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Numerical Modeling of Distribution of Air Pollutants in Near Zone Taking into Account Local Meteorological Conditions

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***Abstract*—The paper presents a three-dimensional numerical model developed by the authors, which describes the change over time of thermodynamic and microphysical characteristics of the atmosphere in the computational domain, the distribution of impurities on a local scale (up to 50 km) from various sources, taking into account the actual or forecast fields of meteorological parameters. The model differs in that it takes into account the microphysical processes of interaction of impurities with the cloud environment. To obtain three-dimensional prognostic fields of meteorological parameters at the initial time (when initializing the model), a combination of data from the global forecasting system GFS and data from remote observations using Doppler meteorological radars is used. Validation of the model on various test data is carried out. Numerical experiments were performed using orography and the actual distribution of wind in the atmosphere. The use of data of instrumental measurements and forecast system allows obtaining a detailed analysis of the environmental situation in the study area.**

Keywords—numerical modeling; pollutant transport; local conditions; distribution of pollutants; meteorological parameters fields

I. Introduction

The issues of transport of light and gaseous impurities in the cloud atmosphere for tens and hundreds of kilometers, their deposition and leaching are of great interest in modern conditions in the light of the frequent occurrence of short-term anthropogenic sources of harmful substances of high power.

Studies of the spread of impurities include field experiments, the development of methods for short-term prediction of atmospheric pollution, the development of methods for modeling the spread of impurities. Significant results have been achieved on these issues [3, 4, 7, 8]. First of all, this applies to theoretical studies of the spread of impurities in the atmosphere and calculations of air pollution, the introduction of scientific developments in the practice of monitoring the purity of the atmosphere, the development of methods for short-term forecasting of dangerous weather conditions in terms of air pollution. Thus, the study of the spread of impurities in the atmosphere by means of mathematical modeling is one of the promising developing areas and is important for environmental protection, atmospheric physics and many other areas. The construction of mathematical models of atmospheric impurities distribution allows researchers to solve a wide range of problems, including the study of regional features of environmental pollution. At the same time, the creation of regional models that allow describing the distribution of impurities correctly is the most difficult. Despite the wide range of existing models for the spread of impurities [3, 4, 12, 14], the diversity of environmental conditions necessitates the creation of models that take into account the influence of many additional factors in the spread of impurities, such as meteorological conditions and terrain. In particular, this problem requires further development for regions with a wide range of local features and local conditions [6, 10, 12-19]. The improvement of numerical prediction methods is facilitated by a more complete account of the physical and chemical atmospheric processes that determine atmospheric pollution. Moreover, the more accurate and complete data models operate, the more accurate forecasts can be obtained.

Let us focus on some of the common models used in the US, EU, Canada and other countries.

The main developers of the model AERMOD [1, 2] are the companies Lakes Environmental (Canada) and BREEZE (USA). The AERMOD model includes three core modules: AERMOD (a dispersion model of an impurity in the atmosphere), AERMET, and AERSURFACE tool set to create the input data associated with the state of the atmosphere and terrain, the AERMAP software, designed to bind a model to the data of local terrain and objects in three settings. In addition, the models of this class contain a number of tools to take into account the peculiarities of the spread of impurities over the roads, water barriers, forests, etc. The use of models of this class is associated with significant costs and efforts in the preparation of input data and makes sense in the assessment of environmental risks from industrial sources of pollution.

The CALPUFF model [5] is a modern non-stationary meteorological and air quality modeling system developed by ASG scientists. It is supported by model developers and distributed by TRC. The model was adopted by the U.S. environmental protection administration (EPA) as a privileged model to assess long-range transport of pollutants and their impacts on Federal areas. The simulation system consists of three main components and a number of post-processing and pre-processing programs.

It should be noted that the improvement of numerical methods of forecasting is facilitated by a more complete account of the physical and chemical atmospheric processes that determine atmospheric pollution. Moreover, the more accurate and complete data models operate, the more accurate forecasts can be obtained.

The aim of this work was to develop a three-dimensional unsteady numerical model of the propagation of pollutants in the atmosphere, taking into account hydrothermodynamic and microphysical processes, and algorithms for the use of three-dimensional initial data obtained from the global forecast system GFS [20] and as a result of instrumental measurements, in particular, Doppler meteorological radars.

II. Model and Methods of Analysis

A. Model description

The method of numerical integration of the atmospheric diffusion equation is often used to predict air pollution from a group of sources. This approach assumes the solution of the equation of turbulent diffusion of an impurity taking into account a nonstationary component:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=k_x\frac{\partial^2 C}{\partial x^2}+k_y\frac{\partial^2 C}{\partial y^2}+ +k_z\frac{\partial^2 C}{\partial z^2}+S(x,y,z), \tag{1}$$

The equation is solved numerically without taking into account the initial rise of the impurity. Thus, the implementation of the solution consists in the direct integration of a non-stationary three-dimensional diffusion equation to determine the expected impurity concentration at the points of interest, taking into account the specific area of the sources.

Distinctive features of calculations for the study of air and soil pollution over long distances is the need to take into account the following processes [6, 8]:

- deposition of impurities on the underlying surface;
- washouts with rain and fog;
- transformation of the impurities with long-term being in the air.

The regional numerical model developed by the author describes the change over time of thermodynamic and dynamic characteristics of the atmosphere in the computational domain, the distribution of impurities in the region from stationary sources, taking into account the initial actual or forecast fields of meteorological parameters. The model includes a system of equations of hydrothermodynamics to describe regional atmospheric processes, similar to those presented in [6,11], and equations for the rate of measurement of the concentration of multicomponent gas impurities of the following type [6]:

$$\frac{\partial C_i}{\partial t}+u_j\frac{\partial C_i}{\partial x_j}=F_i^{gas}-P_i^{nucl}-P_i^{cond}+ +P_i^{phot}+\frac{\partial}{\partial x_j}K_{jj}\frac{\partial C_i}{\partial x_j}, \tag{2}$$

$$\frac{\partial \varphi_k}{\partial t}+(u_j-\delta_{j3}w_g)\frac{\partial \varphi_k}{\partial x_j}=F_k^{aer}+P_k^{nucl} +P_k^{cond}+P_k^{phot}+\frac{\partial}{\partial x_j}K_{jj}\frac{\partial \varphi_k}{\partial x_j}. \tag{3}$$

where j = (u_1 = u, u_2 = v, u_3 = w), (x_1 = x, x_2 = y, x_3 = z); (u,v,w) - components of the wind velocity vector in the direction of x,y,z, respectively; C_i, i = 1,...,N_g, j_k = 1,...,N_a – the concentration of gas impurities and aerosols; N_g , N_a - the number of gas components and aerosol fractions, respectively; wg is the gravitational settling velocity; F^{gas} and F^{aer} - sources of trace gases and aerosols (e.g., fires or smokestacks); P^{nucl}, P^{cond}, P^{coag} and P^{phot} are nonlinear operators nucleation, condensation, coagulation and photochemical transformation, respectively. In this case, equations (1) – (2) are considered in the region

$$D_t = D\times[(0,T]),$$
$$D=\{(x,y,z); x\in[-X,X], y\in[-Y,Y], z\in[z_0,H]\},$$

where H is the upper bound of the integration domain. To account for orography, the model uses a generalized coordinate system $(\overline{x},\overline{y},\sigma)$ associated with the terrain,

$$x \equiv \bar{x}, \quad y \equiv \bar{y}, \quad \sigma = \frac{z-\xi(x,y)}{H-\xi(x,y)}\hat{H},$$

where H and $\hat{H}$ the height of the lower and upper boundaries, respectively, in the z-coordinate system, and $\xi(x,y)$ - a function describing the terrain [6].

The initial conditions are specified in the form:

$$C_i(x,y,z) = C_i^0(x,y,z); \quad \varphi_i(x,y,z) = \varphi_i^0(x,y,z), \quad (4)$$

The boundary conditions at the lateral boundaries of the region have the following form:

$$\varphi_i\big|_\Omega = \varphi_i^b, \text{ if } u_n < 0,$$
$$\left.\frac{\partial \varphi_i}{\partial n}\right|_\Omega = 0, \text{ if } u_n \geq 0, \quad (5)$$

where Ω is the lateral surface, n is the external normal to Ω, and u_n is the normal component of the velocity vector.

The turbulent diffusion equations (2)-(5) are solved by the component-by-component splitting method [11, 16]. The difficulties are caused by the need to calculate the coefficients of turbulent diffusion depending on the state of the atmosphere [12, 14].

Transfer of multicomponent gas impurities is calculated taking into account the microphysical processes of leaching by precipitation and fog. Removal of trace gases from the air is carried out by various mechanisms. They include absorption and deposition on the earth's surface, self-purification in the processes of cloud and fog formation, leaching by precipitation, etc. [13].

B. *Background Information*

The initial information to initialize the model is the meteorological information and data on the characteristics of the source.

To calculate the wet leaching of impurities by precipitation, the model uses radar observations. With the help of Doppler weather radar DMRL-C, at airports at regular intervals (10 min), maps of the distribution of clouds and precipitation over a large area are built [13]. Data on precipitation intensity allow calculating the flow of impurities to the surface of the earth as a result of leaching. Figure 1 presents data obtained by Doppler weather radar DMRL-C.

The model makes it possible to calculate the spread of impurities from various sources using real data of the wind field and clouds in the atmosphere obtained from the processing of sensing data, for example, maps of horizontal wind and reflectance. The use of Doppler DMRL-C data significantly improves the analysis of the environmental situation in the study area.

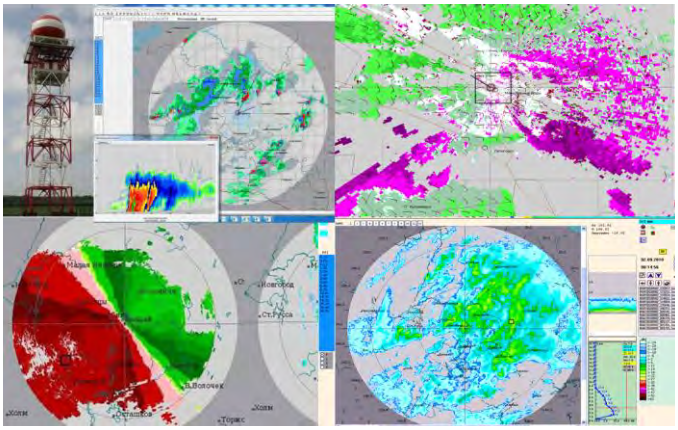

Fig. 1. Map of horizontal wind according to DMRL-C. Arrows indicate direction and speed of wind.

III. Results of Calculations

On the basis of the constructed model, preliminary calculations for various meteorological data are carried out. A stationary source was simulated, chosen as the region representing a spatial rectangular parallelepiped with sides of 12×12×10 km, the Y axis pointing to the North, the X axis – to the East. In the field of specified meteorological parameters on the version of the GFS [9, 20]. The control time t_1 was 5 min (300 s), t_2 was 10 min (600 s), t_3 was 20 min (1200 s). For figure 2 the results of test calculations are presented – the isosurfaces of the impurity concentration are given at the given moments of time. The impurity cloud is carried by the wind and expands due to turbulent diffusion, the maximum concentration of particles increases over time.

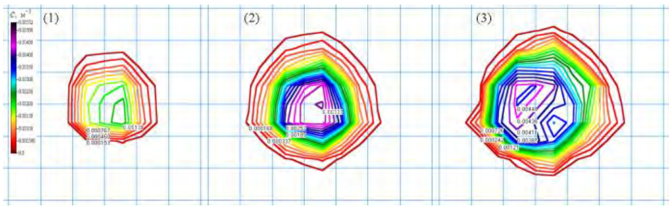

Fig. 2. The isosurface concentration of particles at times t_1=5 (1), t_2=10 (2) and t_3=20 min (3).

Test calculations showed high accuracy of the calculation schemes used in the model. The model allows calculating the distribution of impurities from various sources using real data of the wind field and clouds in the atmosphere.

The results of the calculations performed using different initial data are very different from each other. The change in the structure of wind in the atmosphere leads to a significant change in the nature of the interaction of the impurity cloud with the atmosphere. It is important to predict the possibility of a sharp increase in the concentration of impurities in the air. It can be caused by adverse weather conditions for dispersion of impurities. When forecasting the conditions of increasing concentrations of pollutants in the atmosphere, in addition to weather conditions, it is necessary to take into account the peculiarities of the emission regime associated with the time of year, time of day, days of week, etc. [4, 6, 8]. Using the output of global atmospheric models as predictors in cloud modeling allows us to more adequately reproduce the evolution of convective clouds in natural development and under active influence.

Using the output data of the model NOAA Global Forecast System as input to the cloud models saves time for operational application of the latter. Also, the use of these global models to some extent makes up for the lack of data of upper-air sensing. It is essential that global and mesoscale model data become available to an increasing number of professionals and users.

In order to obtain more complete prognostic fields of meteorological parameters, a combination of data from the global forecasting system (GFS) and data from remote observations by meteorological radars is used [13].

An example of calculating the spread of light impurities is shown in Fig. 3. The vertical distribution of the thermodynamic parameters of the atmosphere and other meteorological parameters are based on the data of the Global GFS system. The conditions of formation of maximum permissible levels of environmental pollution from man-made sources (fires, accidents, etc.) are analyzed with the use of meteorological data on CBD. It has been found that the flows of impurities to the surface due to dry deposition and leaching of sediments during the fires of oil storage at distances of more than 50 km are generally small for a few hours. The accumulation of oxides during the three-day period of oil storage fires is more significant and can be 0.2 mg/m^2 at distances of 50-100 km with the considered meteorological parameters.

The use of combined data significantly improves the analysis of the environmental situation in the study area.

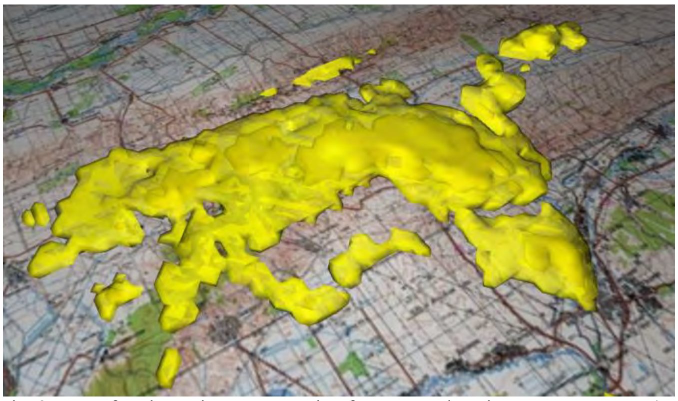

Fig. 3. Isosurface impurity concentration from several stationary sources at t=45 min.

IV. Discussion

Above the areas of the earth's surface having different temperatures, the air temperature is also different, i.e. horizontal temperature contrasts are formed. Temperature contrasts arising in this way in the atmosphere can propagate to altitudes of several hundred meters. Above the warm part of the earth's surface, in the warmer air, at some altitude, the atmospheric pressure will be higher than above the cold part in the colder air, i.e. there are horizontal baric gradients. Under their influence, air currents, including mesoscale, develop.

Transport is closely related to meteorological conditions and features of the earth's surface. The direction of transport of emissions is determined by the direction of the wind, and the height of the rise of emissions by its speed. As the wind speed increases, the mixing of gases with the surrounding air becomes more intense, which leads to dilution of emissions. At the same time, the high wind speed prevents the rise of emissions, limiting their spread in the vertical direction. Similarly, the direction of emission propagation is affected by the temperature of individual layers of air. Under normal atmospheric stratification, emissions can easily rise up, in the case of inversion-their rise is limited. Inversion leads to increase in the concentration of emissions, with the result that when sufficient solar radiation can be observed the formation of smog.

The main factor affecting the distribution and concentration of impurities is wind [5, 19]. The nature of dispersion and transport of impurities depends significantly on the wind speed. Moreover, the influence of wind speed on the dispersion of impurities depends on the types of emission sources. For low emission sources, the maximum concentration is achieved with weak winds from 0 to 1 m / s due to the accumulation of impurities in the surface layer. In the case where the source is located inside the calm layer, based on the results of the integration of the diffusion equation, it follows that at a fixed height of the source the concentration increases indefinitely. In cities with numerous low sources and abundance of transport, concentration increases with decreasing of speed to 2 m/s [8]. The air temperature has a great influence on the content of impurities in the atmosphere. When the temperature decreases, the temperature difference between the emissions and the surrounding air leads to a greater vertical rise of impurities and a decrease in their effect on the surface layer of the atmosphere. Solar radiation plays an important role in the formation of air pollution. Substances that enter the atmosphere from sources of emissions at high solar radiation intensity, as a result of the photochemical reaction, are transformed into various secondary products, which often have more toxic properties. To start a photochemical reaction under the influence of solar radiation, low initial concentrations of impurities are sufficient, which can create potential opportunities for the formation of high levels of air pollution [10].

Natural clouds, precipitation and fog can have a significant impact on the change in the concentration of impurities. The process of capture of impurity particles by raindrops reduces its concentration in the air and increases it on the earth's surface. The rate of change of impurity particles in time is proportional to the product of particle and droplet concentrations [15]:

$$\frac{dn}{dt} = -K(r_i, R_k) n_i N_k, \tag{6}$$

where and respectively the number of particles impurity and drops (rain, fog, clouds) radius and 1 cm^3; – the coefficient of proportionality, in general, depending on the radii and particles and drops. Depending on the size of the impurity particles, the radii of which are in the range from 10^{-7} to 10^{-3}, many factors influence the capture of aerosol particles: Brownian and convective diffusion, turbulent exchange, polarization effects, hydrodynamic and electrostatic effects. The change in the concentration of impurities also depends on such characteristics as the lifetime of the particle, the longer the lifetime of the particle the higher the concentration of impurities. In the study of the influence of precipitation on the concentration of pollutants, it is noted that after their completion, there are rarely increased concentrations [1, 17]. With the increase in the amount of precipitation increases the degree of purification of air, at the same time it can be concluded that precipitation reduces background air pollution, which is the result of the total action of all sources of impurities.

The accumulation of impurities in the atmosphere due to weak winds and inversions is enhanced in fog conditions. The results of theoretical calculations [8] show that the effect of accumulation of impurities from the higher and lower layers is observed in the mists. As a result of this effect, the concentration of impurities in the air and droplets in the fog increases. Water drops, absorbing impurities, to form a new, more harmful substances.

In the presence of inversion and fog, the content of impurities is 20-30% higher than only in the fog, and 6 hours after the beginning of the fog in the presence of inversion, this difference is 30-60% [8].

When releasing gases, account must be taken of the height of the source above the ground, the rate of release, the total amount of gas, its temperature and velocity of propagation. At the same time, it is important to know the composition and mass of emissions to assess atmospheric pollution. All these data can be obtained by measuring equipment. The conditions for the transfer of emissions are much more complex. While the transport of dust is primarily dependent on particle size and density, as well as on the movement of air flows, the distribution of gases is mainly determined by their solubility in water and the ability to chemically interact with atmospheric components. Their presence in the atmosphere depends on whether the transport is limited to a 100 km zone or whether the distribution is global. For example, among gases with a tendency to global distribution, CO_2 can be called, while SO_2 and NO_2 are stored in the atmosphere from several days to several weeks. This defines a significant difference between the concentrations of pollutants in areas exposed to the emissions, compared to those where the emissions do not exist.

A mathematical model of the distribution of impurities in the local area, taking into account the actual or forecast fields of meteorological parameters. Algorithms and software modules of the model implementation on the computer are developed. The scheme of application of DMRL-C data for the construction of the wind field in the design area is introduced. Developed algorithms and software modules the use of these prognostic global models GFS for the construction of the wind field in the computational domain. The method of application of the results of calculations of thermodynamic parameters of the atmosphere by the global model GFS for solving applied problems is tested.

The efficiency of combining data from different sources for initialization in the development of air pollution models is shown.

The main factors affecting the distribution and concentration of impurities are identified and analyzed.

Taking into account the meteorological parameters allows for a more detailed study of air pollution. A numerical analysis of the spread of harmful impurities in the near zone in the area of pollution from stationary sources, with different meteorological parameters, including the wind shear in the atmosphere.

The conditions of formation of maximum permissible levels of environmental pollution from anthropogenic sources (fires, accidents, etc.) are analyzed. If the combination of dangerous 3-5 m/s wind speed and unstable stratification is unfavorable for high sources, these conditions are not dangerous for low sources. Dangerous for low sources is the combination of surface inversions and calm, when ground concentrations from high sources will be minimal.

Numerical methods allow for more accurate results by taking into account changes in emissions from the source over time and the availability of information on the expected characteristics of weather conditions and emission regimes from sources. However, it can be argued that projections will be effective only when it is feasible to control or completely eliminate emissions and to avoid their impact in the event of adverse weather conditions.

V. Conclusion

Thus, in the work on the basis of numerical modeling a number of issues of mesoscale distribution of impurities in the cloud atmosphere, which are important for the prediction of dangerous environmental situations, are investigated.

The results obtained contribute to the improvement of methods for calculating air pollution in the local area. The proposed model and methods can be used to develop a scientifically based forecast on the concentration of pollutants and in further applied research on the meteorological aspects of the spread of pollutants in the surface layer. When creating information systems to ensure meteorological and environmental safety of human life, the ability to calculate the spread of pollution and quantitative assessment of their flows to the underlying surface, allow to predict the development of adverse situations, and, if necessary, to take measures to prevent harmful effects on humans, fauna and flora.

It should also be noted that the results of numerical simulation of the formation of the microstructure of hail clouds and the formation of an electric charge in them showed that the clouds are complex interactions of various physical processes, the role of which is great and can not be neglected. The same can be said about the physics of the spread of gas impurities and aerosols. Obviously, dissolving in cloud drops, impurities begin to influence the further development of microphysical processes. These issues require separate consideration.

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