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Mathematical Modeling and Computational Experiment of the Process the Atmospheric Transport of Salt-Dust Aerosols from the Aral Sea Basin

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***Abstract*— Atmospheric transport of salt-dust aerosols is a sophisticated effect mainly depending on the meteorological situation. Since the dried bottom of the Aral Sea is considered as emissions source, precisely the wind removal of aerosol particles is implied here. It should be noted that the wind erosion of the ground cover can be considered as a special case of the hydrodynamics of multiphase flows, which is of particular scientific interest. In this regard, vertical wind profile, which depends on the roughness of the ground cover and the stability of the atmosphere, become to one of essential aspects for outdoor airflow simulations. Thus, the aim of this work is to study the influence of the vertical wind profile on the atmospheric transport of salt-dust aerosols. The results of computational experiments on the airflow characteristics at various heights, values of the ground-level wind speed and the roughness coefficient are presented in the paper. As well as the results of numerical calculations demonstrating the influence of the horizontal and vertical components of the wind speed on the distribution of suspended aerosol particles within the considered area.**

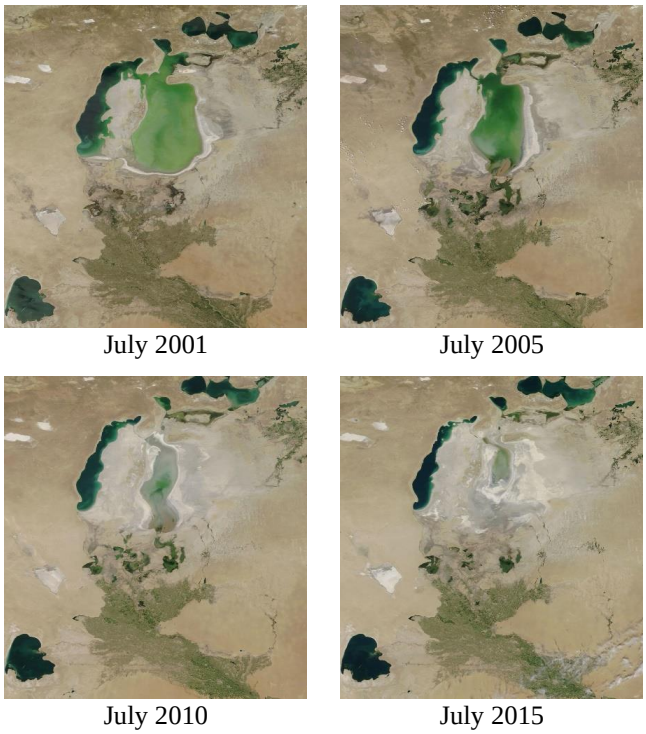
Keywords—air pollution; transport-diffusion equations; wind profile; power law; roughness coefficient; GIS

I. INTRODUCTION

Comprehensive studies of the Aral Sea basin and surrounding areas have long been the subject of interest of hydrologists, soil scientists, ecologists and other specialists. The issue of studying the natural environment of that region in connection with the ecological disaster that began more than 50 years ago is of particular attention for many researchers.

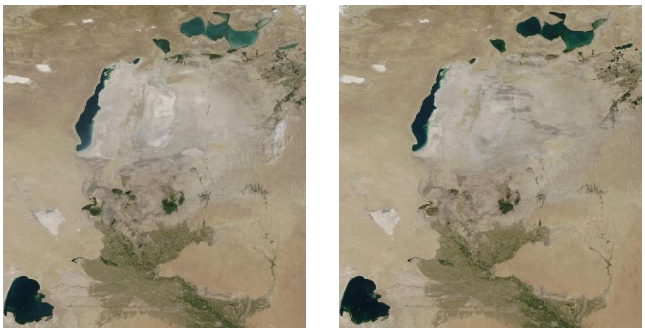
As a result of cooperation between Uzbek and foreign specialists over the past two decades there have been implemented many research projects in the Aral Sea region [1]. Nowdays, based on the analysis of these studies, it is possible to make well-founded generalizations and conclusions on the characteristics of the natural complex of that region influenced by drained bottom of Aral Sea. At the same time, of course, it is not possible to predict all the possible consequences of ongoing environmental processes in the long term.

One of main consequences of the shallowing of the Aral Sea was a formation of Aralkum - colossal salt desert at the junction of three sandy deserts. The Aralkum now extends over an area of almost 5 million hectares (Fig. 1).



July 2001 July 2005

July 2010 July 2015



July 2020 July 2021

Fig. 1. Changes in the water area of the Aral Sea captured by MODIS (2001-2021 years).

The drained bottom of the Aral is a vivid example of arid salt accumulation. Continuous salinization is also facilitated by the evaporation of highly mineralized groundwater lying close to the earth surface (Fig. 2). The Aralkum soils mineralization varies from 5 to 20 kg/m^3, therefore there is practically no vegetation, the soil cover is weakly fixed and consequently subject to intense wind erosion.

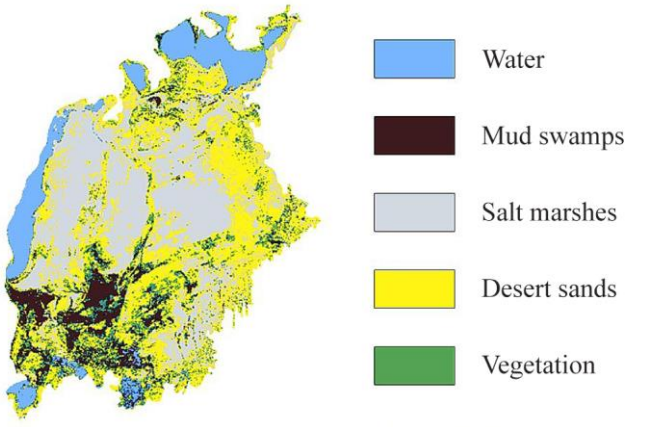


Fig. 2. Thematic map of the former water area of the Aral Sea (2021 y.) [2].

A review of thematic publications shows that atmospheric transport of salt-dust aerosols in the Aral Sea region has not been sufficiently studied to date. In particular, there is no common opinion on the issues of particles removal from the underlying surface, the spatio-temporal evolution of pollutants concentration under dust storms, etc. [3].

The dried bottom of the Aral has become the main source of large dust storms and emissions of salt-dust aerosols in the Aral Sea region. The growing number of dust storms was directly affected by increased temperature difference, which gained the wind speed gradients and the intensity of the convective movement of air mass. A large part of salt and dust particles raised from the dried bottom is often transferred to the irrigated areas and increases the turbidity of the atmosphere in the Aral Sea region. The last one, in turn, affects the long-wave radiation, which enhances the greenhouse effect.

It is well known that the wind speed in the atmospheric boundary layer (ABL) increases with height. Near the ground, air mass always moves slower due to friction resistance varying by terrain roughness types. With distance from the ground surface, the effect of friction decreases and the wind speed grows. The ABL height where the effect of friction is felt can extend up to several thousand meters above the earth's surface. Moreover, various types of underlying surface, such as: desert landscape, agricultural land, forests, hills, buildings, ponds, lead to different vertical wind speed gradients (vertical wind profile) which is always determined for each specific area.

Experimental measurements of vertical wind profiles are performed using aerological radio sounding or lidar scanning [7]. However, such measurements require an appropriate technical infrastructure and in general are advisable only where accurate determination of the wind impact is critical, for example, the construction of high-rise structures, wind power plants, airports, etc. [8].

Therefore, when solving various applied problems associated with atmospheric processes, mathematical methods are usually used to describe the spatial variability of air mass movement. The development of mathematical models of emission, transport and diffusion of air pollutants is usually carried out under known conditions, restrictions and assumptions that do not contradict the physical nature of these processes as well as the fundamental conservation laws. Mathematical models built in view of actual meteorological data and orography of considered area can reproduce the airflow parameters with fairly high accuracy.

Hence, mathematical modeling of air pollutants transport and diffusion in the atmosphere is the subject of interest of numerous researchers who have already achieved significant theoretical and applied results.

Variety of approaches to atmospheric dispersion modeling the process of impurity propagation in the atmosphere is takes plase because the absence of some general physical and mathematical model that takes into account all possible factors and disturbances that affect the studying process. The choice of one or another approach is determined by the specific statement of the problem, the requirements for the accuracy of modeling and the quality of the model overall [4].

In a raw of the most common approaches there are: Gaussian models; Eulerian models, in particular, based on k-theory; Lagrangian models; CFD models based on complete or Reynolds-averaged Navier-Stokes equations [5].

Recently, the models based on artificial intelligence methods have received some development [6]. Such models still have certain disadvantages, however, their benefits include the ability to process inaccurate input data and the ability to adapt to changing environmental conditions.

Because of the fact that atmospheric dispersion is mainly impacted by turbulent mixing in th ABL, the leading approach to modeling is undoubtedly considered to be the semi-empirical theory of turbulent diffusion.

In any case the necessary data set that makes up the information model of atmospheric transport of air pollutants and that is used as input parameters can be conditionally divided the following groups:

- spatial data, including a digital description of terrain elevations and ground cover;
- regional weather and climate characteristics, including: time averaged and actual meteorological data;

- sets of different coefficients: environmental absorption, atmospheric stratification, turbulence, surface roughness, particles deposition rate etc;
- physico-mechanical and chemical properties of pollutants.

The values of these parameters for any considered area can be determined empirically, from appropriate reference books or by certain functional dependencies.

Owing to the development of GIS technologies and web services, the relevant spatial and meteorological data for almost anywhere on the Earth are generally accessible in machine-readable form. And software interfaces and formats for processing are standardized. This allows us to significantly simplify and speed up the automation of data collection and processing to build information models, generate the necessary databases and develop our own software for solving scientific and engineering problems.

In light of the above, the main goal of this work is to study the influence of vertical wind profile on the transport and diffusion of salt-dust aerosol emissions in the atmosphere over Aral Sea region.

II. METHODS

A. Mathematical model

Within the scope of semi-empirical theory of turbulent diffusion in the atmosphere and taking into account such factors as meteorological conditions, sedimentation rate of pollutant particles; interaction of pollutant particles with the land cover surface; mass transfer through the boundaries of the considered area and the absorption capacity of the environment, we propose the following model described by three-dimensional transport and diffusion equation in spherical coordinates:

$$\frac{\partial\theta}{\partial t}+\frac{u}{r\sin\psi}\frac{\partial\theta}{\partial\varphi}+\frac{v}{r}\frac{\partial\theta}{\partial\psi}+w_a\frac{\partial\theta}{\partial r}+\sigma\theta=$$
$$=\mu\left(\frac{1}{r^2\sin^2\psi}\frac{\partial^2\theta}{\partial\varphi^2}+\frac{1}{r^2\sin^2\psi}\frac{\partial}{\partial\psi}\left(\sin\psi\frac{\partial\theta}{\partial\psi}\right)\right)+ \quad (1)$$
$$+\frac{\partial}{\partial r}\left(\kappa\frac{\partial\theta}{\partial r}\right)+\delta Q.$$

with appropriate initial and boundary conditions

$$\theta\big|_{t=0}=\theta^0; \quad (2)$$

$$-\mu\frac{\partial\theta}{\partial\varphi}\bigg|_{\varphi=\varphi_0}=\xi\left(\theta_E-\theta\right);\ \mu\frac{\partial\theta}{\partial\varphi}\bigg|_{\varphi=\varphi_N}=\xi\left(\theta_E-\theta\right); \quad (3)$$

$$-\mu\frac{\partial\theta}{\partial\psi}\bigg|_{\psi=\psi_0}=\xi\left(\theta_E-\theta\right);\ \mu\frac{\partial\theta}{\partial\psi}\bigg|_{\psi=\psi_M}=\xi\left(\theta_E-\theta\right); \quad (4)$$

$$-\kappa\frac{\partial\theta}{\partial r}\bigg|_{r=r_0}=\left(\beta\theta-f_0\right);\ \kappa\frac{\partial\theta}{\partial r}\bigg|_{r=r_L}=\xi\left(\theta_E-\theta\right). \quad (5)$$

Here $\theta(r,\psi,\varphi,t)$ – concentration of air pollutant (kg/m^3); θ^0 – initial concentration; θ_E – concentration coming through the boundaries of the considered area; ξ – coefficient of mass transfer through the boundaries; r, ψ, φ – spherical coordinates; M, N, L – area dimensions (m); t – time (h); u, v, w – the components of wind speed (m/s); $w_a=\left(w-w_g\right)$; w_g – sedimentation rate of pollution particles (m/s); σ – air mass absorption capacity (1/s); μ, κ – respectively horizontal and vertical turbulence coefficients (m^2/s); δ – Dirac delta function; Q – emission rate (kg/m^{3}s); f_0 – volume flow rate of aerosol particles from ground surface (m^3/s); β – coefficient of interaction between aerosol particles and underlying surface.

The solution of the problem (1)-(5) is traditionally found in two stages: spatial discretization and temporal integration. At the first stage we perform parametrization of the ABL. This requires availability of initial meteorological and spatial data, as well as closure relations for the unknown terms of equation (1).

At the second stage, we find a numerical solution of the problem using finite-difference approximation and time fractional steps methods. In order to use the finite-difference method to approximate the problem solution, we first discretize the problem's domain by dividing it into the following grid:

$$\Omega_{r\psi\varphi t}=\Big\{\left(\varphi_i=i\Delta\varphi,\ \psi_j=j\Delta\psi,\ r_k=k\Delta r,\ t_n=n\ \Delta t\right);$$
$$i=\overline{0,N};\ j=\overline{0,M};\ k=\overline{0,L};\ n=\overline{0,N_t};\ \Delta t=\frac{T}{N_t}\Big\}.$$

In order to obtain a difference analogue of (1)-(5) we apply appropriate implicit difference scheme with second order of accuracy. Next we reduce obtained equations to systems of linear equations matrices of which have three diagonal dominance and which are solved by Thomas algorithm. Finally, the resulting solution $\theta^*(r,\psi,\varphi,t)$ within domain Ω is integrated over the desired time interval $[0,T]$.

B. Describtion of vertical profile of wind speed

As it was mentioned above, the description of the vertical profile of the wind speed is of great importance when it comes to solving the problem of atmospheric dispersion of air pollutants. There are number of mathematical methods was already developed for calculating wind speed profiles [1, 4, 10-12]. Nevertheless, this issue is still relevant, and scientific research in this direction continues.

In most countries, as well as in the CIS countries, approximations by power-law and logarithmic functions are most widespread [9]. For the power law function the solution of the transport-diffusion equations can be obtained in an analytical form, and for the log law the solution can be obtained only by numerical method. The log law is more accurate at low altitudes up to 100 m. At altitudes from 100 m to the upper boundary of the atmospheric boundary layer, the power law is more accurately fulfilled (for neutral stability) [10].

Since we interested in heights of up to the upper boundary of the ABL, in this work, the power-law dependence was used to study the effect of the roughness coefficient of the underlying surface on the vertical wind profile.

Here, we describe the vertical wind profile by the following expressions:

$$u(r,t)=|\upsilon|\left(\frac{r}{r_1}\right)^k\cos\lambda,\ \ v(r,t)=|\upsilon|\left(\frac{r}{r_1}\right)^k\sin\lambda, \qquad (6)$$

where $u(r,t)$, $v(r,t)$ – zonal and meridional components of wind speed at the height r; $|\upsilon|$ – modulus of known wind speed at reference height r_1; λ – deflection angle; k – dimensionless coefficient that depends on atmospheric stability and roughness class of ground surface. The vertical wind speed is assumed to be negligibly small.

The formulas (6) are quite obvious except for the exponent k. In the regulatory documents of most EU countries, it approximately equals to 1/7 or 0.143. In the USA, for different localities, the value k is taken equal 0.23 ± 0.03. In the CIS countries for the flat part of the territories is recommended $k=0.2$ [11].

The k is often taken constant in calculations for certain territory. However, using the standard value e.g. $1/7$ for a fairly wide area can give very erroneous estimates. For example, even under the condition of indifferent stratification, over an open surface of water bodies, the value $k=0.11$ is more suitable than $k=0.143$.

For the purpose of study the impact of underlying surface roughness on the vertical wind profile we used satellite imagery SRTM and MODIS (Fig. 3). The first provides digital elevation model data, while the second provides the ability to automatically recognize types of the earth's surface and build thematic maps.



Fig. 3. Satellite image of a part of considered area.

The roughness of the underlying surface was classified according to [11], the coefficient values vary from 0.0 for the water surface to 0.44 for large cities with tall buildings.

To reproduce the wind speed fields at given heights in the calculation domain, the values of this meteorological parameter, sought by (6), were reduced to the nodes of calculation grid.

Moreover, in order to adequately describe the real regime of the air flow, it is necessary to keep in mind that the deformation of the field of wind speed depends on the linear dimensions of the obstacles. Reconstruction of the initial characteristics of the wind occurs at a distance of not less than twenty times the height of these obstacles, and for single obstacles – at a distance not less than their tenfold height [12].

Since, within the area under consideration, over time, the wind flow can pass over areas with different roughness coefficients (Fig. 4), unnatural transitions or gaps may form during the mathematical description of the wind speed fields.

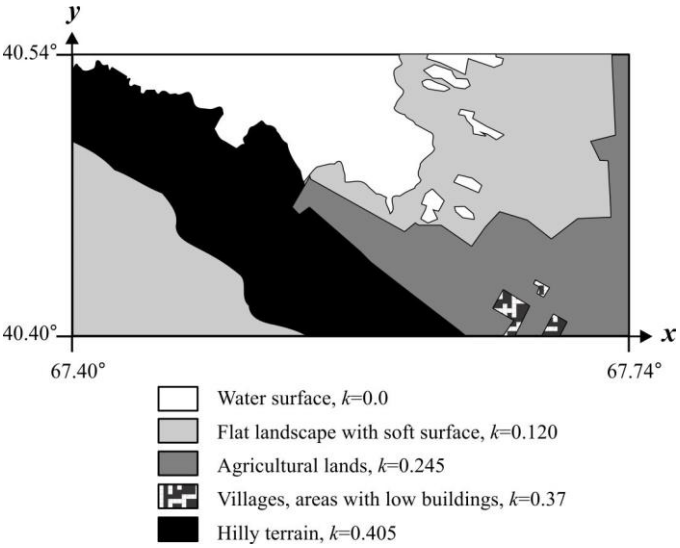


Fig. 4. The thematic map of the surface roughness of the considered area, shown in Fig. 1.

Smoothing of surfaces can be achieved by additionally applying interpolation methods, for example, radial basis functions and spline functions with tension [13].

Also it sholud be noted that the digital description of underlying surface given in the form of thematic map (Fig. 4) is used as $\beta(r,\psi,\varphi)$ function values at $r=r_{surf}$ (topographic surface). Thus, in (1)-(5), the coefficient of interaction of aerosol particles with the underlying surface is taken into account.

III. Results

Based on the developed mathematical model, numerical algorithm and datand a processing capabilities available in QGIS, SAGA and ENVI software, there was developed Python app. Computational experiments to study the characteristics of the air flow at different heights were carried out at different values of the surface wind speed and the roughness coefficient of the underlying surface.

It is expected from the results of numerical calculations (Fig. 5) that the increase in the air mass velocity along the height of the atmospheric boundary layer is mainly affected by wind speeds at the surface of the earth (here the vane level is 10 m) and the surface roughness class.

Computational experiments (Fig. 6) established that with an increase in the roughness coefficient ($V_0=3.5$ m/s), the wind speed increases with height according to the log law. Such growth occurs to a certain height $H\approx2000$ m, and after that the wind speed changes slightly and the effect of the roughness effect disappears.

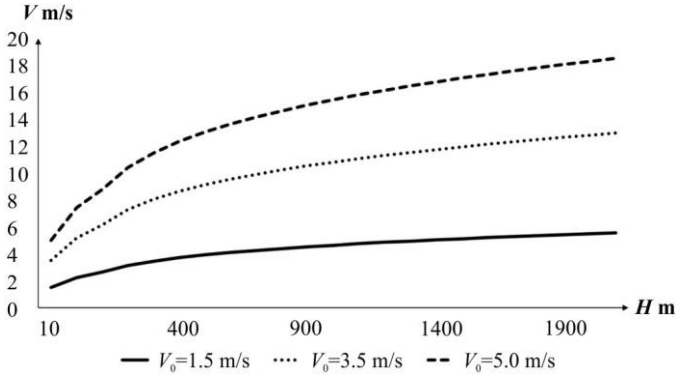


Fig. 5. The change in wind speed along the height of the atmospheric boundary layer with th surface roughness coefficient $k = 0.245$ and various glound-level wind speeds.

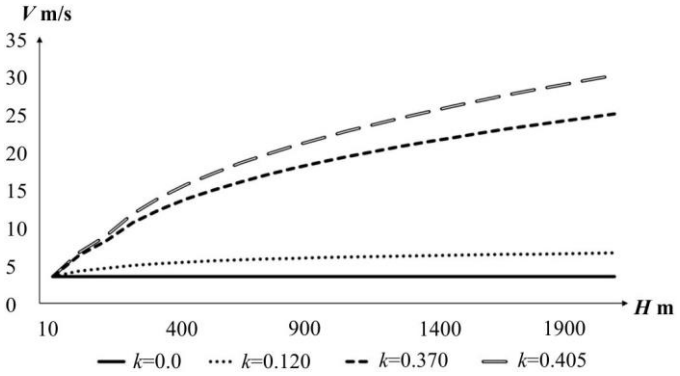


Fig. 6. The change in wind speed along the height of the atmospheric boundary layer, $V_0 = 3.5$ m/s.

As can be seen from the curves in Fig. 6, the nature of the movement of the air mass when passing over the water surface ($k = 0$) practically does not change with height, and in the case of passage along land areas with significant heterogeneity of the relief ($k = 0.405$) – a speed gradient is observed.

To forecast the distribution of salt-dust particles in the southern Aral Sea region, let us use the proposed mathematical model.

Areal sources are considered to be located in the northeastern part of Aral Sea basin. Computational experiments were carried out when in the time period $[0, t_5]$ the wind was directed to the south, in the time period $[t_5, t_{10}]$ – to the southwest.

Numerical experiments were carried out for various values of the turbulence coefficient. In the first case, aerosol transport was uniform at all heights, depending on the wind speed and direction. With unstable stratification, κ values rise upto 200-400 m and quickly falls with more height, tending to zero at the upper boundary of the ABL (1000-1600m). With stable stratification, κ grows insignificantly in the surface layer and decreases with heights above 400-600 m.

Figures 7 and 8 show the contour plots of the function $\theta(r, \varphi, \psi, t) \cdot 10^8$ at the time $t = 5$ h, $t = 10$ h when the sources are situated at the northeastern part of southern Aral Sea region. In figure 9 the contour plot are shown for $t = 10$ h when the sources are situated at in the middle part of the dried bottom and with weak unstable atmosphere stratification.



Fig. 7. $\theta(r, \varphi, \psi, t) \cdot 10^8$ function contour plot at $t = t_5$.

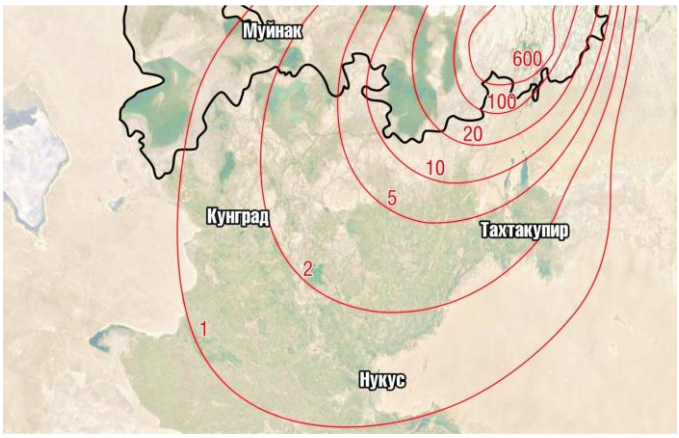


Fig. 8. $\theta(r, \varphi, \psi, t) \cdot 10^8$ function contour plot at $t = t_{10}$.

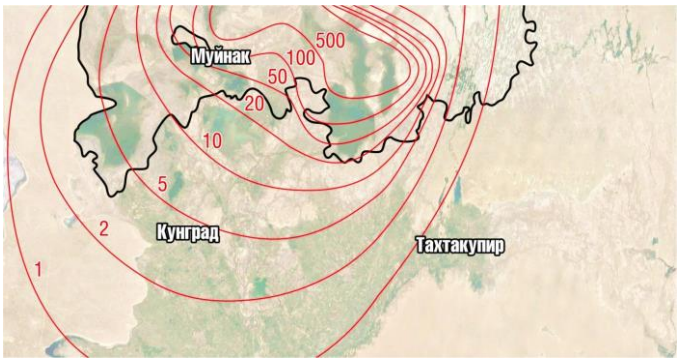


Fig. 9. $\theta(r, \varphi, \psi, t) \cdot 10^8$ function contour plot at $t = t_{10}$.

Figures 10 and 11 show contour plots of the concentration of aerosol particles sedimented on the underlying surface.

As can be seen from the numerical calculations, when the north wind is blowing (Fig. 7) aerosol does not reach Nukus city and when it is the northeast wind aerosol reaches Nukus (Fig. 8). That means the spread of aerosol particles in the atmosphere is significantly affected by the horizontal component of the wind speed and its direction.

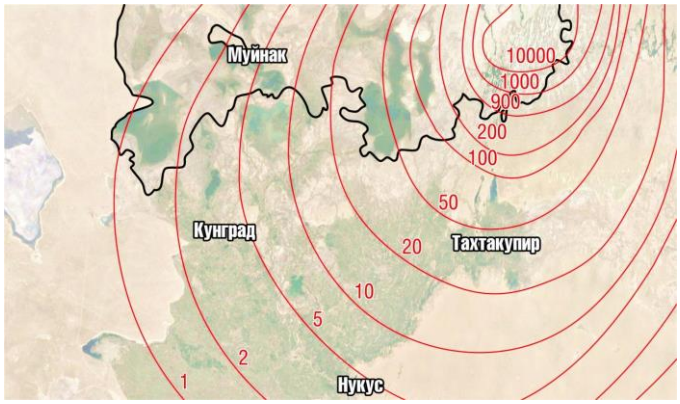


Fig. 10. The concentration of sedimented aerosol particles $\theta(r_{surf},\varphi,\psi,t)\cdot 10^6$ at time $t=t_{10}$. Corresponds to the experiment showed in Fig. 8.

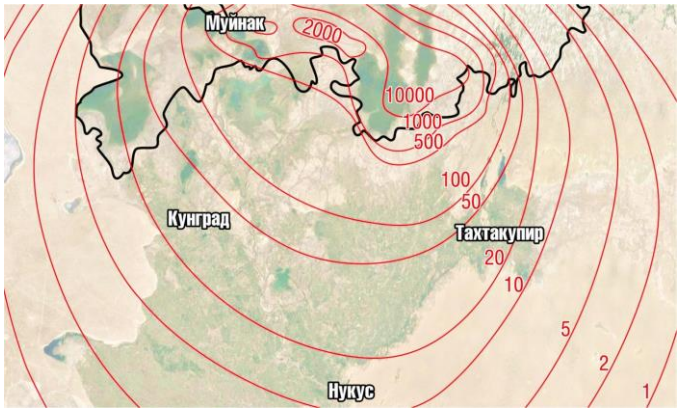


Fig. 11. The concentration of sedimented aerosol particles $\theta(r_{surf},\varphi,\psi,t)\cdot 10^6$ at time $t=t_{10}$. Corresponds to the experiment showed in Fig. 9.

The datasets of a number of experimental studies show that various parts of the dried bottom of the Aral Sea most of the year have high erodibility rates – from 60 to 2800 ton/km^2 [3].

In this aspect, it is interesting to analyze the experimental data of the Central Asian Research Institute of Irrigation (SANIIRI) collected over several decades. Samples of settled dust according to SANIIRI data show that particles with a radius of more than 0.25 mm fell unevenly at various observation stations, for example, in Surkulya (10 km from source) they make up 97.87%, in Dzhiltirbas (170 km from source) – 8.91%. With distance from solonchaks, the precipitation of particles with a radius of >0.25 mm does not reach one percent (Nukus city).

The consentration of fine particles with radius of 0.01 mm deposited in Nukus consists 23.38 - 52.97% of whole salt-dust emission in summer and 20.56 - 40.79% in winter.

The results of modeling presented in this work generally agree with the experimental data of SANIIRI and numerical calculations of other authors [18]. That actually confirms the adequacy of the proposed mathematical model.

IV. Conclusion

Knowing and taking into account the patterns of changes in wind speed with altitude depending on the type of land cover and the roughness coefficient of the underlying surface are a prerequisite for the adequacy of the results of mathematical modeling of the process of dispersion of harmful emissions in the atmosphere. Moreover, it is highly desirable to keep in mind the possibility of dynamically changing the roughness coefficient of the underlying surface when solving specific applied problems.

As the analysis of published scientific works and the results of this study show, the use of a constant value of this parameter for various types of the earth's surface can lead to significant errors in estimating the flow regime of the wind flow even if the atmosphere is stratified indifferently.

The analysis also showed that the use of the logarithmic dependence of the change in the vertical profile of the wind gives more accurate results up to a height of about 100 m, and at heights up to the upper boundary of the atmospheric boundary layer, it is preferable to use a power dependence.

The considered approach to the construction of wind fields at different heights, based on the use of existing mathematical methods and GIS technologies, allows us to accurately describe the transport and diffusion of impurities in the atmosphere and evaluate the distribution of the concentration of harmful particles.

As follows from an analysis of the results of numerical calculations, the distribution of the concentration of suspended aerosol impurities in the region under consideration largely depends on the horizontal component of the air mass velocity in the atmospheric boundary layer. Moreover, with an increase in the roughness coefficient, the horizontal wind speed increases with height, and the area of influence of the discharge plume proportionally expands with time, thereby reducing the level of concentration of aerosol particles.

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