Modeling the salt-dust aerosols distribution in the atmosphere, taking into account the soil erosion

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Abstract. In the general case, when modelling the process of air pollution dispersion, it is necessary to take into account factors associated with the interaction of air mass with the underlying earth surface or wind erosion. The main purpose of this work is to study the factors affecting the amount of particulates carried upward from the soil into the air due to wind erosion. The study of this aspect is very relevant for the analysis of environmental situation in the Aral region of Uzbekistan. The major share of harmful substances emission in Aral Sea region is undertaken by dust, salts and toxic chemicals blown up from dried bottom of the Aral Sea. Thus, in mathematical modelling of atmospheric dispersion process, it is necessary to take into account the physic and mechanical properties of the particles and basic forces acting on them. In the paper there are presented certain numerical calculations for studying the process of soil erosion depending on the air mass velocity of the atmosphere, the size and density of particles, and the acting forces. The basic forces that play a significant role in the process of soil erosion were determined by carried numerical calculations.

1. Introduction

The issues of developing mathematical models, effective computational algorithms and software tools designed to address environmental problems are as significant and relevant today as ever. Considerable scientific interest is associated with the problems of monitoring and forecasting the atmospheric dispersion of polluting emissions.

The processes of transfer and diffusion of anthropogenic or natural pollutants are quite complex, and they are influenced by many factors. The sufficient adequate description of these processes claims to take into account various parameters in formulating the models, such as: air mass movement velocity, atmospheric turbulence, meteorological variability, topographical features, physical and mechanical properties of harmful particulates, deposition of pollutant particles, absorptive capacity of the environment etc.

It is for that reason the atmospheric dispersion of pollutants is usually described by partial differential equations with the corresponding initial and boundary conditions so-called convection (advection)-diffusion equations. These equations can be expressed in a finite difference form, which paves the way to a wide variety of numerical solutions [1].
There are numerous works on this scientific direction have been published over recent years. These researches focused on various aspects of modelling the atmospheric dispersion process. For example, the dimensionality of solving problems, experiments with difference schemes, the order of approximation, a degree of influence of individual parameters or phenomena (wind profiles, turbulence, dry and wet deposition, chemical transformations, wind erosion, source properties, etc.) over the distribution of contaminants concentration in the atmosphere and on the underlying surface.

Indeed, in a study of Moreira and Albuquerque [2] was obtained a semi-analytical solution of the two-dimensional advection-diffusion equation taking into account the longitudinal wind speed as a function of the distance from emitter and the vertical height relative to the plume. The model proposed by the authors also takes into account the transformation of pollutants and the process of removing contaminants due to chemical reactions and dry deposition. The main purpose of the model was to study the dispersion of air pollutants in urban conditions in the presence of cumulative effect of large-scale and mesoscale winds. The results obtained by the authors showed that the movement of air mass that occurs under the influence of urban heat-generating zones advects pollutants upward, which increases the intensity of air pollution in urban areas.

Elperin with his colleagues proposed a two-dimensional model of adsorption of atmospheric trace gases by aerosol particles of pollutants emitted from an industrial source [3]. The model developed by the authors is based on a joint application of the theory of turbulent diffusion in the atmospheric boundary layer, the Gaussian plume model and the model of gas adsorption by porous solid particles. The final model allows to analyse the spatio-temporal evolution of the concentration of adsorbate in the gas phase and in solid particles. The computational experiments carried out by the authors for various meteorological conditions and atmospheric stability classes showed good convergence of obtained results with the available experimental data.

Sullivan and Ajwa in their study [4] focused on modelling the processes of pollutants transfer from contaminated surfaces into the atmosphere as a result of wind erosion, and subsequent deposition of harmful particles in remote areas. The authors' study was aimed at long-term forecasting of the negative impact associated with the movement of harmful substances from contaminated areas to residential areas. The authors compared several empirical models of wind erosion. Thus, the importance of using empirical models was shown not only for assessing the erosive ability of earth soils, but also for determining the spatio-temporal evolution of the concentration of contaminants.

Overall, the analysis of published scientific literature showed an increasing interest in modelling the process of transport and diffusion of harmful substances in the atmosphere, when the drained parts of the seas, degraded agricultural lands, overburden dumps and other surface areas are treated as harmful emission sources.

This is a very topical issue in the case of the Aral region of Uzbekistan, which territory is vulnerable to impact of wind regime. As a result a large amount of dust, salts and toxic chemicals are emitted annually from the surface of the exposed bottom of the Aral Sea into the atmosphere and then are transported by air mass over long distances [5].

Therefore, unlike our previous works [6, 7, 8], where the issues of developing models and numerical algorithms for forecasting the distribution of air pollutants emitted by industrial facilities were considered, the main purpose of this work is to study the factors affecting the amount of particulates carried upward from the soil into the air due to wind erosion.

2. Problem statement
In order to study the factors that significantly affect the process of air pollution as well as the soil erosion, let us consider the mathematical model which is described by the complete hydromechanics equation:
\[
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} + \left(w - w_g\right) \frac{\partial \theta}{\partial z} + \sigma \cdot \theta = \\
= \mu \cdot \Delta \theta + \frac{\partial}{\partial z} \left(k \cdot \frac{\partial \theta}{\partial z}\right) + Q \cdot \delta(x, y, z);
\]

\[
\theta(x, y, z, 0) = \theta(x, y, z);
\]

\[
-\mu \left. \frac{\partial \theta}{\partial x} \right|_{x=0} = \gamma(\theta - \theta_a) ; \quad \mu \left. \frac{\partial \theta}{\partial x} \right|_{x=L_s} = \gamma(\theta - \theta_a) ;
\]

\[
-\mu \left. \frac{\partial \theta}{\partial y} \right|_{y=0} = \gamma(\theta - \theta_a) ; \quad \mu \left. \frac{\partial \theta}{\partial y} \right|_{y=L_s} = \gamma(\theta - \theta_a) ;
\]

\[
-k \left. \frac{\partial \theta}{\partial z} \right| = \gamma(\beta \cdot \theta - F_0), \quad z = 0 ;
\]

\[
k \left. \frac{\partial \theta}{\partial z} \right| = \gamma(\theta - \theta_a), \quad z = H.
\]

The variables and parameters of this model were given in detail in the papers [6, 7, 8]. When \( h_z = 0 \) we have an elevated source at the level \( z = h_z \) \((F_0 = 0)\) and at ground sources \( F_0 \neq 0 \) \((Q = 0)\).

3. Solution method

Let us consider problem (1) - (6) in area \( D = (0 < x < a, 0 < y < b, 0 < z < H) \), when the source is located on the surface layer.

The value \( F_0 \) is a function of \( x, y, z, t \) and should be determined from experimental data depending on meteorological conditions, properties of the underlying surface, size and density of dust particles.

Due to the linearity of equation (5), the source strength can be normalized so that the maximum value of \( F_0 \) corresponds to unity. Then, multiplying by the normalizing factor, we obtain the sought for impurity concentrations. Accordingly, the turbulence coefficient also depends on meteorological conditions [7]. From the statement of problem (1) - (6), it is seen that to calculate the volume of particles entrained from the soil surface due to erosion, it is necessary to determine the vortex lifting force \( F_l \), which depends on several factors: the lift coefficient, the radius of soil particles, air density, and flow velocity outside the boundary layer.

According to Zhukovsky [9] the determination of lifting force and lift coefficient is based on the experimental determination of the critical flow velocity and can be determined if the vertical rise of particles corresponds to the critical velocity. When a finely dispersed particle is in a state of unstable equilibrium or protrudes above an overall surface, it does not rise vertically, but begins to move horizontally, and the reason for its motion is frontal pressure, not a lifting force.

In view of the foregoing and assuming that the particles differ only in size, we use the equation of the balance of forces in projections on the vertical axis at the time of flow separation \( U = U_k \) and we obtain:

\[
F_l = mg + F_c.
\]

Here, \( F_l, F_c \) are the frontal and cohesive forces of particles, respectively, \( m \) is the mass of particles, \( g \) is the force of gravity.
Further, assuming that the particles have the shape of a sphere with radius \( r \) and density \( \rho_p \), we obtain:
\[
k_p \pi r^2 \rho_p U_k = \frac{4}{3} \pi r^3 (\rho_p - \rho_a) g - k_f \mu_a \pi r w_h + F_c.
\]

For a more detailed study of the key parameters that significantly affect the vertical motion of aerosol particles in the atmosphere, introduce the following notation:
\[
k_p = k_1; \quad x = \pi r^2 \rho_a U_k^2; \quad y = \frac{4}{3} \pi r^3 (\rho_p - \rho_a) g; \quad b = F_c.
\]

Based on the materials of experimental data on multi-fractional soils in a wind tunnel and on literature sources [10, 11], the following equation was compiled
\[
y = kx - b,
\]
which is solved by the least squares method. Numerical calculations showed that there is a close relationship between the parameters \( y \) and \( x \). The value of the lift coefficient \( k \) varies in the range from 0.03 to 0.18. As it is seen from the analysis and generalization of numerical calculations, experimental data and the results of other authors, it is possible to obtain the value of the lift coefficient 0.12 for a wide range of particle sizes (from 0.01 to 3 mm) and densities (from 1400 to 11350 kg/m\(^3\)). Then, this coefficient can be used to model the process of transport and diffusion of aerosol particles in the atmosphere, considering soil erosion; for example, for predicting and monitoring the ecological state of the Aral Sea region.

In most cases, the particles have a spherical shape, so the frontal drag force and lifting force can be calculated as:
\[
F_f = 0.0078 \pi r^2 \rho_a U^2;
\]
\[
F_l = 0.12 \pi r^2 \rho_a U^2.
\]

From equations (10) and (11) it follows that at \( U \) equal to critical velocity, the motion of particles begins precisely under the action of a lifting force, which is an order of magnitude greater than the frontal drag force.

4. Results
Numerical calculations were performed for various densities (from 1400 kg/m\(^3\) to 1135 kg/m\(^3\)) and particle sizes. The results of calculations showed that with increasing particle density, the cohesion force increases linearly.

Figure 1. Change in cohesion force of particles \( F_c \) depending on atmospheric air mass velocity.
As can be seen from figure 1, one of the key factors that impacts the change in cohesion force of particles is the atmospheric air mass velocity.

As the atmospheric air mass velocity increases, the cohesive force of particles increases exponentially. Numerical calculations showed that this growth is especially noticeable at $U>4$ m/s. Similarly, the frontal drag force increases with increasing velocity of the atmospheric air mass velocity (figure 1).

It was noted in Zhukovsky’s studies, to construct the wind erosion theory, not only the separation force that tears the soil particle off the surface is important, but the force that transports it through the air [9].

The curves in Figure 2 show that the lifting force and the drag force of the particles increase depending on the growth of atmospheric air mass velocity. An exponential increase in the particle lifting force is especially noticeable when the wind velocity $U_k$ exceeds the critical values.

![Figure 2. Change in lifting force and frontal drag force of particles depending on the atmospheric air mass velocity: a – lifting force $F_l$, b – frontal drag force $F_f$, particle radius $r=0.01$ mm, $\rho_p=1.2754$.](image)

Figure 3 shows the changes in the lifting force and the drag force of the particles depending on their radius. As follows from numerical calculations and the curves in Figure 3, with increasing diameter of the particles, their lifting force exponentially increases, and the frontal drag force increases imperceptibly with increasing particle diameter. Numerical calculations show that one of the main parameters that affect the drag force is an atmospheric density. With an increase in the atmospheric density, the drag force of particles increases linearly, while it does not affect the change in the lifting force of particles.

![Figure 3. Change in lifting force and frontal drag force of particles depending on their radius: (a – lifting force $F_l$, b – frontal drag force $F_f$, $\rho_a=1.2754$).](image)
The numerical calculations (figures 1 - 3) and a comparison of the obtained values of equations (10) and (11) allow us to state that upon reaching the critical values of flow velocity and the levelled surface, the particle motion begins precisely under the action of the lifting force, since it approximately an order of magnitude greater than the frontal drag force. Numerical calculations showed that in the case of fine aerosol particles constrained by similar ones on all sides, the critical wind velocity is the only way to start the vertical motion of particles.

From the analysis of numerical experiments [12], we can conclude that for the process of saltation and particle elevation from the surface, the vortex lifting force is required that is calculated by equation (11).

5. Conclusion
Numerical calculations showed that the vortex lift coefficient is constant, and it does not depend on the shape of particles and their density.

The analysis of numerical calculations showed that the main driving force of wind erosion is the vortex lifting force, which is an order of magnitude greater than the shear stress.

From the analysis of calculation results, it follows that the atmospheric density does not play significant role in changing the lifting force. It grows exponentially depending on changes in atmospheric air mass velocity.

Thus, based on the results of this study and developed mathematical software, it is possible to determine the amount of salt and dust particles emitted from the dried parts of the Aral Sea due to soil erosion caused by critical increase in wind velocity near the Earth's surface.

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