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SECTION 2. Applied mathematics.
Mathematical modeling.

ADVANCED MODEL OF TRANSFER PROCESS AND DIFFUSION OF HARMFUL SUBSTANCES IN THE ATMOSPHERIC BOUNDARY LAYER

***Abstract**: This work considers the actual problem related to solving the problem of forecasting and environmental monitoring of air pool of industrial regions, where there is an imbalance of sanitary environmental standards due to the large number of emissions of harmful substances and active fine aerosol particles, and carbon dioxide gases into the atmosphere. In the article for solving the above mentioned problem there is a full mathematical model developed to conduct a comprehensive study of the process of transfer and diffusion of pollutants released into the environment from production facilities, which is described by a system of differential equations in partial derivatives with appropriate initial and boundary conditions. To derive a mathematical model of the object there were used the basic laws of mechanics and hydro thermodynamic (conservation equations of mass, energy, balance of power, the state, etc..), Taking into account the main parameters that play a significant role in the process of transport and diffusion of pollutants in the atmosphere: the wind speed and its directions; terrain; absorption coefficient of harmful aerosol fine particles in the atmosphere, etc. We obtain the differential equation for calculating the rate of deposition of fine and aerosol particles, propagating in the boundary layer of the atmosphere, when the principal parameters are considered, which affect the rate of particle deposition: the mass and radius of aerosol particles, density of the atmosphere, air resistance force.*

***Key words**: mathematical model, transfer and diffusion of pollutants, climatic factor, mechanics, hydro thermodynamics.*

***Language**: English*

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Introduction

The rapid development of spheres of production, mining and development of oil, gas and ore deposits, processing of raw materials and general-purpose products, construction of production facilities and settlement blocks has set humankind acute problem – protection of the environment. As a result of a sharp increase of harmful emissions in the industrial regions, the concentration of harmful substances in the atmosphere exceeded the maximum allowable by health norms. Problems related to coal mining, nonferrous metals and other minerals have led to soil erosion and contamination of vast areas of secondary materials and waste production that are a source of pollution of the air-water areas of cities and regions.

It also should be noted that emitted by thermal power stations, factories and production facilities, gas impurities undergo complex chemical reactions, as a result of which new, more toxic substances arise, which did not exist in the original emissions. These inorganic substances are especially harmful emissions of nitrogen oxides and sulfur oxides and carbon dioxide, etc. As we know, all thrown out harmful substances from industrial production objects in the environment (the ground layer of the atmosphere) end up as a material substance is deposited on the surface of the earth, and the heavy precipitated mainly by the gravitational field, and the light - a result of the diffusion process.

The growth of human impact on the environment caused by the intensive use of natural resources, production of energy from the bowels of the earth, as well as the development of material production, has led to the disruption of ecological balance as a locally - in particular areas of the globe, as well as globally - across the planet as a whole. This is especially evident in countries with rapid growth in the productive capacity of production facilities and primary processing of raw materials, as an example in the countries of India, China, North Korea, Singapore, etc.

In the reports of ITAR-TASS for December 2016 in China, France, Mongolia, the Balkans and other regions have been declared critical levels of air pollution. In particular, in Beijing the measures for the elimination of environmental threats to measures included stopping for a few days of the industrial facilities, lessons in schools, childcare institutions, and restrictions on the movement of vehicles inside the megalopolis.

As a result of ecology imbalance in the globe, cancer, asthma, and other allergic diseases began to grow sharply, the reduction of many species of fauna and flora occurred.

It is necessary to emphasize that in order to study, forecast and monitor the state of the atmospheric pool of industrial regions, as well as to assess the impact of anthropogenic factors it is necessary to develop a tool which can be used to solve the above mentioned problems. One of the most effective and constructive methods and tools for solving the problems is - mathematical modeling and computing experiments on a computer, with which you can give a qualitative and quantitative assessment of the ecological state of the environment of the region.

Review of Literature

The problems of mathematical modeling of the transfer processes, diffusion and transport of harmful substances (carbon dioxide gases, fine aerosol active and passive particles) were taught in the schools created under the direction of G.I. Marchuk, V.V. Penenko, A.E. Aloyana, L.T. Matveeva, V.P. Dymnikova I.E. Naatsa, E.A. Zakarin, I.A. Kibel, L.N. Gutmann, F.B. Abutalieva, as well as foreign scientists W.J. Layton, J.H. Ferziger, J.W. Deardorff. M. Germano., U. Piomelli., L.C. Berselli, G.S. Winckelmans, W.C. Reynolds, H. Zidisk, K.A. Velds, K.I. Nappo, J. Gotaas, M. Mullioland, S. Trap, M. Maties, V. Edelman etc.

To solve the urgent global problems there are established science centers and schools under the guidance of leading specialists in various branches of science dealing with problems of environmental protection, protection of water resources from external technological factors, the impact of the transformations in the ecosystem, etc. Scientific schools and centers obtained significant results of theoretical and applied character. The literature review shows that the list of urgent problems to be solved with the help of mathematical modeling, environmental issues occupies a special place.

Korchagin P.V. and others [1-3] developed a kinematic model of spreading of the reactant particles in the cloud, which describes by a system of quasi-linear partial differential equations of parabolic type, axisymmetric jet, typical for cumulonimbus clouds, which takes into account transfer processes, diffusion, generation and dissipation of turbulence on the development and investigated the behavior of the approximate solution depending on the selected grid

Lisanov M.V. [4] considered the problem of modeling the scattering of hazardous gaseous emissions in the atmosphere. Three main approaches are noted for modeling of the process: Gaussian dispersion model called dispersion models; The model is based on the integral conservation laws of substance; models based on the numerical solution of a system of conservation equations - numerical simulation.

In this work, there is developed a mathematical model, which describes the following processes: the cloud movement at variable wind speed vertical; gravitational spreading; scattering cloud in the vertical direction due to atmospheric turbulence; heating or cooling of the cloud due to air mixing; heat exchange cloud with the underlying surface.

The Authors at the study of the process of transfer and diffusion of harmful particles in the atmosphere took into account the changes in the mass and the internal energy of the cloud and its physical characteristics and equalized the results of model calculations with experimental data. According to the results of the numerical calculations the following conclusions were drawn: standard methods, based on Gaussian models cannot predict with sufficient precision the spread of harmful substances (heavy gas) as a multiple rocket launcher, as well as from the permanent sources of harmful substance emissions in the atmosphere.

The article [5] presents the main approaches to the creation of computer models of atmospheric phenomena. The current models of the distribution of the substance in the atmosphere, dust and pollen filters were reviewed and the advantage of the Finnish Meteorological Institute's SILAM model was showed. The physical side of the problem is related to the analysis of emission, the spread and absorption of pollutants are considered in this work.

Berlyand M.E. [6] showed the significant factors affecting the process of transfer and diffusion of harmful substances: the atmospheric circulation regime, its thermal stability; atmospheric pressure, humidity, temperature mode; temperature inversions, their frequency and duration; wind speed, repeatability of air stagnation and weak winds (speeds of up to 1 m/s); duration of fog; topography, geology and hydrogeology of the area; soil and vegetation conditions (soil type, water permeability, porosity, particle size distribution of soils, vegetation state, the composition of species, age, site class); background values of indicators of pollution of natural components of the atmosphere; condition of the animal world.

Volkov V.Yu, [7] developed a distributed automated system through the use of modern information technologies allowing to increase the efficiency of research and forecasting the spread of pollutants emitted by chemical-technological enterprises in the atmosphere of the industrial region.

The papers [8-9] are devoted to a critical analysis of the applicability of physical and mathematical models of atmospheric diffusion for studies of air pollution with harmful emissions of road transport. We consider the specific characteristics of the exhaust gas composition, patterns of migration and metabolism in a stratified atmosphere. Air pollution monitoring map is demonstrated using the ring road of St. Petersburg as an example.

Belosludtsev A.A. [10] constructed a mathematical model to describe the non-stationary three-dimensional dynamics of pollution, including from non-stationary sources for a particular specified by the physical state of the atmosphere. In the proposed approach it is used a direct numerical integration of the exact equations impurity transport in the atmosphere, taking into account the main physical factors that approximates this method to conduct computational experiments. On the basis of the developed mathematical model it is created an information system for computer modeling of the process of pollution spreading from industrial sources located on the territory of the enterprise.

The adequacy of the model to the process is verified using the current detection algorithms.

Chernyavskiy S. [11] conducted analytical research of processes of emissions enterprises' dissemination in the atmosphere. The carbon dioxide ($CO2$) is considered as a major atmospheric pollutant. In the work is presented the Green's function for the problem of one-off instant of emission of harmful impurities in the standard atmospheric boundary layer with a given wind field and an expression is derived for the concentration of impurities in a stationary case and by continuously operating sources of pollution. The levels of equal pollution of atmosphere are built and their transformation by the change of the source's parameters are analyzed.

In paper [12] the task of modelling of gaseous impurities' emissions in the atmosphere is considered in a new mathematical formulation, which allows to take into account the mutual influence of various dynamic processes occurring by the implementation of the production cycles or as a result of accidents at industrial enterprises.

Smirnov E.A. [13] created an information system for mathematical modeling of the process of transfer and diffusion of pollutants in the atmosphere with the use of software applications «ArcGIS», which reflects the real state of the air in the regions. But here it should be noted that under this system the results can be obtained only at certain areas, and they cannot give an adequate picture of the air state in the rest of the territory.

Aloyan A.E. [14] devoted his research to the development of mathematical models of the dynamics and kinetics of the process of transfer and diffusion of gas and aerosol impurities in the atmosphere. In the work is shown the model of multicomponent impurities' transfer taking in to account of photochemical transformation and formation of aerosols in the troposphere of the northern hemisphere, taking into account the kinetic processes of enucleation, condensation and coagulation.

Chub A.I. in paper [15] presented the software of the process of inflammable objects' placement and their optimization taking into account the terrain and spatial form.

Sukhinov A.I. [16] developed computer model for research, forecasting and monitoring of transport of hazardous substances from motor vehicles into the environment. It is shown numerical realization of the model on a computer using the finite volume method based on distributed algorithm developed for computing.

The modeling of the field of wind flows based on Navier-Stokes equations' system taking into account the compressibility and turbulence of the air environment, the terrain is offered in [17], and SIMPLE-algorithm is used as a numerical method.

Kordzadze A. [18] conducted the research based on developed regional models of the process of diffusion of substances described hydro-thermodynamic equation, namely the equation of molecular heat conduction in the active layer of soil, taking into account the heat balance of the underlying surface (water, earth). Developed by researcher a comprehensive mathematical model is made up of individual blocks, each of which represents a mathematical model describing the hydro-thermodynamic processes in separate environmental objects. The authors investigate the environmental problems associated with the distribution of pollutants from the known sources and determine the probable location of the source in an aqueous medium.

The process of transfer and diffusion of pollutants in the atmosphere taking into account different climatic factors and external disturbers is considered in [19]. The work deals with the transfer of pollutants from the source based on the advection of pollutants from the average air flow, mixing polluting atmospheric turbulence and mass diffusion. In addition, it gives the study process under various physical and mathematical aspects related to the transport and diffusion of pollutants in the atmospheric boundary layer by weak and strong winds.

Here it should be emphasized, that the question of mathematical modeling of pollutant's spread transported by water is of considerable interest.

In article [20] the problem related to the process of dissemination of harmful substances in the environment is considered and it is modeled as a set of four simple models: overland water flow, seepage, migration of pollutants runoff and pollutant deposition (accumulation) on the ground. The model is based on the diffusion equation with additional terms on the right side. In the developed mathematical model of the process are taken into account the influence of topography, lithologic structure of the territory and the intensity of the pollution from the absorption rate of the earth surface. The shape, the boundaries and the topology of problem solving varies with the time depending on the appearance of dry "islands" surrounded by water.

Khan Y. [21] devoted the work to the dispersion and diffusion process of reactive primary pollutants emitted from elevated line sources in a stable boundary layer of the atmosphere with the generalized wind speed and the quadratic function of the vertical height. For this setting, an exact solution was found with the help Laplace's transform for linear sources in the atmospheric boundary layer. It takes into account the chemical reaction that occurs as a result of interaction with the air mass, as well as the conversion of gaseous pollutants in the solid particles and their deposition on the surface of the considerable area.

In the papers [22-26] a mathematical software for solving the problem of motion of multicomponent air environment, taking into account the transfer and diffusion of pollutants in the atmosphere, the changes in the thermal regime of the atmosphere, phase transition, as well as the influence of vegetation.

The work [27] is devoted to the transfer of hazardous substances in the air flow of the atmosphere's surface layer over long and medium distances.

Analysis of these sources showed, that in the studies of the authors is not considered a process of transfer and diffusion of multi-component pollutants in the atmosphere, where the a significant role play the main factors: the rate of deposition of the gel particles, depending on the line size and weight; speed of the air mass of the atmosphere in three directions, u, v and w; terrain of the considered industrial region; heat transfer between the liquid and gaseous phases; the changes of the density state and their temperature etc. which vary in the day and time of year.

It should also be noted that by the mathematical modeling of the process of dissemination of harmful substances in the atmosphere in the works of many authors assumed that the spread of harmful substances emitted from the sources does not reach the boundaries of the area under consideration for solving the problem and there is no inflow and outflow of harmful substances through them.

During this study of the process of transfer and diffusion of harmful substances in the atmosphere, there were made the efforts to fill this gap.

Based on the foregoing, the aim of this work is to develop mathematical models and numerical algorithms for solving the problem of transfer and diffusion of aerosol emissions in the boundary layer of the atmosphere.

Problem Statement

To simulate the process of transfer and diffusion of pollutants in the atmosphere, based on the basic laws of hydro thermodynamics and hydromechanics of the process we obtain the equations of pollutant's transfer in the atmosphere:

$$\begin{aligned}&\frac{\partial\theta}{\partial t}+u\frac{\partial h\theta}{\partial x}+v\frac{\partial h\theta}{\partial y}+\\&+\left(w-w_g\right)\frac{\partial h\theta}{\partial z}+h\sigma\theta=\\&=\frac{\partial}{\partial x}\left(\mu h\frac{\partial\theta}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu h\frac{\partial\theta}{\partial y}\right)+\\&+\frac{\partial}{\partial z}\left(\eta h\frac{\partial\theta}{\partial z}\right)+\delta_{i,j,k}I,\end{aligned}\qquad(1)$$

which takes into account the air mass velocities, terrain, and the coefficient of diffusion and turbulence, the speed of deposition of harmful substances on the earth's surface, the absorption coefficient of harmful substances in the atmosphere.

Taking into account aggregation state of harmful compounds emitted into the atmosphere, we can write the equation describing the transition of water from liquid to gaseous state and vice versa [1-2]:

- when the source is supplied with gas

$$\begin{aligned}&\frac{\partial\theta_1}{\partial t}+u\frac{\partial h\theta_1}{\partial x}+v\frac{\partial h\theta_1}{\partial y}+w\frac{\partial h\theta_1}{\partial z}=\\&=\frac{\partial}{\partial x}\left(\mu h\frac{\partial\theta_1}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu h\frac{\partial\theta_1}{\partial y}\right)+\\&+\frac{\partial}{\partial z}\left(\eta h\frac{\partial\theta_1}{\partial z}\right)+\delta_{i,j,k}I_1;\end{aligned}\qquad(2)$$

- when the source is supplied with water in gaseous state

$$\begin{aligned}&\frac{\partial\theta_2}{\partial t}+u\frac{\partial h\theta_2}{\partial x}+v\frac{\partial h\theta_2}{\partial y}+w\frac{\partial h\theta_2}{\partial z}=\\&=\frac{\partial}{\partial x}\left(\mu h\frac{\partial\theta_2}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu h\frac{\partial\theta_2}{\partial y}\right)+\\&+\frac{\partial}{\partial z}\left(\eta h\frac{\partial\theta_2}{\partial z}\right)+\delta_{i,j,k}I_2+\frac{v_g}{\rho_p};\end{aligned}\qquad(3)$$

- when the source is supplied with water

$$\frac{\partial \theta_3}{\partial t}+u\frac{\partial h\theta_3}{\partial x}+v\frac{\partial h\theta_3}{\partial y}+ +\left(w-w_g\right)\frac{\partial h\theta_3}{\partial z}+h\sigma_1\theta_3 = =\frac{\partial}{\partial x}\left(\mu h\frac{\partial \theta_3}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu h\frac{\partial \theta_3}{\partial y}\right)+ +\frac{\partial}{\partial z}\left(\eta h\frac{\partial \theta_3}{\partial z}\right)+\delta_{i,j,k}I_3-\frac{v_g}{\rho_p}; \tag{4}$$

- when the source is supplied with soot

$$\frac{\partial \theta_4}{\partial t}+u\frac{\partial h\theta_4}{\partial x}+v\frac{\partial h\theta_4}{\partial y}+ +\left(w-w_g\right)\frac{\partial h\theta_4}{\partial z}+h\sigma_2\theta_4 = =\frac{\partial}{\partial x}\left(\mu h\frac{\partial \theta_4}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu h\frac{\partial \theta_4}{\partial y}\right)+ +\frac{\partial}{\partial z}\left(\eta h\frac{\partial \theta_4}{\partial z}\right)+\delta_{i,j,k}I_4. \tag{5}$$

To determine the concentration of harmful substances in the atmosphere, depending on the orography of the terrain and weather climatic factors necessary to set initial and boundary conditions:

$$\left.\begin{aligned} &\theta_i(x,y,z)=\theta_{i,H}(x,y,z) \text{ при } t=0,\\ &\mu\left.\frac{\partial\theta_i}{\partial x}\right|_{x=0}=\left(\theta_i-\theta_{i,H}\right),\mu\left.\frac{\partial\theta_i}{\partial x}\right|_{x=L_x}=\left(\theta_i-\theta_{i,H}\right),\\ &\mu\left.\frac{\partial\theta_i}{\partial y}\right|_{y=0}=\left(\theta_i-\theta_{i,H}\right),\mu\left.\frac{\partial\theta_i}{\partial y}\right|_{y=L_y}=\left(\theta_i-\theta_{i,H}\right),\\ &\left.\frac{\partial\theta_i}{\partial z}\right|_{z=0}=\xi\theta_i-\tilde{f},\ \left.\frac{\partial\theta_i}{\partial z}\right|_{z=L_z}=0, \end{aligned}\right\} \tag{7}$$

where: i=1, 2, 3, 4.

Here, - $\theta_1,\ \theta_2,\ \theta_3,\ \theta_4, \theta_{i,H}$ respectively the concentration of harmful substances emitted in water form in a gaseous state, gas in the source, liquid water, soot and their original value in the atmosphere; $u,\ v,\ w$ - wind speed in three directions; $v_g=f\left(\rho_n-\rho_1\right)$ - mass evaporation rate; ρ_n - the density of the saturated vapor; μ - the diffusion coefficient; η - the coefficient of turbulence; ξ - interaction coefficient with the underlying ground surface; h - function describing the orographic surface of the earth; $I_1,\ I_2,\ I_3,\ I_4$ - power of emission sources respectively for harmful gas, water in a gaseous form, liquid water and soot; $\tilde{f}$ - A source of emission of harmful substances from the settling surface of the earth; $\sigma_1,\ \sigma_2$ - coefficient of absorption of harmful substances in the atmosphere (water in liquid form, and soot); $\delta_{i,j,k}$ - Dirac function; w_g - deposition rate of harmful particles.

Solution Method

The statement of the problem (1) - (7) implies, that for its numerical integration, it is necessary to calculate of the velocity of the air mass of the atmosphere in three directions respectively in u, v and w.

To determine the rates of movement of air masses in the atmosphere in three directions u, v and w consider the hydrodynamic equations by Navier-Stokes:

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}= =\frac{1}{\rho}\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)+ +\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\eta\frac{\partial u}{\partial z}\right)-g_x, \tag{8}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}= =\frac{1}{\rho}\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial x}\right)+ +\frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(\eta\frac{\partial v}{\partial z}\right)-g_y, \tag{9}$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}= =\frac{1}{\rho}\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial w}{\partial x}\right)+ +\frac{\partial}{\partial y}\left(\mu\frac{\partial w}{\partial y}\right)+\frac{\partial}{\partial z}\left(\eta\frac{\partial w}{\partial z}\right)-g_z, \tag{10}$$

$$\frac{\partial w_g}{\partial t}+u\frac{\partial w_g}{\partial x}+v\frac{\partial w_g}{\partial y}+w\frac{\partial w_g}{\partial z}= =\frac{1}{\rho}\frac{\partial P}{\partial x}+\frac{\partial}{\partial x}\left(\mu\frac{\partial w_g}{\partial x}\right)+ +\frac{\partial}{\partial y}\left(\mu\frac{\partial w_g}{\partial y}\right)+\frac{\partial}{\partial z}\left(\eta\frac{\partial w_g}{\partial z}\right)-G_z-R_s, \tag{11}$$

with initial and boundary conditions

$$\begin{aligned} &u(x,y,z,0)=\dot{u}(x,y,z);\\ &v(x,y,z,0)=\dot{v}(x,y,z);\\ &w(x,y,z,0)=\dot{w}(x,y,z);\\ &w_g(x,y,z,0)=\dot{w}_g(x,y,z). \end{aligned} \tag{12}$$

$$\left.\begin{aligned}
&\mu\left.\frac{\partial u}{\partial x}\right|_{x=0}=\left(u-\dot{u}_0\right),\mu\left.\frac{\partial u}{\partial x}\right|_{x=L_x}=\left(u-\dot{u}_0\right),\\
&\mu\left.\frac{\partial v}{\partial y}\right|_{y=0}=\left(v-\dot{v}_0\right),\mu\left.\frac{\partial v}{\partial y}\right|_{y=L_y}=\left(v-\dot{v}_0\right),\\
&\eta\left.\frac{\partial w_g}{\partial z}\right|_{z=h_v}=\varphi(x,y,h_v,t),\\
&\eta\left.\frac{\partial w_g}{\partial z}\right|_{x=L_z}=0,\eta\left.\frac{\partial w}{\partial z}\right|_{z=0}=0,\\
&\eta\left.\frac{\partial w}{\partial z}\right|_{x=L_z}=0.
\end{aligned}\right\}\quad(13)$$

Here P - pressure; $g_{(x,y,z)}$ -the projection of the components of the gravitational acceleration, $R_s = w_g(6\pi kr - 1/2 * c\rho_a S w_g)$ - the power of the air resistance, m - particle mass, *r*-radius of the particles, S - cross sectional area of the particles, ρ_a - atmospheric density, c - dimensionless quantity equal to 0.5.

To calculate the density of emitted substances into the atmosphere, taking into account the mass conservation law for fluid flowing through the fixed volume, the continuity equation will be obtained.

$$\begin{aligned}
&\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=\\
&=\frac{\partial}{\partial x}\left(\mu\frac{\partial\rho}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial\rho}{\partial y}\right)+\\
&+\frac{\partial}{\partial z}\left(\eta\frac{\partial\rho}{\partial z}\right)+I_g
\end{aligned}\quad(14)$$

with appropriate initial and boundary conditions:

$$\rho(x,y,z)\big|_{t=0}=\rho_c,$$

$$\left.\begin{aligned}
&\mu\left.\frac{\partial\rho}{\partial x}\right|_{x=0}=\left(\rho-\rho_0\right),\mu\left.\frac{\partial\rho}{\partial x}\right|_{x=L_x}=\left(\rho-\rho_0\right),\\
&\mu\left.\frac{\partial\rho}{\partial y}\right|_{y=0}=\left(\rho-\rho_0\right),\mu\left.\frac{\partial\rho}{\partial y}\right|_{y=L_y}=\left(\rho-\rho_0\right),\\
&\left.\frac{\partial\rho}{\partial z}\right|_{z=0}=0,\ \left.\frac{\partial\rho}{\partial z}\right|_{z=L_z}=0.
\end{aligned}\right\}\quad(15)$$

Since impurities emitted into the environment have a certain temperature, which plays a significant role in the spread of harmful substances into the atmosphere, consideration of this factor is necessary. The equation describing processes of transfer and heat diffusion and heat exchange with the environment is as follows:

$$\begin{aligned}
&\frac{\partial\Phi}{\partial t}+u\frac{\partial\Phi}{\partial x}+v\frac{\partial\Phi}{\partial y}-w_g\frac{\partial\Phi}{\partial z}=\\
&=\frac{\partial}{\partial x}\left(\mu\frac{\partial\Phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial\Phi}{\partial y}\right)+\\
&+\frac{\partial}{\partial z}\left(\eta\frac{\partial\Phi}{\partial z}\right)+\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)+\\
&+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right)+\delta_{i,j,k}I_T.
\end{aligned}\quad(16)$$

Here Φ - the thermal energy; w_g - The rate of deposition of suspended particles; λ - coefficient of thermal conductivity; I_T - Function describing the distribution and power of the heat source. Since we consider the propagation of a multi-component environment, then for the coefficient of thermal conductivity and thermal energy is a fairly relation

$$\Phi=\sum_{i=1}^{L}\Phi_i\theta_i=\sum_{i=1}^{L}\rho_i c_i\theta_i T_i.$$

In our formulation for heat transfer problem in a multi-component environment can be considered the cases:

- Heat transfer for gas

$$\begin{aligned}
&R_1\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(R_2\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(R_2\frac{\partial T}{\partial y}\right)+\\
&+\frac{\partial}{\partial z}\left(R_2\frac{\partial T}{\partial z}\right)+\bar{q}_2 v_g-\alpha_v\left(T-T_s\right),
\end{aligned}\quad(17)$$

where $R_1=\sum_{i=1}^{2}\rho_i c_\rho\theta_i$; $R_2=\sum_{i=1}^{2}\left(\rho_i c_\rho\mu+\lambda_i\right)\theta_i$; v_g - the mass evaporation rate; ρ, c_ρ - density and heat capacity of gas phase; $\bar{q}$ - Specific heat of transformation, T, T_s - the temperature of the gas and condensed phases; α_v - heat transfer coefficient;

- Transfer of heat to the condensate

$$\begin{aligned}
&R_3\left(\frac{\partial T}{\partial t}-w_0\frac{\partial T_s}{\partial z}\right)=\\
&=\frac{\partial}{\partial x}\left(\left(R_3\mu\right)\frac{\partial T_s}{\partial x}\right)+\frac{\partial}{\partial y}\left(\left(R_3\mu\right)\frac{\partial T_s}{\partial y}\right)+\\
&+\frac{\partial}{\partial z}\left(\left(R_3\mu\right)\frac{\partial T_s}{\partial z}\right)-\alpha_v\left(T-T_s\right),
\end{aligned}\quad(18)$$

where $R_3=\sum_{i=3}^{4}\left(\rho_i c_{\rho_i}\theta_i\right)$; c_{ρ_i}, θ_i, ρ_i - specific heat capacity, volume fractions i-th phase and the true density; T, T_s - the temperature of the gas and condensed phases.

To solve (17) - (18) we give initial and boundary conditions:

$$T(x,y,z)=T_0(x,y,z);\quad(19)$$

$$\left.\begin{aligned}
&\lambda\frac{\partial T}{\partial x}\bigg|_{x=0}=(T-T_0),\ \lambda\frac{\partial T}{\partial x}\bigg|_{x=L_x}=(T-T_0),\\
&\lambda\frac{\partial T}{\partial y}\bigg|_{y=0}=(T-T_0),\ \lambda\frac{\partial T}{\partial y}\bigg|_{y=L_y}=(T-T_0),\\
&\lambda\frac{\partial T}{\partial z}\bigg|_{z=0}=(T-T_0),\ \lambda\frac{\partial T}{\partial z}\bigg|_{z=L_z}=(T-T_0).
\end{aligned}\right\}\quad(20)$$

To determine the vapor pressure in terms of temperature, we use the equation of Mendeleev-Clapeyron and through differentiation obtain

$$\frac{\rho}{P}\frac{\partial P}{\partial t}=\frac{\partial\rho}{\partial t}+\frac{\rho}{T}\frac{\partial T}{\partial t}.\qquad(21)$$

Here ρ_i, R, M - density, universal gas constant, molar mass; k_1 - coefficient of thermal conductivity.

To solve equation (8) - (12) we split by the physical parameters and obtain the three tasks, the first one can be written in the difference analogue:

$$\left.\begin{aligned}
&\frac{u^{n+1/3}-u^n}{\Delta t/3}+\left(u\frac{\partial u}{\partial x}\right)^{n+1/3}+\\
&+\left(v\frac{\partial u}{\partial y}\right)^{n+1/3}+\left(w\frac{\partial u}{\partial z}\right)^{n+1/3}=-G_x,\\
&\frac{v^{n+1/3}-v^n}{\Delta t/3}+\left(u\frac{\partial v}{\partial x}\right)^{n+1/3}+\\
&+\left(v\frac{\partial v}{\partial y}\right)^{n+1/3}+\left(w\frac{\partial v}{\partial z}\right)^{n+1/3}=-G_y,\\
&\frac{w^{n+1/3}-w^n}{\Delta t/3}+\left(u\frac{\partial w}{\partial x}\right)^{n+1/3}+\\
&+\left(v\frac{\partial w}{\partial y}\right)^{n+1/3}+\left(w\frac{\partial w}{\partial z}\right)^{n+1/3}=-G_z,\\
&\frac{w_g{}^{n+1/3}-w_g{}^n}{\Delta t/3}+\left(u\frac{\partial w_g}{\partial x}\right)^{n+1/3}+\\
&+\left(v\frac{\partial w_g}{\partial y}\right)^{n+1/3}+\left(w\frac{\partial w_g}{\partial z}\right)^{n+1/3}=-G_z-R_s,
\end{aligned}\right\}\quad(22)$$

the second one:

$$\left.\begin{aligned}
&\frac{u^{n+2/3}-u^{n+1/3}}{\Delta t/3}=\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial x}\right)^{n+2/3}+\\
&+\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)^{n+2/3}+\frac{\partial}{\partial z}\left(\eta\frac{\partial u}{\partial z}\right)^{n+2/3},\\
&\frac{v^{n+2/3}-v^{n+1/3}}{\Delta t/3}=\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial x}\right)^{n+2/3}+\\
&+\frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial y}\right)^{n+2/3}+\frac{\partial}{\partial z}\left(\eta\frac{\partial v}{\partial z}\right)^{n+2/3},\\
&\frac{w^{n+2/3}-w^{n+1/3}}{\Delta t/3}=\frac{\partial}{\partial x}\left(\mu\frac{\partial w}{\partial x}\right)^{n+2/3}+\\
&+\frac{\partial}{\partial y}\left(\mu\frac{\partial w}{\partial y}\right)^{n+2/3}+\frac{\partial}{\partial z}\left(\eta\frac{\partial w}{\partial z}\right)^{n+2/3},\\
&\frac{w_g{}^{n+2/3}-w_g{}^{n+1/3}}{\Delta t/3}=\frac{\partial}{\partial x}\left(\mu\frac{\partial w_g}{\partial x}\right)^{n+2/3}+\\
&+\frac{\partial}{\partial y}\left(\mu\frac{\partial w_g}{\partial y}\right)^{n+2/3}+\frac{\partial}{\partial z}\left(\eta\frac{\partial w_g}{\partial z}\right)^{n+2/3},
\end{aligned}\right\}\quad(23)$$

and the third one:

$$\left.\begin{aligned}
&\frac{u^{n+1}-u^{n+2/3}}{\Delta t/3}=-\frac{1}{\rho}\frac{\partial P}{\partial x},\\
&\frac{v^{n+1}-v^{n+2/3}}{\Delta t/3}=-\frac{1}{\rho}\frac{\partial P}{\partial y},\\
&\frac{w^{n+1}-w^{n+2/3}}{\Delta t/3}=-\frac{1}{\rho}\frac{\partial P}{\partial z}.\\
&\frac{w^{n+1}-w^{n+2/3}}{\Delta t/3}=-\frac{1}{\rho}\frac{\partial P}{\partial z}.
\end{aligned}\right\}\quad(24)$$

Here η - coefficient of turbulent exchange.

Next, multiplying the system of equations (24) by $\rho\Delta t/3$ and differentiating with respect to the variables x, y, z, respectively, at the end we get

$$\left.\begin{aligned}
&\left(\rho\frac{\partial u}{\partial x}\right)^{n+1}=\left(\rho\frac{\partial u}{\partial x}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial x^2},\\
&\left(\rho\frac{\partial v}{\partial y}\right)^{n+1}=\left(\rho\frac{\partial v}{\partial y}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial y^2},\\
&\left(\rho\frac{\partial w}{\partial z}\right)^{n+1}=\left(\rho\frac{\partial w}{\partial z}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial z^2},\\
&\left(\rho\frac{\partial w_g}{\partial z}\right)^{n+1}=\left(\rho\frac{\partial w_g}{\partial z}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial z^2}.
\end{aligned}\right\}\quad(25)$$

Substituting system (25) into (13) we get the following:

$$\begin{gathered}\frac{\partial\rho}{\partial t}+\left(\frac{\partial(\rho u)}{\partial x}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial x^2}+\\+\left(\frac{\partial(\rho v)}{\partial y}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial y^2}+\\+\left(\frac{\partial(\rho w)}{\partial z}\right)^{n+2/3}-\Delta t/3\frac{\partial^2 P}{\partial z^2}=\\=\left(\mu\frac{\partial^2\rho}{\partial x^2}\right)+\left(\mu\frac{\partial^2\rho}{\partial y^2}\right)+\left(k_0\frac{\partial^2\rho}{\partial z^2}\right)+I_g.\end{gathered}\tag{26}$$

Using equation of state (26) we obtain an equation for calculating the pressure field:

$$\begin{gathered}\left(\frac{\rho}{P}\frac{\partial P}{\partial t}\right)=\Delta t/3\frac{\partial^2 P}{\partial x^2}+\Delta t/3\frac{\partial^2 P}{\partial y^2}+\\+\Delta t/3\frac{\partial^2 P}{\partial z^2}-\frac{\rho}{T}\frac{\partial T}{\partial t}-\left(\rho\frac{\partial u}{\partial x}\right)^{n+2/3}-\\-\left(\rho\frac{\partial v}{\partial y}\right)^{n+2/3}-\left(\rho\frac{\partial w}{\partial z}\right)^{n+2/3}+\\+\left(\mu\frac{\partial^2\rho}{\partial x^2}\right)+\left(\mu\frac{\partial^2\rho}{\partial y^2}\right)+\left(k_0\frac{\partial^2\rho}{\partial z^2}\right)+I_g.\end{gathered}\tag{27}$$

With the help of the equation (27) we got, we can calculate the field of pressure distribution in the considered layer of the atmosphere.

Thus, we developed a three-dimensional mathematical model of the process of the spread of harmful substances in the atmospheric boundary layer, taking into account the terrain and the characteristics of the underlying surface.

During the development of this model there were used: the equation of motion of a multicomponent air environment, model of pressure calculation, model of heat flow, which is described by the equations of heat conduction and gas condensate.

With the help of the given model you can calculate the key indicators and parameters that affect the process of transfer and diffusion of harmful multicomponent compound emitted from industrial facilities, construction areas and drained parts of seas and lakes.

Conclusion

Mathematical models of transfer and diffusion of pollutants in the form of water, gas and soot in a multicomponent air environment, which take into account such factors as the transition of water from a liquid to a gaseous state, a turbulent exchange, convective motion, precipitation of substances, heat transfer between the liquid and gaseous states, and variable density and temperature, as well as consideration of the terrain that greatly affects the dynamically changing state of the object of study.

An equation was derived to calculate the rate of deposition of the gel particles in the process of transfer and diffusion of the gel particles, depending on the line size and mass, the speed of movement of the air mass of the atmosphere in three directions and force of air resistance.

While developing a mathematical model of process of harmful substances' spread in the atmosphere, an equation for calculating the pressure field was derived, which takes into account the compressibility of the medium, the thermal expansion, the turbulent mixing of the air mass of the atmosphere.

The peculiarity of the developed mathematical models of transfer and diffusion of harmful substances in the boundary layer of the atmosphere and the movement of the air environment is connected with the account of turbulent compound in the equation of continuity of the environment, as well as consideration of the effect of orographic surface of the ground vegetation on the distribution of aerosol particles in the atmosphere.

In the developed mathematical model of the process is taken into account the transfer and diffusion of harmful components through borders of solving problems' section, with the help of the boundary condition of the third kind, which corresponds to the actual physical nature of the considered process.

The developed mathematical model, taking into account the above factors more adequately describes the process as compared to other known models offered by other authors.

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