vaporization and condensation. They highlight one of the key tasks of modern atmospheric physics: studying the variability of the gas and aerosol composition of air, as well as assessing the impact of atmospheric impurities on the environment. In subsequent works, Suxinov A.I. and co-authors [2] presented a mathematical model describing the transport of pollutants and heat, the influence of phase transitions, and the impact of vegetation cover on the spread of harmful substances in the atmosphere. These studies help to more accurately predict changes in air composition and their ecological consequences.

The research of Stockie J.M. [3] and Yerramilli A. with co-authors [4] is aimed at modeling the processes of pollutant distribution in the atmosphere. Stockie J.M. applies the Gaussian model for the analysis of turbulent diffusion and advection, which allows for the solution of inverse problems in determining the characteristics of emission sources. In turn, Yerramilli A. and his colleagues use a combined approach based on the HYSPLIT and WRF models to assess trajectories and concentrations of pollutants. These works demonstrate the importance of mathematical modeling in forecasting air pollution and solving environmental monitoring problems.

Studies [5-6] are focused on analyzing the processes of transfer, diffusion, and transformation of pollutants in the atmosphere. The work [5] examines the mechanisms of harmful substance distribution over medium and long distances, as well as trajectory and evolutionary models of aerosol particle movement, followed by a comparison of calculated data with field measurements. In work [6], a mathematical model of the dynamics and kinetics of gas and aerosol impurity transfer was developed, taking into account photochemical processes, aerosol formation, and their evolution in the troposphere of the Northern Hemisphere. These studies contribute to more accurate forecasting of atmospheric pollution and its impact on the environment.

The work [7] shows significant factors influencing the process of transfer and diffusion of harmful substances: atmospheric circulation regime, its thermal stability; atmospheric pressure, air humidity, temperature regime; temperature inversions, their recurrence and duration; wind speed, recurrence of air stagnation and weak winds (up to 1 m/s); duration of fogs; terrain relief, geological structure and hydrogeology of the region; soil and vegetation conditions (soil type, water permeability, porosity, soil granulometric composition, vegetation state, rock composition, age, bonitet); background values of pollution indicators of natural atmospheric components; state of the animal world.

Research [8-10] is aimed at developing and improving methods for modeling processes in the atmosphere. In the work [10], the processes of transfer and diffusion of active aerosol particles are considered, taking into account chemical transformations in the atmosphere, and the main chemical reactions influencing the composition of the air environment are described. These studies contribute to a more accurate analysis and forecasting of the ecological consequences of atmospheric pollution. The works [8-9] present mathematical models, numerical algorithms, and software for predicting and monitoring the movement of multicomponent air and the spread of pollutants, including phase transitions such as vaporization and condensation.

In the study [11], an analytical analysis of the processes of distribution of harmful emissions from industrial enterprises in the atmosphere was carried out, with an emphasis on carbon dioxide (CO_2) as the main pollutant. Green's function for modeling the single instantaneous emission of impurities in the standard ground-level layer of the atmosphere at a given wind field is presented. Expressions describing the concentration of pollutants, both under stationary conditions and with a continuous emission source, were also obtained.

Research [12-14] focuses on developing and applying computer models for analyzing atmospheric processes and the distribution of pollutants. In the work [12], a model for forecasting and monitoring emissions of harmful substances from motor vehicles, implemented based on the control volume method and a distributed calculation algorithm, is presented. In the work [13], a model of wind flows based on the Navier-Stokes system of equations, taking into account compressibility, turbulence, and terrain relief, using the SIMPLE algorithm, is proposed. The article [14] examines the basic principles of building computer models of atmospheric phenomena, provides an overview of modern models for the distribution of impurities in the atmosphere, and analyzes dust and pollen filters, including the advantages of the SILAM model of the Finnish Meteorological Institute.

The conducted research showed that to create an accurate mathematical model of the process, several key factors must be considered. Firstly, soil erosion, which, with unstable stratification of air masses, significantly affects the concentration of pollutants in the atmosphere. Second, the speed of movement of air flows in three directions over time. Thirdly, changes in the diffusion and turbulent mixing coefficient along the vertical in conditions of stable and unstable stratification. Fourthly, the dynamics of wind direction change over time, taking into account the characteristics of the terrain. Fifthly, the variability of the interaction coefficient, which depends on the characteristics of the underlying surface and orographic conditions.

2. Materials and Methods

Statement of the Problem

For effective monitoring and forecasting of the ecological state of industrial regions, as well as for making management decisions, let's consider a situation where industrial enterprises emit harmful aerosol particles into the atmosphere with an intensity Q at a height z = h. These particles are then transported and dispersed by air currents. The main objectives of mathematical modeling of pollutant transport and diffusion processes in the atmosphere are: monitoring and forecasting the concentration of aerosol particles, analyzing the influence of key parameters and weather-climatic factors on the pollution process, as well as determining the optimal location of industrial facilities and the permissible emission levels, at which sanitary standards will be met in individual zones and the region as a whole.

Solving the problem of optimal enterprise placement, taking into account sanitary norms, traditionally requires repeated integration of the direct problem for various placement options of the sources.

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

with the corresponding initial and boundary conditions:

$$\theta^*(x,y,z,t)=\theta_T^*(x,y,z,T) \quad (2)$$

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

$$-\mu\frac{\partial\theta^*}{\partial y}\bigg|_{y=0}=\gamma\left(\theta_t-\theta^*\right);\ \ \mu\frac{\partial\theta^*}{\partial y}\bigg|_{y=L_y}=\lambda\left(\theta_t-\theta^*\right); \quad (4)$$

$$\kappa\frac{\partial\theta^*}{\partial z}\bigg|_{z=0}=\beta\cdot\theta^*-F_0\left(x,\mathrm{y},z\right);\ \ \kappa\frac{\partial\theta^*}{\partial z}\bigg|_{z=H_z}=\gamma\left(\theta_t-\theta^*\right) \quad (5)$$

Where θ^* - concentration of the diffusing substance, θ^0 - initial concentration (g/m^3), θ_E - concentration entering through the boundaries of the territory under consideration (g/m^3), x,y,z - coordinate system, u,v,w - wind speed in three directions (m/s), w_g - impurity settling velocity (m/s), σ - atmospheric absorption coefficient of impurity (s^{-1}), α - coefficient characterizing the capture of particles by vegetation elements, k_r - radioactive decay coefficient ($k_r=\ln 2/T_{1/2}$, $T_{1/2}$ -

half-life of the radionuclide under study), μ, κ - diffusion and turbulence coefficients respectively (m^2/s), Q - source of radionuclides, δ - Dirac function, f_0 - the lifting of particles into the atmosphere from the underlying surface of the earth, β - particle-surface interaction coefficient, ξ - dimensionality reduction parameter, L_x, L_y - length and width of the area under consideration respectively (m), H_z - height, Λ - wet deposition coefficient.

t - time, x, y, z - coordinates, u, ϑ, w - components of wind velocity in x, y, z directions respectively, w_g - particle settling velocity, κ - coefficient of turbulent mixing, μ - diffusion coefficient, σ - absorption coefficient, β - coefficient of interaction with the underlying surface, $P(x, y, z, t)$ - emission rate of harmful substances into the atmosphere from stationary sources; $F_0(x, y, z)$ - quantities of salt and aerosol particle emissions from the earth's surface; θ_b - concentration of suspended matter entering through the boundaries of the problem domain.

A coupled model (1) - (5) has been developed for the problems of aerosol particle dispersion in the atmosphere, taking into account sources of harmful emissions in the atmosphere and addressing soil erosion.

a. $\kappa = const,\ u, v, w\ \text{-}\ const;$

b. $$\kappa = \begin{cases} v + \kappa_1 \dfrac{z}{z_1}, & z \le h, \\ v + \kappa_1 \dfrac{h}{z_1}, & z > h, \end{cases}$$

c. $\kappa = \kappa(z),\ v = v(z),\ w = w(z),\ \ v = |v| z^n;$

where h - ground layer height, ν - turbulent viscosity.

3. Results and Discussion

Within the framework of the developed model and corresponding algorithms, a set of software solutions has been created that enables the calculation of a functional for determining the optimal placement of new industrial facilities with minimal environmental pollution. This study incorporated numerical calculations that took into account factors such as wind speed at ground level, soil moisture, surface roughness coefficient, and other physical and mechanical soil parameters.

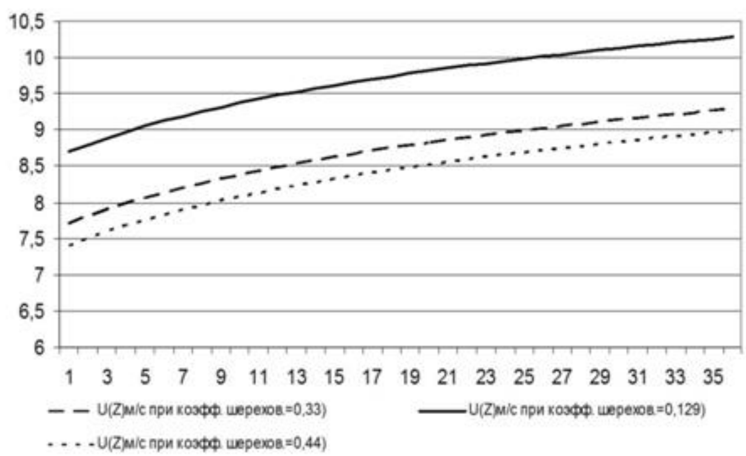

Figure 1. This graph shows the change in horizontal wind speed in various atmospheric layers

depending on the roughness coefficient.

According to the curves in Figure 1, as the ground roughness coefficient increases, the horizontal component of wind speed decreases proportionally. This is especially noticeable when the higher the roughness coefficient, the greater the influence this factor has on wind speed.

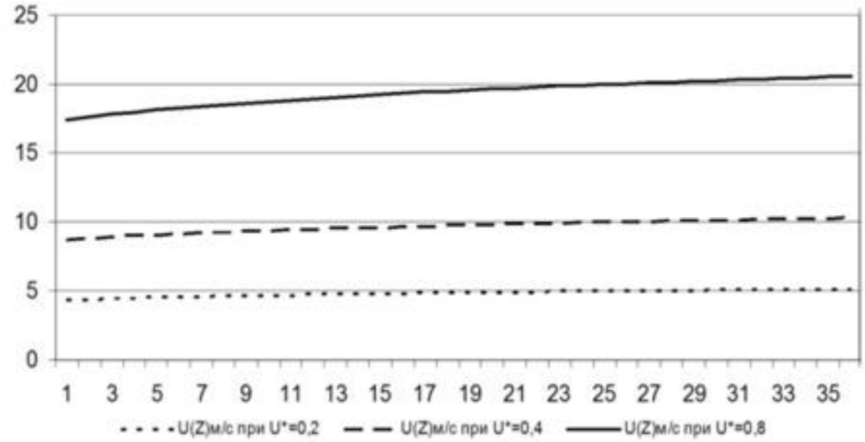

Figure 2. The graph shows changes in wind speed with height as a function of friction velocity.

Figure 4 shows that the vertical wind speed directly depends on the dynamic friction velocity. An increase in the dynamic friction velocity leads to a proportional increase in the vertical wind speed near the surface, and after a certain height threshold, it remains constant.

In this study, unlike the work of G.I. Marchuk, a three-dimensional formulation of the problem of harmful aerosol particle dispersion in the atmosphere is considered, taking into account the inflow and outflow of substances through the boundaries of the examined area. Industrial facilities act as sources of harmful emissions, and under unstable wind stratification conditions of the underlying earth surface, an additional source of harmful emissions also arises due to soil erosion.

4. Conclusion.

An integrated mathematical model of the research subject was developed to observe and predict ecological conditions in atmospheric basins of industrial areas, as well as to optimally locate production facilities. The primary factor of atmospheric pollution in the analyzed region, associated with soil erosion, is described by a differential equation. Solving this equation allows for determining the volume of harmful substance emissions depending on weather and climatic conditions. To ensure compliance with sanitary standards in specific zones of the region, an optimization problem is formulated. The solution to this problem enables precise determination of pollution source coordinates based on their emission capacity and weather and climatic conditions.

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