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SIMULATION OF RADIONUCLIDE DISPERSION IN THE AIR AND ON THE SOIL SURFACE[†]

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Mathematical and numerical methods are used to simulate physical and chemical processes when building models of pollutants dispersion in the air and on the soil surface. Based on meteorological data and information on the source of emissions, these models characterize both the primary pollutants entering the atmosphere directly and the secondary ones formed as the result of complex chemical reactions. These models are important for the air quality management system, as they allow monitoring emissions into the atmosphere, predicting their distribution, as well as developing effective strategies intended for reducing harmful substances in the atmosphere. The article presents an overview of computational methods used to simulate the pollutants dispersion in atmospheric air and on the soil surface, such as the Gaussian torch model, the Lagrangian dispersion stochastic model, and the Eulerian model of atmospheric diffusion. The practical application of the considered models showed sufficient reliability and validity of the air and soil pollution levels forecast. The simulation uses computer programs that include algorithms for solving the mathematical equations that control pollutant dispersion. The dispersion models are used to estimate the concentration of air pollutants or toxins. They can also be used to predict future concentrations under certain scenarios. They are useful for studying the pollutants that disperse over long distances and can initiate reactions in the atmosphere. Such software products are as follows: AEROPOL, AERMOD, GRAL, TAPM CSIRO, CALPUFF, HYSPLIT, etc. A method of processing information about the pollution sources and the environmental parameters, based on the HYSPLIT program, is proposed to form maps of the volume and surface activity of radionuclides. This method was applied to analyze the process of the plutonium isotopes dispersion as a result of the movement of air masses in the places of fires in April 2020 in the exclusion zone of the Chornobyl NPP, as well as the associated hazard for the population health and the environment.
Keywords: *turbulent diffusion equation, impurity scattering in the atmosphere, point source, near-surface concentration level, atmospheric pollution, volumetric activity of radionuclides*.
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Currently, the atmospheric pollution is increasing due to the anthropogenic influence of industrial enterprises, nuclear power plants, transport, industrial and household waste dumps, and urban construction. The problem of environmental protection requires a large amount of experimental research invested in monitoring of the environment state. Environmental monitoring systems, which include automatic (stationary) and mobile air pollution monitoring stations, have been created to effectively control the quality of the atmosphere. One of the main tasks of environmental monitoring is the collection of data on concentration of pollutants. This information is necessary for further analysis and forecasting of air and soil quality when making management decisions as to ensuring the environmental safety. Monitoring of the environment state allows analyzing data and determining the impact of atmospheric pollution on the quality of the environment and on the health of population.

Theoretical studies are needed to develop models that include identification of pollution sources, quantification of pollutant release rates, understanding of the process of the emission transportation from the source to the point of discharge, and knowledge of the physical and chemical transformation processes of the released substances, that may occur during this transportation.

The creation of models for the estimation of the concentration fields and source parameters using the observation data and model representations of the impurity dispersion processes allows more reliable control of the main parameters of the technogeneous pollution of the area. This approach makes it possible to determine the information capability of the observation systems and to optimize the position and the number of sampling points.

THE TECHNIQUES OF SIMULATION OF THE POLLUTANTS DISPERSION IN THE ATMOSPHERIC AIR

When building models of air quality, mathematical and numerical methods are used to simulate physical and chemical processes that affect the substances dispersion in the atmosphere. Based on meteorological data and information about the source of emissions (emission concentration, smokestack height, etc.), these models characterize both primary pollutants, which enter the atmosphere directly, and secondary pollutants, which are formed as a result of complex chemical reactions in the atmosphere. These models are of great importance for the creation of an atmospheric air quality management system, as they allow controlling emissions into the atmosphere, predicting their dispersion and developing effective strategies for reducing harmful substances in the atmosphere.

The development and improvement of new models is associated with the development of computer technology and the appearance of previously unavailable satellite meteorological data. This allows taking into account a large number of

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pollutants and their interaction, a large number of emission sources of various configurations, and the influence of complex atmospheric processes.

The process of the dispersion of pollutants occurs due to their being transferred by air masses and the diffusion caused by turbulent air pulsations. Almost all the impurities sooner or later deposit on the Earth's surface, the heavy ones – under the influence of the gravitational field, the light ones – as a result of the diffusion process. The pollutants get into atmospheric air, water, soil, and later into the living organisms. The assessment of contamination of the atmosphere and the underlying surface with impurities is carried out using mathematical models built on the basis of partial differential aerodynamic equations, as well as their finite-difference approximations. These models are also known as atmospheric dispersion models.

Theoretical and experimental studies of processes of the impurities diffusion and features of their spatio-temporal dispersion are the basis for an objective assessment of the state and trends of changes in atmospheric air pollution of soil, vegetation, and water bodies.

The most significant amount of fundamental research in the field of the environment is performed in the USA and European countries. In many countries, the air quality is assessed using the AQI index (air quality index). This index is used by all the world environmental government bodies to inform the public about the level of air pollution, as well as to forecast air pollution [1, 2].

To obtain indicators of atmospheric air pollution, some up-to-date models for calculating the concentrations of pollutants in the atmosphere are needed.

The success of developing air pollution models depends on understanding the laws of pollutants dispersion. The main factors determining the dispersion of a pollutant are advection (horizontal transport) and vertical diffusion. The wind speed determines both the mechanism of transportation of impurities and atmospheric turbulence [3].

The input information that is required when building a model includes three main groups of parameters: source parameters, environment parameters, and boundary conditions.

The source parameters include the rate of the impurity release, the type of the source (point, linear, surface), the nature of the source functioning (instantaneous, continuous), the properties of the pollutant, and its chemical activity.

The group of environmental parameters includes: the temperature gradient (vertical, horizontal), wind direction and speed, cloud cover, radiation, precipitation, rate of temperature and pressure change, values of background concentrations of impurities in the air.

The group of boundary conditions is formed by the surface properties (roughness, topography), inversion height, surface temperature, and surface air currents.

The accuracy of the model depends on the completeness of accounting for the variables included in each group. The simulation allows obtaining the dispersion of impurity concentration in space and time, evaluating the processes of impurity deposition, washing-out, chemical interaction, and sorption [3].

There are four main approaches to solving the problem of the substance scattering of in a moving gaseous medium [4]:

1. Direct experimental research, which is related to the use of instrumental methods for determining the form of emissions, trajectory of the pollution spread, diffusion conditions. This approach is used to solve tasks of operational forecasting and management, but not long-term planning.

2. The theory of similarity is used in modeling in those cases when, it is impossible to correctly assess the boundary conditions and directions of air flows due to the complexity of the topography and buildings, and therefore the hydraulic models have to be used.

3. The theory of pollutant diffusion is based on the law of mass conservation. It assumes the uniformity of the main movement along the coordinate axes and the use of the common methods of averaging the turbulent characteristics consisting of average and pulsational components. The solution of the semi-empirical diffusion equation is widely used to calculate the dispersion of impurities in the atmosphere.

4. The classical statistical theory describes atmospheric turbulence in terms of its intensity, scale, and spectral properties. It allows studying the history of the movement of individual particles and determining the statistical characteristics necessary for the description of diffusion.

The type of random process, used in the study of turbulence and diffusion, can be characterized as stationary, homogeneous, isotropic, and Gaussian.

Since each approach has its advantages and disadvantages, the choice of any of the listed approaches depends on the fact how adequate the conditions of the pollution process under study are in this case. The progress in the development of atmospheric diffusion understanding is achieved by combining the use of the theory with carefully planned observations and experiments.

One of the last stages of simulation is related to the choice of the coordinate system. Some models use the moving Lagrangian coordinate system, some other ones use the fixed Euler coordinate system. The models using Lagrangian coordinates allow determining the substance concentration at any moment along the curvilinear trajectory of its dispersion, and here it is not necessary to integrate the model along all three spatial coordinates. The model with Euler coordinates allows obtaining a solution at any point in space and for any moment of time. Such a model turns to be convenient in the case of a large number of point sources.

The final stage in the process of the model building is the selection of its basic version, which is characteristic of the adopted approach to simulation. This basic model can be static or dynamic, deterministic or stochastic, linear or non-linear, stationary or non-stationary by analogy with the models, which are used in chemical technology. Fig.1 presents the classification of mathematical models designed for the atmospheric pollution assessment and forecast.

Figure 1. Block diagram of the mathematical models classification of the pollutants dispersion in the surface layer of the atmosphere

Forecasting models are used to simulate atmospheric air pollution processes. Long-term and operational forecasting models are distinguished. For long-term forecasting, the calculation (analytical, approximation) models, based on the solution of the turbulent diffusion equation, have become the most widespread. They are "torch", "clew", "box" models, and finite-difference ones. For operational forecasting, statistical models of linear and non-linear regression, as well as models of heuristic self-organization (method of group accounting of arguments) are widely used. For operational forecasting of air pollution in case of emergency and volley emissions, the calculation (analytical methods) " clew " models should be used, which are employed to forecast the spread of impurities from instantaneous point sources. The most common are forecasting models that are obtained with the solution of the turbulent diffusion equation taken into account. The phenomena of pollutant transfer and diffusion are described by the equation [2]:

$$\frac{dC}{dt} = div(K \cdot gradC) - grad(CU) \pm Q \tag{1}$$

turbulent diffusion convection source

where C is the concentration of the pollutant; K = (k_x, k_y, k_z) is the vector of turbulent diffusion coefficients; U = (u, v, w) is the vector of the averaged velocity field of the air medium; Q is the pollutant emission rate of the source.

The choice of the initial and boundary conditions, which are necessary to solve equation (1), depends on the operating conditions of the source and the properties of the underlying surface.

On the basis of equation (1), four main types of models are obtained: "clew", "torch", "box" and finite-difference ones. In general, solving equation (1) using analytical methods is impossible. This becomes possible either by simplifying the equation or by using numerical methods.

Thus, the presence in equation (1) of the assumptions about the absence of convective transfer, non-isotropy of the medium and the location of the source outside the analyzed area, leads to the equation:

$$\frac{\partial C}{\partial t} = k_x \frac{\partial^2 C}{\partial x^2} + k_y \frac{\partial^2 C}{\partial y^2} + k_z \frac{\partial^2 C}{\partial z^2}. \tag{2}$$

The fundamental solution of this equation has the form of Gaussian function. This solution is used in the models of "clew" and "torch" type.

The model of "clew" type assumes an instantaneous source of pollution. The process of transferring the forming cloud ("clew") from the source under the wind influence is considered in the moving coordinate system. The equation of the non-stationary Gaussian model has the form:

$$C(x,y,z,t) = \frac{Q}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z} \cdot exp\left\{-\frac{1}{2}\left[\left(\frac{x-U_t}{\sigma_x}\right)^2 + \left(\frac{y-V_t}{\sigma_y}\right)^2 + \left(\frac{z-W_t}{\sigma_z}\right)^2\right]\right\}, \quad (3)$$

where C(x, y, z, t) is the concentration of the pollutant at the point with coordinates x, y, z at time t; U, V, W are the average values of wind speed in x, y, z directions at time t; σ_x, σ_y, σ_z are the standard deviations of "clew" dimensions in x, y, z directions, respectively; Q is the amount of the substance released by the pollution source at time t [4].

The model allows determining concentrations on the curved trajectory of the "clew" movement. In addition, it allows taking into account the change in atmospheric stability. Operating with the "clew" model involves real-time observation of the wind field. Integrating the model over space allows obtaining a solution for the instantaneous volumetric source.

The shortcomings of the model include: the requirement of a large amount of meteorological data (measurements of wind speeds along all three coordinates), the difficulty of determining the initial height of the gravity center of the "clew", the complexity of the calculation program.

The “torch” model (stationary Gaussian model) is based on the assumption of a continuously operating point source. It is obtained by integrating equation (1) over time. The equation of the "torch" model looks like this:

$$C(x,y,z,H) = \frac{Q}{2\pi\sigma_y\sigma_z U} exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\}, \quad (4)$$

where C(x, y, z, H) is the concentration dispersion along the x, y, z coordinates; Q is the pollutant release rate; U is the average wind speed; σ_y , σ_z are standard deviations of the "torch" dimensions in the horizontal and vertical directions at the given x; H=h+Δh is the effective height of the "torch"; h is the pipe height; Δh is the rise of the "torch") due to its buoyancy [4].

The major advantage of the "torch" model is its simplicity and the possibility to calculate the concentration fields basing on a relatively small number of experimentally determined parameters.

The "box" model is used for the rough estimation of the pollutant released from large surface sources. In this model, it is assumed that inside the analyzed volume of air, the concentration does not depend on the coordinates y and z, and the particles of the substance do not move relative to the environment. The wind speed is assumed to be the same with height. Such an assumption is usually made in the absence of more precise meteorological data. Besides, it is necessary the diffusion of the jet in the transverse and vertical directions to be small. This assumption is valid if the source of pollution is limited by buildings, topographic irregularities (mountains, hills) and the inversion height.

In addition to the single "box" model, there are known options for building of the multi-box models intended to estimate the concentrations from the distributed emission sources. In these cases, the atmosphere is divided on the system of "boxes", and then the impurity fluxes between the boxes and the concentrations in each of them are calculated. The "boxes" are usually bounded below by the earth surface, and above by the height of the inversion or an arbitrarily chosen upper boundary.

Such a model is, in fact, a finite-difference analogue of the diffusion equation under the condition of vertical homogeneity of the medium, the absence of diffusive components, and the transfer occurring only due to advection being taken into account. Basing on such models, the impurity concentrations in the entire region are calculated for the same time.

The multi-box model has the following disadvantages: 1) the complete mixing is assumed to occur in the vertical direction; 2) the absence of diffusion between the "boxes" is assumed; 3) the accuracy of the model corresponds to the accuracy of the first-order differential equation.

Another broader class of models was obtained as a result of replacing the diffusion equation with simpler equations and using numerical methods for their solution, they are "finite-difference" models. These models are based on the approximation of the air basin by three-dimensional cells to obtain the numerical solution. The main problems here are due to the model stability and accuracy.

The practical application of the models considered above showed sufficient reliability and validity of the forecast of air pollution levels created by individual powerful point sources.

Subject to the implementation methodology, the known methods of forecasting atmospheric processes can be divided into numerical, statistical, and pattern recognition methods [4, 5].

The forecasting methods, being developed on the basis of mathematical description of the impurities dispersion, in which the turbulent diffusion equation is used, are numerical. Such methods are universal with respect to the source, medium characteristics, and boundary conditions and allow the use of turbulent exchange parameters. Numerical methods of forecasting are used to solve the following tasks:

1. Forecast of maximum impurity concentrations from the sources, that is, the calculation of maximum concentrations created at a certain distance from the source.
2. Forecast of integral characteristics of air pollution from the plane source.
3. Forecast of the highest concentration from dispersed sources.

For the forecast of air pollution from individual sources and from a group of sources, the methods of numerical integration of the atmospheric diffusion equation are used directly.

The forecast of air pollution in cities and industrial areas using the statistical models is carried out by statistical methods. The latter ones are based on statistical analysis of observations. It is assumed that during the analysis period, as well as during the forecast period, the emissions and location of the sources practically do not change. This is associated with certain errors and limitations of the results of analysis and forecasts, which are not characteristic of numerical methods, so the specified assumption is used for relatively short forecast periods, i.e. from a few hours to a few days. Besides, with a large number of sources and their insufficient power, it can be assumed that the increase in emissions from some of them is compensated by the decrease from the other ones. Therefore, the growth of average and total air pollution in the city is mainly associated with the changes in meteorological conditions or the synoptic situation.

The Important factors for ensuring the accuracy of the air pollution forecast are the choice of model parameters and the synoptic situation and sets of meteorological factors being taken into account.

To study the influence of meteorological conditions of air pollution, it is possible to apply the method of pattern recognition. The task of identifying the sources of air pollution can be considered as a typical task of pattern recognition. The image recognition is the classification of the initial data into a certain class using the choice of the existing features or properties, which characterize these data, from the total set of features. The subject of recognition combines a number of scientific disciplines. They are combined by the search for a solution to the common problem of distinguishing elements, which belong to a specific class among many different elements belonging to several classes.

ANALYSIS OF THE SOFTWARE DESIGNED FOR SIMULATION OF ATMOSPHERIC POLLUTION DISPERSION

The simulation of atmospheric dispersion is the mathematical simulation of the process of the pollutant's dispersion in the surrounding atmosphere. The simulation is carried out using computer programs that include algorithms to solve the mathematical equations, which govern the pollutant dispersion. The dispersion models are used to estimate concentrations of air pollutants or toxins emitted from the sources, such as industrial enterprises, motor traffic, or accidental emission of chemicals. They can also be used to predict future concentrations under certain scenarios. They are most useful for studying pollutants that disperse over long distances and can initiate reactions in the atmosphere.

Many up-to-date programs, designed to simulate dispersion, include a preprocessor module for inputting meteorological and other data, and a postprocessor module for graphical representation of the output data and mapping of the area exposed to the air pollutants. The diagram of the area under exposure may also include isopleths showing the areas having from minimum to high concentration, which represent the greatest risk for health.

In many countries of Europe and in the USA, currently, when numerically predicting the spread of impurities in the boundary layer of the atmosphere, the Gaussian "torch") model, or the dispersive Lagrangian stochastic model, or the Eulerian model of atmospheric diffusion is chosen.

The Gaussian model assumes that pollutant dispersion occurs in a Gaussian dispersion. Such models are usually used to predict the "torch") emitted by a stationary emission source. Gaussian-type models dominate in the majority of regulatory documents of many countries of the world, regulating the procedure and rules for calculating surface concentrations up to the distances of 50 km.

The Gaussian "torch" model functions in a stationary mode, the meteorological parameters do not change in time and space. This model is most often used to predict the spread of long-term atmospheric pollution from the sources located at the level of the earth surface or at some height. The application of the model is limited to the local scale. This technique is recommended by the United States Environmental Protection Agency (EPA) for calculations that are of a regulatory nature.

The Gaussian "torch" model is implemented in many software products. In fact, this is currently the most common method of atmospheric pollution simulation: CALINE4 [6], HIWAY2 [7], CAR-FMI [8], AEROPOL [9], ADMS5 [10], etc.

One of the most well-known systems for simulation of the pollutants spread in atmospheric air, which uses the Gaussian "torch" technique, is AERMOD [11].

AERMOD is the model developed by AERMIC (a joint working group of scientists from AMS (American Meteorological Society) and EPA) for regulation of atmospheric air pollutions. AERMOD is an up-to-date advanced "torch" model. This model uses the pollutant dispersion based on the atmospheric boundary layer turbulence structure and the scaling concept; it is capable of handling simple and complex terrain. AERMOD considers pollution from three types of "torches": main, indirect and penetrating (Fig. 2) [12].

For steady conditions, the expression for AERMOD concentration (C_s) has the Gaussian form and is similar to that used in many other steady-state "torch" models:

$$C_s(x,y,z) = \frac{Q}{u\sigma_{zs}\sqrt{2\pi}} F_y \sum_{m=-\infty}^{\infty}\left[exp\left(\frac{\left(z-h_{es}+2mz_{ieff}\right)^2}{2\sigma_{zs}^2}\right) + exp\left(\frac{\left(z+h_{es}+2mz_{ieff}\right)^2}{2\sigma_{zs}^2}\right)\right], \quad (5)$$

$$F_y = \left(-\frac{1}{\sqrt{2\pi\sigma_y}} exp\left(-\frac{y^2}{2\sigma_y}\right)\right) \quad (6)$$

where u is the wind speed; F_y is the lateral dispersion function; z_{ieff} is the effective mechanical height of the mixed layer; σ_{zs} is the total vertical dispersion; h_{es} is the height of the "torch") (the height of the emission source plus the height of the "torch" itself).

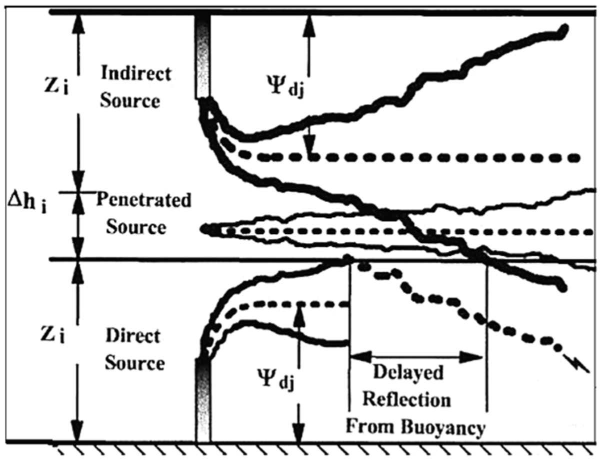

Figure 2. Schematic of the torch simulation in AERMOD [12]

In AERMOD, the total concentration (C) is calculated by formula (7) by summing the contribution from three sources:

$$C(x,y,z) = C_d(x,y,z) + C_p(x,y,z) + C_r(x,y,z). \tag{7}$$

The concentration from the main source is calculated by formula:

$$C_d = (x,y,z) = \frac{Qf_p}{\sqrt{2\pi u}} F_y \sum_{f=1}^{2} \sum_{m-0}^{\infty} \frac{\lambda_f}{\sigma_{zj}} \left[exp\left(-\frac{\left(z-\psi_{dj}-2mz_j\right)^2}{2\sigma_{zj}^2}\right) + exp\left(-\frac{\left(z+\psi_{dj}+2mz_j\right)^2}{2\sigma_{zj}^2}\right)\right], \tag{8}$$

$$\psi_{dj} = h_s + \Delta h_d \frac{xw_j}{u}, \tag{9}$$

where Δh_d is the plume height of the emission source; h_s is the plume height, with the height of the emission source taken into account; w_j is the vertical velocity for the upflow (j = 1) and dispersion of the downflow (j = 2); σ_{zj} and ψ_{dj} are the parameters of the emission source height and vertical dispersion. The subscript j=1 is used for the upflows and j=2 for the downflows.

The concentration from the indirect source is calculated according to the following formula:

$$C_r(x,y,z) = \frac{Qf_p}{\sqrt{2\pi u}} F_y \sum_{f=1}^{2} \sum_{m=0}^{\infty} \frac{\lambda_f}{\sigma_{zj}} \left[exp\left(-\frac{\left(z+\psi_{rj}-2mz_j\right)^2}{2\sigma_{zj}^2}\right) + exp\left(-\frac{\left(z-\psi_{dj}+2mz_j\right)^2}{2\sigma_{zj}^2}\right)\right], \tag{10}$$

where, $\psi_{rj} = \psi_{dj} - \Delta h_i$, and Δh_i is the plume from an indirect source.

For the penetrating source the expression for concentration (C_p) has Gaussian form in both vertical and transverse directions. The concentration caused by this source is determined by the formula:

$$C_p(x,y,z) = \frac{Q(1-f_p)}{u\sigma_{zp}\sqrt{2\pi}} F_y \sum_{m=-\infty}^{\infty} \left[exp\left(-\frac{\left(z-h_{ep}+2mz_{ieff}\right)^2}{2\sigma_{zp}^2}\right) + exp\left(-\frac{\left(z+h_{ep}+2mz_{ieff}\right)^2}{2\sigma_{zp}^2}\right)\right], \tag{11}$$

where z_{ieff} is the height of the upper reflecting surface in the stable layer, and σ_{zp} is the total dispersion for the penetrating source.

The complete AERMOD simulation system consists of two processors: a meteorological preprocessor (AERMET) and a mapping program (AERMAP), as well as the dispersion model itself. The detailed information on the development of the model is described on the EPA resource [11].

The Lagrange's method and the Euler's method for describing turbulence are used when solving different problems, independently or mutually complementing each other.

The Euler's models are built on the solution of the semi-empirical equation of turbulent diffusion, which is integrated on a finite-difference Euler's grid. The representation of turbulence by Euler is related to the assignment of the field of random variables in space and time by means of an equation or a system of equations, such as the equations of hydrodynamics. By successively averaging these equations, a system of equations describing any processes in a turbulent environment is obtained. In this case, the argument is the set of coordinates of points in space, and the components of the velocity vector of the medium movement and the values of the impurity concentration at this point in space are functions of these coordinates and time [3, 13].

The Eulerian model of atmospheric diffusion rather easily solves the problems associated with predicting the mesoscale transfer of emissions. However, due to the use of a relatively coarse grid (horizontal linear size is several kilometers or more) there are difficulties in presenting concentration gradients from the point and line sources [3].

The Eulerian models differ among themselves subject to the method of obtaining the meteorological values, i.e. wind speed and turbulent diffusion coefficient. These models, unlike the Gaussian models, are rather complex and require significant software processing time. Currently, there are a large number of implemented Eulerian models of pollutant transport in the atmosphere. However, many of them are suitable only for the areas of about several tens of kilometers, what does not allow studying the long-range impurity transfer.

In the Lagrange method, an infinitesimal particle with coordinates at a fixed time is considered. And when it is moving, its coordinates are considered at the subsequent moments as functions of the time of the initial coordinates, with further averaging of the trajectory parameters or groups of trajectories according to the environment fluctuations. The particle velocities are derivatives of coordinates and time. The impurity from a point source is usually represented as an ensemble of discrete "balls" or particles. For each "ball" the trajectory of its movement in the time- and space-varying wind field is calculated and the diffusion transfer is also calculated. This is done, for example, using the stochastic models, and often the turbulent structure is assumed to be the Gaussian. Studying the transfer and scattering of a large number (several thousand) of tracer particles allows simulating the drift and dispersion of the impurity in the turbulent atmospheric boundary layer. The impurity concentration at any point in space is represented as the sum of contributions from each Lagrangian element.

The Lagrangian model of the atmospheric pollution spread is represented as a sequence of "torches", inside each of which the substance has a certain dispersion. This approach is more flexible than the principle of the Gaussian "torch", as it is closest to the physical essence of the matter scattering in the atmosphere. The Lagrange model allows simulating the process that is non-stationary in time and space, and quite correctly takes into account the changes in the direction of the wind, the complex topography of the area, and chemical transformations of the matter. This technique gives correct results when simulating both the instantaneous or short-term emission and the long-term emission, for example, for a seasonal or annual cycle. The Lagrange model is an effective tool in the study of atmospheric pollution propagation processes. The approach, in which the movement of individual particles is tracked, gives more opportunities to obtain qualitatively new results, as compared to the Euler approach. However, solving the problem of describing the matter movement by calculating the speed of its movement in the nodes of the coordinate grid imposes a number of restrictions. For example, if the substance is a certain amount of radionuclides, then the process of describing the decay and/or transformation into other types of radioactive particles with this approach is difficult. On the contrary, the Lagrangian approach offers a simple solution to this problem.

A few decades ago, the use of Lagrange models was practically impossible due to the large volume of necessary calculations, but now, with the growth of up-to-date computing power, it is quite possible.

The application of the Lagrangian model is justified, when it is important to take into account temporal and spatial changes in meteorological conditions. Also, the model makes it possible to estimate the pollutant spread in calm weather much better.

This class of models is relatively young, as compared to the Gaussian "torch" model. There are several software implementations of this approach: GRAL [14], TAPM CSIRO [15], CALPUFF [16], HYSPLIT [17].

One of the examples of the Lagrangian cloud model implementation is HYSPLIT [18]. More precisely, HYSPLIT uses a combined Lagrangian-Eulerian model, which is widely used in the up-to-date pollutant dispersion modeling systems.

In order to take into account the shortcomings of the analyzed approaches, some hybrid models of impurity propagation in the atmosphere were proposed, in which the Lagrangian dispersive stochastic approach is used at the initial stage of emission propagation, and the Eulerian model of atmospheric diffusion is used to predict the further transfer and transformation of pollution over long distances. Nevertheless, when using this method, there are still problems associated with the combination of two different approaches for the description of the impurity.

To obtain the pollutant concentration cards, the task of selecting the necessary software product arises. Installing and running all the pollutant propagation modeling systems is a time-consuming task: for each software product, it is necessary to find the raw data in a certain format, learn the architecture and startup procedure, and install certain software and hardware. Therefore, the choice of the most effective system is based on the study of domestic and foreign research.

As a result of the up-to-date models analysis, the HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory), was chosen, which had been developed at the NOAA Air Mass Laboratory (USA) and the Australian Bureau of Meteorology [19].

The HYSPLIT model allows for three-dimensional modeling of the process of formation and spread of an air pollution cloud from the given source. The HYSPLIT model combines two classical approaches: Lagrangian and Euler, the advection and diffusion equations are solved independently in the Lagrangian formulation, and the concentration calculations are performed within the framework of the Euler approach on the fixed spatial grid. The input meteorological information that is required for HYSPLIT is borrowed from the calculation data of the meteorological models, which are based on the results of the in-situ measurements. Generally, this information is presented on the regular spatial grid and includes the data on the vertical dispersion of horizontal and vertical wind components, temperature and pressure, as well as the surface pressure, and some other parameters.

HYSPLIT functions in the dialog mode and has a detailed user manual; it can be operated online from the NOAA page or via an executive program.

The user kit contains a library of programs for each specific application. There is a need to have a grid of weather data in one of several geographic projections at certain intervals. This data, in the form of the archival materials or the results of weather forecast models, are available on the Internet in the form of the already formatted data for input into HYSPLIT.

In addition, there are programs intended to convert NOAA output information, The National Center for Atmospheric Research (NCAR), or European Center for Medium-Range Weather Forecasts (ECMWF) source data into the format, which is suitable for the HYSPLIT model.

The impurities concentration in the air is calculated at the points of intersection of the grid coordinates (in latitude and longitude) for the air flows, and for the individual particles – in the form of cell-averaged concentrations. The model contains a ground coordinate grid, the sizes of bumps, and the terrain information at 1° resolution in the Northern Hemisphere. The model allows consideration of dry and wet deposition of impurities, radioactive decay and restoration of the suspension state.

The main initial parameters for the simulation are as follows:

• The initial time (year, month, day, hour);

• The position (initial values of latitude, longitude and altitude);

• The initial time and duration of dispersion (i.e. run duration);

• The impurity characteristics (number of types, speed and duration of the radiation);

• The size of the calculation grid (including the mixing height and the height of each vertical level on the concentration grid);

• The particle properties (diameter, density and shape, deposition rate, molecular weight, coefficient of chemical interaction with the surface, diffusion rate, half-life, suspension rate, etc.) and sampling time.

Currently, in some Eastern European countries, all the calculations of atmospheric pollution are carried out applying special software tools, i.e. the unified programs for calculating atmospheric pollution, which are an appendix to "Methods for calculation of the harmful substances concentration in the atmospheric air" [20]. In 2018, its new edition came into force, but the approach to simulation had not changed significantly ("Methods for calculating the dispersion of emissions of harmful (polluting) substances in the atmospheric air" [21]).

The unified program for the calculation of atmospheric pollution allows determining the concentrations of pollutants in atmospheric air by calculation. The program can be applied to any sources of emissions of polluting substances, regardless of which branch of the national economy they belong to.

A number of software products are based on this approach: the "Ecolog" program series of the "Integral" company [22], the Unified Program for the Calculation of Atmospheric Pollution "ECOcenter-Standard" [23], and others.

METHODOLOGY OF PROCESSING THE INFORMATION ON THE RADIONUCLIDES DISPERSION IN THE AIR AND ON THE SOIL SURFACE

Adaptation of the modeling system to a specific region or a specific task is a separate complex task [24, 25]. The method of processing information about pollution sources and environmental parameters for the formation of pollutant concentration maps consists of the following stages: analysis of the parameters required for processing; simulation of the pollution dispersion; visualization of simulation results (both archival and predictive).

This method was applied to analyze the process of Pu isotopes dispersion due to the movement of air masses in the places where fires occurred in April 2020 in the exclusion zone of the Chernobyl NPP and the associated dangers for the population and the environment [25]. The HYSPLIT program was used to study the pollutants spatial dispersion.

The maps of volumetric and surface activity of radionuclides in the air and in the process of their falling on the ground in the period of April 8-13, 2020 were constructed. Fig. 3 presents the map of Pu radionuclides volumetric activity in the air on April 9, 2020, due to the fire in the area of Kopachi village to Chistogalivka village.

Figure 3. Volumetric activity of Pu isotopes in the air on April 9, 2020 due to the fire in the area of Kopachi village to Chystohalivka village (per day), the source height being 20 m [25]

Fig. 4 presents the map of the surface activity of Pu isotopes in the process of their falling on the soil on April 9, 2020 in this area.

As a result of the analysis of the dispersion of Pu radionuclides in the territory under consideration, it was established that due to the presence of this element, the radioactivity in the air and in the process of radioactive particles falling on the ground was low. Despite the high radio toxicity of Pu isotopes, the contribution of their radioactivity to the radiation effect on the population during inspiration or consumption of food products will be insignificant.

The risk of fires in the exclusion zone of Chernobyl increases with the climate change, and the measures to prevent them should be considered in some emergency programs. This information will allow to gain some important insights about the dynamics of accumulation, transformation and migration of Pu and ^{241}Am isotopes. There is also an opportunity to study the impact of ionizing radiation from the fires in the exclusion zone of the Chernobyl NPP on the environment.

Figure 4. Surface activity of Pu isotopes in the process of their falling on the ground on April 9, 2020 due to the fire in the area of Kopachi village to Chistohalivka village (per day), the source height being 20 m [25]

CONCLUSIONS

An analysis of the up-to-date methods of simulation of the pollutants dispersion in atmospheric air, as well as the software complexes, which are based on them, has been carried out.

A method of processing the information about the pollution sources and environmental parameters for the formation of pollutant concentration maps, based on the HYSPLIT software complex has been proposed.

The expediency of using the HYSPLIT pollutant dispersion model for the analysis of Pu isotopes dispersion due to the movement of air masses in the places, where fires occurred in April 2020 in the exclusion zone of the Chornobyl NPP, is shown.

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МОДЕЛЮВАННЯ ПОШИРЕННЯ РАДІОНУКЛІДІВ У ПОВІТРІ ТА НА ПОВЕРХНІ ҐРУНТУ

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При побудові моделей поширення забруднюючих речовин у повітрі та на поверхні ґрунту використовуються математичні та чисельні методи для моделювання фізичних та хімічних процесів. На основі метеорологічних даних та інформації про джерело викидів, ці моделі характеризують як первинні забруднюючі речовини, що потрапляють безпосередньо в атмосферу, так і вторинні забруднювачі, що утворюються внаслідок складних хімічних реакцій. Ці моделі мають значення для системи управління якістю атмосферного повітря, оскільки дозволяють контролювати викиди в атмосферу, прогнозувати їх поширення та розробляти ефективні стратегії щодо скорочення шкідливих речовин в атмосфері. У статті наведено огляд обчислювальних методів, які застосовуються при моделюванні поширення забруднюючих речовин в атмосферному повітрі та на поверхні ґрунту, такі як модель гаусового факела, лагранжева дисперсійна стохастична модель, ейлерова модель атмосферної дифузії. Практичне застосування розглянутих моделей показало достатню надійність та достовірність прогнозу рівнів забруднення повітря та ґрунту. Моделювання виконується за допомогою комп'ютерних програм, що включають алгоритми для вирішення математичних рівнянь, які керують дисперсією забруднювача. Моделі розсіювання використовуються з метою оцінки концентрації забруднювачів повітря чи токсинів. Їх також можна використовувати для прогнозування майбутніх концентрацій за певних сценаріїв. Вони корисні для вивчення забруднюючих речовин, які розсіюються на великі відстані і можуть розпочинати реакцію у атмосфері. До таких програмних продуктів належать: AEROPOL, AERMOD, GRAL, TAPM CSIRO, CALPUFF, HYSPLIT тощо. Запропоновано метод обробки інформації про джерела забруднення та параметри навколишнього середовища для формування карт об'ємної та поверхневої активності радіонуклідів на основі програми HYSPLIT. Цей метод був застосований для аналізу процесу поширення ізотопів плутонію внаслідок руху повітряних мас у місцях виникнення пожеж у квітні 2020 р. у зоні відчуження Чорнобильської АЕС та пов'язані з цим небезпеки для населення та навколишнього середовища.

Ключові слова: *рівняння турбулентної дифузії; розсіювання домішки в атмосфері; точкове джерело; рівень приземної концентрації; забруднення атмосфери; об'ємна активність радіонуклідів*