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A Mathematical Model for the Study and Forecast of the Concentration of Harmful Substances in the Atmosphere

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Abstract This article contains a brief overview of the problem of studying and forecasting the diffusion of harmful substances in the atmosphere. Authors developed a mathematical model that takes into several parameters of the process and also weather and climate factors. Numerical experiments were conducted based on the given model. The obtained results presented here show the main factors, such as wind speed, soil moisture, soil composition significantly affect the diffusion of harmful substances in the atmosphere.

Keywords: *mathematical model, numerical algorithm, harmful substances, wind speed, humidity, weather and climate factor, soil erosion, resistance force, destruction force, concentration*

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1. Introduction

In recent years, intensive human activities unconcerned about possibilities of nature and laws of its sustainable development have led to the necessity of solving such an acute problem as the protection and preservation of the environment, water resources and Earth's interior from technogenic factors and human impact.

It should be noted that currently there are threats in environmental safety arising everywhere. There is the particular problem of contamination of certain territories by harmful substances released from industrial facilities into the environment (atmosphere) in form of carbon dioxide emissions, harmful particles and ionic compounds. These findings follow from statistical data manipulation related to the state of the environment in recent years, which testify intensive growth of emissions into the atmosphere as a result of increasing production capacity and transportation systems.

In this regard, the problems of aerosol emissions diffusion, analysis, monitoring and forecasting of sanitary norms of considered industrial regions and the optimal placement of newly designed facilities which are being studied are clearly relevant both in global and regional scale.

Another important aspect of the problem is an emission of harmful particles from the soil surface caused by movement of air masses. This problem is particularly relevant for the Aral Sea region. Intensive decrease of the Aral Sea has led to exposure of 30000 km^2 of its bottom made up mostly of salt marshes and saline soils. The salt removal from the dried bottom of the Aral Sea, the determination of its quantity, qualitative composition and pathways are the most important and least enlightened questions in the Aral Sea problem. Their importance is due to strong influence of the salt removal on the environment, soil-reclamation and crop yield over irrigated areas. Increased turbidity of the atmosphere over the region has an effect on long-wave radiation which increases the greenhouse effect.

An air pollution largely depends on conditions which can cause high impurity concentration in the surface layer of the atmosphere. These conditions include humidity, pressure, atmospheric temperature, wind speed and direction, etc. which are changing during the day and seasons. They can be taken into account directly as an information support for the mathematical tool of considered process which is being developed on the basis of new information technologies.

The problems mentioned above have been studied closely by many researchers: D.L. Laikhtman, V.V. Penenko, A.E. Aloyan, V.K. Danchenko, T.C. Ivlev, R.F. Lavrynenko, G.I. Marchuk, V.P. Dymnikov, O.M. Belotserkovniy, A.M. Oparin, N.E. Naats and others who have contributed to the development of these areas. There were obtained significant theoretical and practical results and worked out recommendations in the field of diffusion of harmful substances in the atmosphere.

Some important results on numerical modeling of turbulence and diffusion of impurities in the atmospheric surface layer were shown by D.L. Laikhtman in [1]. In V.V. Penenko's work [2] were described some aspects of the modeling methodology, notably variational principles and methods of optimization for sharing numerical models and monitoring data. Significant achievements in the field of mathematical modeling of atmospheric processes are contained in papers of A.E. Aloyan and his followers [3]. In particular, the authors consider a mathematical model of transport of multicomponent impurity taking into account the photochemical transformation and formation of aerosols in the troposphere of the northern hemisphere with the kinetic processes of nucleation, condensation and coagulation.

Another important issue is the identification of aerosols of different origin. The main approaches to solving this problem, and research results were set forth by V.K. Danchenko and T.C. Ivlev [4]. R.F. Lavrynenko's paper [5] is devoted to the formation of the chemical composition of precipitation. It holds a generalization of observations of the chemical composition of precipitation and cloud water, quantitative characteristics of changes in composition in a space and in a time domain.

G.I. Marchuk and his followers [6] have created an entire methodology of mathematical modeling. They studied its fundamental issues and developed original design approaches to study atmospheric and oceanic circulation, as well as to the solution of the problems of weather forecast, theory of climate and environmental protection.

V.P. Dymnikov and his followers have done their work devoted to mathematical modeling of climate theory. For instance, in [7] were discussed several nonlinear problems of atmospheric physics, which were solved using the Green's function. The paper considers equation sets describing large-scale dynamics of atmospheric processes.

Further development of numerical modeling of atmospheric turbulence and diffusion was reflected in [8] by O.M. Belotserkovniy, A.M. Oparin et al. In particular, in [9] were analyzed fundamental concepts and techniques which are needed to study turbulence. Direct numerical modeling of fully developed turbulence is conducted using new numerical methods, along with this were obtained the main qualitative characteristics of the structure of turbulence in different movement modes: coherent structures, laminar-turbulent flow, transition to chaos. The problem of turbulence and convection was considered in the monograph using numerical experiment.

Also, a long series of papers by N.E. Naats and his colleagues [10-14] deal with mathematical modeling of pollutant transportation concerning the issue of ecological monitoring.

Thus, we can assume that a comprehensive study of spread of harmful substances into the environment using mathematical models and computational experiments in order to identify the conditions of the most accurate description of studied processes requires further development.

Considering the above-mentioned, we have developed the information provision and mathematical model to conduct computational experiments for analysis and prediction of sanitary standards when the spread of harmful substances is taking place as well as for optimal placement of the newly designed industrial facilities.

While conducting computational experiments using this mathematical tool it is possible to determine main factors affecting the ecological status of industrial regions, as well as the optimal placement of the newly designed facilities, depending on climatic factors and the orography of the terrain. In turn, this will improve the air quality in considered region and, as a consequence, whole ecological state of the region, creating more favorable conditions for humans and wildlife.

2. Methods

Statistical data manipulation on the influence of different weather climatic conditions on particles loss from the surface of the earth shows that the basic factor causing soil erosion is the velocity of the incident air flow, and the main factor - soil moisture. Other parameters are playing their certain role in increasing or prevention of erosion, but their influence is ambiguous. That is why while mathematical modeling of diffusion of harmful particles and their concentration changing over the time, it is necessary to consider these parameters, yet the physico-chemical properties of the soil can be considered constant in the calculation formula.

The wind speed and the soil moisture influence on the propagation of harmful particles in the atmosphere and soil erosion in different ways. If there is increasing of wind speed then there is intensity of erosion process, on the other hand the soil moisture boost inhibits the erosion process.

General dependence can be written as:

$$\theta = f(u, w), \tag{1}$$

Here θ - volumetric flow rate of particles entrained by atmospheric front, m^3/s.

To determine type of function (1) let us turn to the analysis of the forces, causing the destruction of soil and resisting this destruction. The destructive forces will be denoted by F. They are always opposed to resistance forces R, which include humidity and other physical and mechanical properties of soil.

If F force overtops R force, the soil eolation process begins. The destruction force is mainly determined by the shear stress of incident flow. The greater number of solid particles in flow, the greater total shearing stress destroying soil. To obtain theoretical dependence we consider an equilibrium process. While dynamic equilibrium the F and R forces' difference must be equal to zero, i.e.,

$$F - R = 0. \tag{2}$$

Let us form the expression for these forces. The relationship between volumetric flow of entrained particles θ and the flow rate can be expressed as:

$$F = \frac{\partial \theta}{\partial u} \cdot \chi, \tag{3}$$

where χ - shear stress, kg/m^2.

For the resisting force R, by analogy with F we take expression

$$R = c_0 \frac{\mu}{l} \frac{\partial \theta}{\partial w} \tag{4}$$

where μ - viscosity of a mixture (air + soil), $kg{*}c/m^2$; l - the distance between individual particles, m; c_0 - the constant of soil.

Substituting (3) and (4) in (2) we have

$$\frac{\partial\theta}{\partial u} - c_0\frac{\mu}{l\chi}\frac{\partial\theta}{\partial w} = 0 \quad (5)$$

Let us consider the separate expression $c_0\mu/(l\chi)$ in equation (5).

If we approximately assume that the shear stress is determined by the external speed u_∞, i.e. $\chi = u_\infty$, then the above expression in equation (5) can be written as

$$c_0\mu/(l\chi) = c_0\mu/(lu_\infty) \quad (6)$$

In (6) the viscosity of the mixture μ is still being dinamic variable, and apart from physical and mechanical properties of soil, is mainly determined by moisture of soil, which provides increasing in cohesive forces between individual particles.

Upon this, the expression (6) can be assumed as dependent on humidity function, i.e.

$$c_0\mu/(lu_\infty) \cong c_0' f(w) \quad (7)$$

Next, the function $f(w)$ will be replaced by a simple dependence

$$f(w) \cong c_0 c_0' w \quad (8)$$

Finally, dependence (8) takes following form

$$c_0\mu/(lu_\infty) \cong c_0 f(w) \cong \cong c_0 c_0' w = k_p w. \quad (9)$$

where k_p – constant of soil, s/m.

Returning to expression (5), we'll have

$$\frac{\partial\theta}{\partial u} - k_p w\frac{\partial\theta}{\partial w} = 0. \quad (10)$$

Thus, for considered problem we have the first-order partial differential equation. Integration of this equation gives us two arbitrary constants (C_1, C_2). Taking into account the constants of soil « k_p », we have to define three constants C_1, C_2, k_p. Therefore, the boundary conditions must be defined for three values of θ. In order to use fewer arguments we accept following boundary conditions:

$$\left.\begin{aligned} \theta = \theta_1: &\quad w = w_1, \quad u = u_1; \\ \theta = \theta_2: &\quad w = w_2, \quad u = u_2; \\ \theta = \theta_3: &\quad w = w_3, \quad u = u_3. \end{aligned}\right\} \quad (11)$$

Thereby, the solution of (11) was obtained as

$$\theta = c_1 w^{c_2/k_p} e^{c_2 u}. \quad (12)$$

Wherein, k_p – is a negative value.

Formula (12) is valid for the $u > 0$ case. According to boundary conditions (11), following expressions were obtained for constants:

$$c_2 = \ln(\theta_1/\theta_2)/(u_1 - u_2), \quad (13)$$

$$k_p = c_2 \ln(w_1/w_2)/\ln(\theta_2/\theta_3), \quad (14)$$

$$c_1 = \theta_1 w^{-c_2/k_p} e^{-c_2 u}. \quad (15)$$

3. Results

To compare theoretically obtained dependence (12) with real experiments, there were calculated coefficients C_1, C_2, k_p for particular soil types according to K. Mirzazhanov [15].

For example, for meadow - alluvial soil type there were obtained: $C_1 = 1,29$, $C_2 = 0,745$, $k_p = -0,515$.

θ values differ from experimental values in range of 10-15%, which can be explained by experimental errors.

Thus, in terms of formulas (13)-(15) according to experimental data we can calculate values C_1, C_2, k_p for different types of soil. Changing of intensity of particles entrainment θ depending on the flow speed u with different levels of soil moisture w is shown in Figure 1-Figure 2.

Changing of intensity of particles entrainment depending on the composition of the soil is shown in Figure 3-4.

In all cases the value of wind speed was assumed as constant – 5 m/s. This is the average value of wind speed in the Aral Sea region.

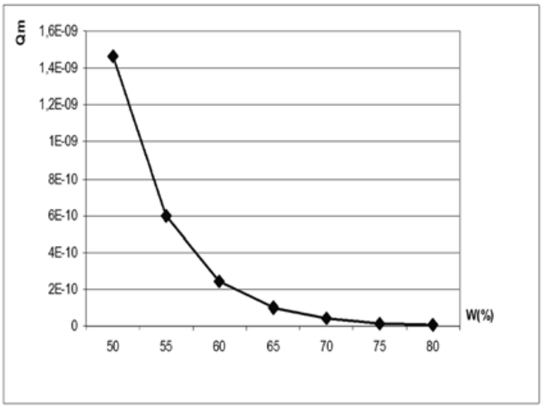

Figure 1. Changing of intensity of particles entrainment θ depending on levels of soil moisture w

As can be seen from Figure 1, the intensity of particles entrainment from the soil surface smoothly decreases with increasing of soil moisture.

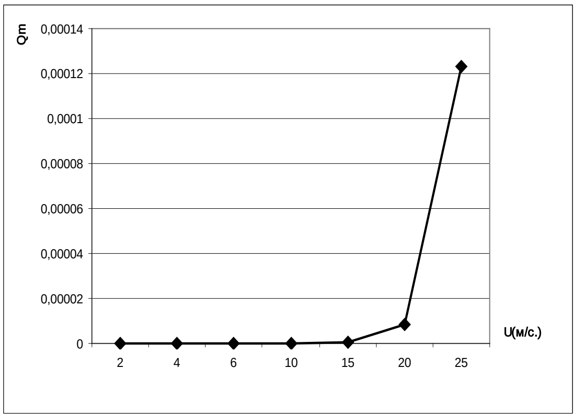

Figure 2. Changing of intensity of particles entrainment θ depending on the flow speed u

Figure 2 shows that when the the air flow reaches critical speed threshold the intensity of particles entrainment dramatically increases. This is due to the fact that the laminar flow turns into turbulent.

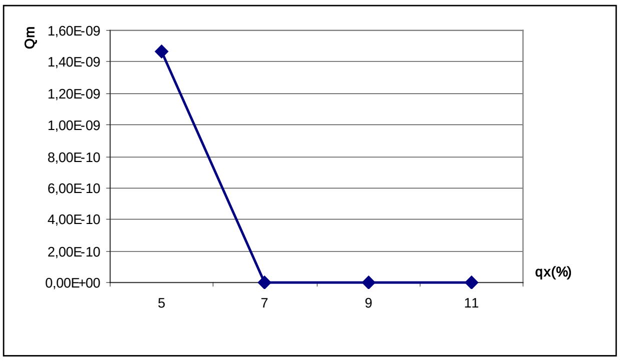

Figure 3. Changing of intensity of particles entrainment depending on the chlorine content in soil

Figure 3 shows that intensity of particles entrainment decreases if chlorine amount in the soil is high. The reason is that chlorine particles have a high degree of adhesion.

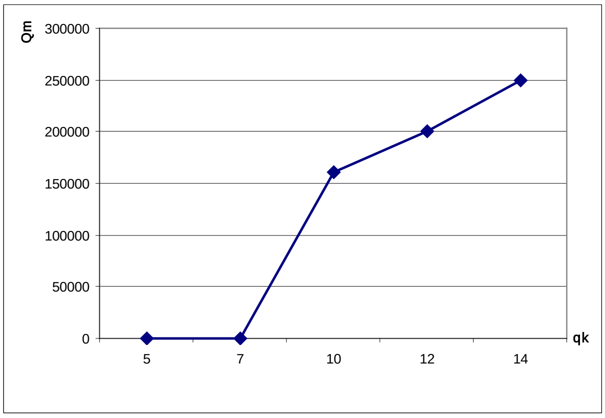

Figure 4. Changing of intensity of particles entrainment depending on the soda carbonate content in soil

If there is high content of sodium carbonate in the soil (Figure 4) the intensity of particles entrainment increases because these particles have less adhesiveness.

Considered model was used in experiments for the forecast of of the concentration of salt and dust particles raised from the dried bottom of the Aral Sea up to the atmosphere [16,17,18]. While conducting those experiments we also took into account the coefficient of interaction with underlying surface. We considered the summer season, characterized by intensity and strength of winds blowing in a southerly direction. The analysis of obtained results indicates that the distribution of salt and dust particles from the dried areas differently depends on characteristics of the underlying surface. However, the establishment of artificial barriers helps to reduce wind strength and prevents transfer of large particles to the nearest areas. With regard to lightweight aerosols, because of the turbulent air flow they raise up and move along the wind direction. Though, the green spaces help to absorb much of laid-down lightweight aerosols afterwards. In this regard, in order to prevent the processes of desertification and deflation of salt and dust particles from the dried bottom of the Aral Sea and from the deltas of the Amu Darya and Syr Darya, there was proposed a scheme to establish the green protective belt in the Southern Aral Sea area.

4. Discussion

As K. Mirzazhanov's experiments were conducted in area of laminar boundary layer of wind tunnel (in the initial section), then calculated coefficients inserted in (12) give θ values only for entrainment within the laminar boundary layer. To use the formula (12) in area of turbulent boundary layer, experiments should be conducted in the wind tunnel in area of turbulent boundary layer and then the constants C_1, C_2, k_p should be determined.

As it follows from the numerical calculations, the most important parameters that influence the process of soil erosion and the state of harmful substances concentration in the atmosphere - are the speed of air mass in the atmospheric boundary layer, soil moisture, soil composition and also the coefficient of harmful substances absorption in the atmosphere, which varies daily and by seasons.

The developed mathematical model allows us to study and forecast the concentration of harmful substances entrained from the soil surface into the atmosphere. Therefore, it could be recommended for monitoring, forecasting and for environmental planning in order to economic rehabilitation of the Aral Sea region or any similar regions.

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