Modelling the pollutants transport in the "air-water" system of a shallow water

T V Lyashchenko¹,4, I A Lyapunova¹, A E Chistyakov ²,³, A V Nikitina¹,³, A A Filina¹ and A L Leontiev¹,³

¹Southern Federal University, Rostov-on-Don, Russia
²Don State Technical University, Rostov-on-Don, Russia
³Science and Technology University "Sirius", Sochi, Russia
⁴Taganrog Management and Economics Institute, Taganrog, Russia

Abstract. The work is devoted to the spread processes mathematical modelling of impurities in a reservoir in areas located far from river runoff. An aerodynamic processes mathematical model is proposed that takes into account a variety factors: increased air humidity, variability of atmospheric pressure and temperature, etc. The model discretization was carried out taking into account the partial filling of the calculated cells, which made it possible to significantly reduce the error at the boundary. For the calibration and verification of the pollutants transport model, the expeditionary research data were used.

1. Introduction
Most of the pollutants coming from industrial facilities and transport are concentrated in the surface atmosphere layer the, and are deposited on the surface of the water or enters the reservoir with precipitation [1-3]. It is known that in the distance of river runoff, more than 60% of pollutants enter the reservoir from the air substances affecting the production and destruction phytoplankton processes. Toxic pollutants enter water bodies from the atmosphere, are absorbed by phytoplankton, and then are transmitted to more highly organized organisms through food chains. Therefore, it became necessary to develop mathematical models to predict changes in the ecological situation in shallow water and coastal areas, including: the pollution spread processes in the border layer of the coastal zone atmosphere; pollutants movement and sediments, the organic sediments decomposition processes [4-6].

The analyzing problems, monitoring and predicting the air environment quality in cities with intensive traffic flows are very important, the health and comfortable people living conditions depend on their solution. From a theoretical and applied view point, significant among the analyzing tasks and forecasting the air environment state are those that take into account the multicomponent nature, including a significant change in humidity, the phase transitions presence, etc., which is especially important for coastal cities. An effective tool for predicting the air quality is mathematical modelling of the variability of its gas and aerosol compositions, as well as assessing the atmospheric impurities impact on the environment, including on adjacent aquatic ecosystems [7]. Many gaseous and aerosols impurities transformation processes occur in a turbulent atmosphere. To reproduce the atmosphere turbulent characteristics variability, the impurities propagation modelling problem solution must be carried out in conjunction with hydrodynamic models [8-10]. At present, in the mathematical modelling field of the pollutions movement processes in the atmosphere and the numerical methods development for these purposes, a situation has arisen in which in the process of ongoing research individual phenomena are
considered, but they are not included in the complex. Therefore, to solve the problems that meet the set task, it is necessary to develop new mathematical models based on the gas dynamics equations and the matter conservation laws, taking into account the multicomponent medium nature.

In practice, special attention is paid to the study of the processes of transfer of pollutants (pollutants) in the air. The air movement and the pollutants spread in it includes four stages [11]. Pollutants matters transport scheme in the "air-water" system is shown in figure 1.

![Figure 1. Pollutants matters transport scheme of in the "air-water" system.](image)

Recently, mathematical modeling in the water bodies hydrophysics field and impurities transport has advanced and went beyond academic research – many industrialized countries use hydrophysical models in the water ecosystems study. Currently, two-dimensional and three-dimensional mathematical hydrophysic models have been developed, but the further scientific research area has not been exhausted, and the use of modern technologies will provide their quantitative and qualitative improvement.

To describe the pollutants transfer in the air and their deposition on the reservoir surface, in this work, interacting motion models of multicomponent air medium and a model describing the pollutants transport processes in the air-water system are proposed. The motion models of multicomponent air medium is used to calculate the velocity vector field and takes into account such factors as: turbulent exchange; variable density; dependence density air on pressure.

2. The air multicomponent medium movement model

Due to complexity of describing the properties and urban relief shape, the influence of such factors as temperature, humidity and air density on the currents nature, the atmosphere mobile turbulent nature, the air environment state is nontrivial. For effective observation, assessment and changes forecasting in the atmosphere state, all these factors must be taken into account in detail. There is still no universal mathematical model for solving such a complex problem. Applying the mass conservation law to a liquid flowing through a fixed infinitesimal control volume, we obtain the continuity equation (1) [12-14]:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial \rho}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial \rho}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial \rho}{\partial z} \right) + I_\rho,
\]

where \( \rho \) is the air density. Similarly, the momentum equation follows from Newton's second law

\[
\rho \frac{dv}{dt} = \rho g + \frac{\partial}{\partial x} \Pi_y,
\]

where \( g \) is the gravity acceleration, \( \Pi_y \) is stress tensor.

For all gases that can be considered a continuous medium, as well as for most liquids, it can be seen that the tension at some point linearly depends on the rate of deformation of the liquid. According to
[2], the general deformation law, which relates the tension tensor to pressure and velocity components, is written in the form

$$\Pi_{ij} = -p\delta_{ij} + \sum_{i,j} \delta_{ij} \mu \frac{\partial v_i}{\partial x_j}, \quad i, j = 1, 2, 3. \quad (3)$$

Here $\delta_{ij}$ is the Kronecker symbol, $\mu$ is the turbulent exchange coefficient.

By transformations from equations (2) and (3) we obtain the motion equation (Navier-Stokes):

$$\frac{dv_i}{dt} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial v_i}{\partial x_j} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial v_i}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial v_i}{\partial z} \right) - g_i, \quad (4)$$

where $v_i$ are the velocity components projections on the axis $Ox_i, i=1,2,3$.

System (4) is considered under initial and boundary conditions. At the initial time moment, the velocity is zero.

$$V(t, x, y, z) = 0. \quad (5)$$

Border conditions:

– on the bottom surface

$$\rho \mu \frac{\partial V}{\partial n}(t, x, y, z) \bigg|_{(x, y, z) \in \Gamma} = -\tau, \quad \frac{\partial V}{\partial n}(t, x, y, z) \bigg|_{(x, y, z) \in \Gamma} = 0; \quad (6)$$

– at the top and side borders

$$\frac{\partial V}{\partial n}(t, x, y, z) \bigg|_{(x, y, z) \in \Gamma} = 0, \quad \frac{\partial V}{\partial n}(t, x, y, z) \bigg|_{(x, y, z) \in \Gamma} = V_0(t, x, y, z), \quad \frac{\partial \rho}{\partial n}(t, x, y, z) \bigg|_{(x, y, z) \in \Gamma} = 0; \quad (7)$$

where $V_n$ is the velocity vector normal component, $V_0$ is the velocity vector value at the upper and lateral computational domain boundaries, $n$ is the outer normal to the boundary surface.

When the liquid surface contacts its vapor at a given temperature, an equilibrium vapor pressure determined for each liquid is established. A small increase in vapor pressure above the liquid surface leads to vapor condensation on this surface, and an infinite small decrease in pressure causes the liquid to evaporate from its surface. To describe the vapor pressure dependence on temperature, we will use the Mendeleev-Clapeyron formula, which can be represented as

$$P = \sum_i \frac{\rho_i}{M_i}RT, \quad (8)$$

where $\rho_i = m_i / V_i$ is density, $V_i = m_i / M_i$, $m$ is mass, $M$ is molar mass, $R$ is universal gas constant, $T$ is temperature.

Let us differentiate the state equation (8) and we get the equation (9):

$$\frac{\partial \rho}{\partial t} = \frac{\rho \frac{\partial P}{\partial t}}{P} - \frac{\rho}{T} \frac{\partial T}{\partial t}. \quad (9)$$

3. Dissipation polluting substances in the atmosphere

It is known that the atmospheric movements spatial scales vary from small eddies to the large air masses movement. Table 1 describes the various atmosphere processes and their spatial scales.
Table 1. The processes scales in the atmosphere.

| Phenomena                                      | Scale (km) |
|------------------------------------------------|------------|
| Air pollution with toxic substances           | 0.1 – 100  |
| Stratospheric ozone destruction               | 1.000 – 40.000 |
| Increase in greenhouse gases                  | 10.000 – 40.000 |
| Acidic precipitation                          | 100 – 2000 |
| The impact on the climate of aerosols         | 100 – 40.000 |
| Transport and oxidation processes in the troposphere | 1 – 40.000 |
| Stratospheric – tropospheric exchange         | 0.1 – 100  |
| Transport and oxidation processes in the stratosphere | 1 – 40.000 |

The wide scales range is explained by the gas impurities and aerosols variability. And, therefore, depending on the spatio-temporal considering processes scales, it is necessary to choose both the corresponding hydrodynamic models and the models for the gas impurities and aerosols transformation to solve a specific physical problem. The impurities transport equation, which describes the small moving vortices mixing with the environment and which is accompanied by the matter transfer, is written as:

$$\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} + (w - w_0) \frac{\partial \varphi}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial \varphi}{\partial z} \right) + f$$

(10)

or

$$\frac{d \varphi}{dt} - w_0 \frac{\partial \varphi}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial \varphi}{\partial z} \right) + f ,$$

(11)

where $w_0$ is the deposition rate, $f$ is a function describing the distribution and power of impurity sources.

Taking into account the transition of water from a liquid to a gaseous state and vice versa, as well as the fact that suspended particles are deposited during the impurities transfer, the equations for the pollutants transport in a multicomponent air medium look like this:

$$\frac{d \varphi_i}{dt} = \frac{\partial}{\partial x} \left( \mu \frac{\partial \varphi_i}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial \varphi_i}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial \varphi_i}{\partial z} \right) + f_i, \quad i = 0, 4,$$

(12)

where $f_0 = f_4 = 0 \quad f_1 = \frac{v}{\rho_n}, \quad f_3 = \frac{v}{\rho_n}$, $v = f (\rho_n - \rho_i)$ is evaporation rate, $\rho_n$ is the density of saturated vapors.

The equations system (12) must be supplemented with the following boundary condition:

$$\frac{\partial \varphi_i}{\partial n} \bigg|_{(x,y,z) \in \Gamma} = 0 .$$

(13)

We use the friction and gravity forces, which are involved in determining the pollutant velocity.

$$kw_0^2 - g (\varphi_1 + \varphi_4 \rho_4) = 0$$

or
where \( w_s \) is the impurities deposition rate.

4. Shallow water hydrodynamics model

During solving the atmospheric impurities propagation problems and their settling on the water surface, it becomes necessary to use the pollution transfer processes modelling to determine the heavy particles accumulation at the reservoir bottom, since their own deposition velocity depends on the heavy impurities transfer peculiarity, which often exceeds the vertical environment movement.

4.1 Shallow water hydrophysics model

The developed model for calculating three-dimensional aquatic environment movement velocity vector fields, temperature and salinity is based on a mathematical model of the shallow water bodies hydrophysics, taking into account the heat and salts transport [15]:

- the motion equation (Navier-Stokes)

\[
\begin{align*}
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = & - \frac{1}{\rho} \frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) + \frac{\partial}{\partial z} \left( \nu \frac{\partial u}{\partial z} \right) - 2 \Omega (\sin \theta \cdot u - \cos \theta \cdot v) \, , \end{align*}
\]

(15)

\[
\begin{align*}
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = & - \frac{1}{\rho} \frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left( \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial v}{\partial z} \right) + \frac{\partial}{\partial z} \left( \nu \frac{\partial v}{\partial z} \right) + 2 \Omega \cos \theta \cdot u \, , \end{align*}
\]

(16)

\[
\begin{align*}
\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = & - \frac{1}{\rho} \frac{\partial P}{\partial z} + \frac{\partial}{\partial x} \left( \mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial w}{\partial z} \right) + \frac{\partial}{\partial z} \left( \nu \frac{\partial w}{\partial z} \right) + 2 \Omega \cos \theta \cdot g \, , \end{align*}
\]

(17)

- continuity equation in the variable density case

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \rho \frac{\partial u}{\partial x} + \rho \frac{\partial v}{\partial y} + \rho \frac{\partial w}{\partial z} = 0 \, ;
\end{align*}
\]

(18)

- heat transport equation

\[
\begin{align*}
\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = & \frac{\partial}{\partial x} \left( \mu \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial T}{\partial z} \right) + \frac{\partial}{\partial z} \left( \nu \frac{\partial T}{\partial z} \right) + f_r \, ;
\end{align*}
\]

(19)

- salt transport equation

\[
\begin{align*}
\frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} + v \frac{\partial S}{\partial y} + w \frac{\partial S}{\partial z} = \rho \frac{\partial}{\partial x} \left( \mu \frac{\partial S}{\partial x} \right) + \rho \frac{\partial}{\partial y} \left( \mu \frac{\partial S}{\partial y} \right) + \rho \frac{\partial}{\partial z} \left( \mu \frac{\partial S}{\partial z} \right) + \frac{\partial}{\partial z} \left( \nu \frac{\partial S}{\partial z} \right) + f_s \, ,
\end{align*}
\]

(20)

where \( \{u, v, w\} \) are the velocity vector components; \( P \) is the total hydrodynamic pressure; \( S \) and \( T \) is salinity and temperature of the aquatic environment; \( \rho \) is the aquatic environment density; \( \mu, \nu \) are horizontal and vertical components of the turbulent exchange coefficient; \( \Omega = \Omega \cdot (\cos \theta \cdot j + \sin \theta \cdot k) \) is the angular Earth's rotation velocity; \( \theta \) is the site latitude; \( g \) is the gravity acceleration; \( f_r, f_s \) are heat and salt sources. (located on the border of the region).

Two components are conditionally separated from the total hydrodynamic pressure: the liquid column pressure function and the hydrodynamic part:

\[
P(x, y, z, t) = p(x, y, z, t) + \rho_0 g z \, ,
\]
where \( P \) is hydrostatic undisturbed liquid pressure; \( \rho_0 \) is the fresh water density under normal conditions.

State equation for density

\[
\rho = \rho + \rho_0,
\]

where \( \rho_0 \) is the fresh water density under normal conditions, \( \rho \) is determined by the equation recommended by UNESCO

\[
\rho = \rho_w + (8.24493 \cdot 10^{-1} - 4.0899 \cdot 10^{-3} T + 7.6438 \cdot 10^{-3} T^2 - 8.2467 \cdot 10^{-7} T^3 + 5.3875 \cdot 10^{-9} T^4) S + \]
\[
+(-5.72466 \cdot 10^{-3} + 1.0227 \cdot 10^{-4} T - 1.6546 \cdot 10^{-6} T^2) S^{\frac{3}{2}} + 4.8314 \cdot 10^{-4} S^2,
\]

where \( \rho_w \) is the fresh water density given by a polynomial

\[
\rho_w = 999.842594 + 6.793952 \cdot 10^{-2} T - 9.095290 \cdot 10^{-3} T^2 + 1.001685 \cdot 10^{-4} T^3 - 1.20083 \cdot 10^{-6} T^4 + 6.536332 \cdot 10^{-9} T^5.
\]

Equation (21) applies to salinity in the range of 0 – 42 \( \% \) and temperature from –2 to 40 \( ^{\circ} \)C. The equations system (15) – (20) is considered under the following boundary conditions:

- at the entrance

\[
V = V_0, \quad \frac{\partial P}{\partial n} = 0, \quad T = T_1, \quad S = S_1,
\]

- bottom boundary

\[
\rho, \mu \frac{\partial V}{\partial n} = -\tau, \quad V_0 = 0, \quad \frac{\partial P}{\partial n} = 0, \quad \frac{\partial T}{\partial n} = 0, \quad \frac{\partial S}{\partial n} = 0, \quad f_T = 0, \quad f_S = 0,
\]

- lateral border

\[
\frac{\partial V}{\partial n} = 0, \quad \frac{\partial V}{\partial n} = 0, \quad \frac{\partial P}{\partial n} = 0, \quad \frac{\partial T}{\partial n} = 0, \quad \frac{\partial S}{\partial n} = 0, \quad f_T = 0, \quad f_S = 0,
\]

- top border

\[
\rho, \mu \frac{\partial V}{\partial n} = -\tau, \quad w = -\omega - \frac{1}{\rho g} \frac{\partial P}{\partial t}, \quad \frac{\partial V}{\partial n} = 0, \quad \frac{\partial T}{\partial n} = 0, \quad \frac{\partial S}{\partial n} = 0, \quad f_T = k(T_0 - T), \quad f_S = \frac{\omega}{h_z - h_w} S,
\]

- at the exit

\[
\frac{\partial V}{\partial n} = 0, \quad \frac{\partial P}{\partial n} = 0, \quad \frac{\partial T}{\partial n} = 0, \quad \frac{\partial S}{\partial n} = 0, \quad f_T = 0, \quad f_S = 0,
\]

where \( \omega \) is liquid evaporation intensity; \( V_0, \ V_T \) are the velocity vector normal and tangential components; \( n \) is the outer normal to the boundary surface; \( \tau = \{\tau_x, \tau_y, \tau_z\} \) is tangential stress vector; \( \rho \) is the aquatic environment density; \( \rho_s \) is suspension density; \( T_0 \) is atmospheric temperature; \( k \) is heat transfer between the atmosphere and the aquatic environment coefficient, \( h_z \) is depth step, \( h_w = \omega \tau \) is a liquid layer that evaporates over time \( \tau \).

4.2 Shallow water biological rehabilitation model

A multi-species phyto- and zooplankton interaction model, taking into account the pollutants influence entering the reservoir on production-destruction processes in the reservoir has the form:
\[
\frac{\partial F_i}{\partial t} + \text{div}(UF_i) = \mu_i \Delta F_i + \frac{\partial}{\partial z} \left( v_i \frac{\partial F_i}{\partial z} \right) + \left( \alpha_i \varphi_i(B) - \theta_i F_z - \epsilon_i \right) F_i - g_i(F_i, Z),
\]

\[
\frac{\partial F_z}{\partial t} + \text{div}(UF_z) = \mu_z \Delta F_z + \frac{\partial}{\partial z} \left( v_z \frac{\partial F_z}{\partial z} \right) + \left( \alpha_z \varphi_z(F_i, F_z) - \lambda(M_z) \right) Z,
\]

where \( F_i \) are the concentrations of green and blue-green algae values, respectively; \( i = 1, m \); \( Z \) is zooplankton concentration; \( j = 1, m \); \( m \) is the pollutants quantity; \( B \) is nutrient concentration; \( M_j \) is metabolite concentration \( i \)-th type; \( j \) is concentration \( j \)-th pollutant; \( \Delta \) is two-dimensional Laplace operator; \( \mu_i, \mu_z, \mu_h, \mu_v, v_z, v_i, v \) are diffusion coefficients in the horizontal and vertical directions of substances \( F_i, Z, B, S_j \); \( M_j, r \in \{1, 2, 3, 4\} \); \( \alpha_i = (\alpha_{i\alpha} + \gamma_i M_i) \) is growth function \( i \)-th type due \( M_i \); \( \alpha_{i\alpha}, \gamma_i \) are growth rate in the absence of metabolite and exposure parameter \( i \)-th type; \( \alpha_z \) is the zooplankton growth rate; \( \varphi_z(F_i, F_z) \) is a function describing growth \( Z \) through consumption of the species \( X_i \) and oppression views \( X_i \); \( g_i(F_i, Z) \) is zooplankton absorption function \( i \)-th type phytoplankton; \( B \) is the nutrient intake rate; \( B_p \) is the maximum possible nutrients concentration; \( \epsilon_i \) is coefficient taking into account mortality \( i \)-th type and eating it by fish; \( \lambda(M_z) \) is the zooplankton mortality function, including the elimination risk due to the metabolite of blue-green algae; \( \alpha_g = \alpha_g(F_i, F_z, M_z, Z) = \epsilon_z F_i + \epsilon_z F_z + \delta_g(M_z, Z) + f - \) growth rate \( B \); \( \delta_g = \delta_g(M_z, Z) \) is concentration growth function \( B \) due to the zooplankton elimination when exposed to it \( M_z \); \( \epsilon_m \) are metabolite decomposition coefficients, \( m = 3, 4 \); \( k \) are excretion coefficients \( i \)-th type; \( f = f(x, y, z, t) \) is the pollution source function; \( \theta_i \) is interspecific competition coefficient \( i \)-th type; \( u \) is the water flow velocities field; \( U = u + u_{ok} \); \( U = (u, v, w) \) is the convective matter transfer rate; \( u_{ok} \) is sedimentation rate \( k \)-th substance, \( k \in \{F_i, F_z, B, S_j, Z, M_1, M_2\} \).

In system (22), the first six equations describe the production and destruction processes of phyto- and zooplankton, taking into account the external-hormonal regulation mechanism. The last system equation (22) describes the pollutants transport in a shallow water body.

The initial conditions for sistem (22) are set in the form:

\[
\varphi_i(x, y, z, 0) = \varphi_{i0}(x, y, z); k \in \{F_i, F_z, B, S_j, Z, M_1, M_2\} \times (x, y, z) \in \overline{G} \quad i = 1, 2, j = 1, m.
\]
Let \( n \) is the outward normal vector to the surface \( \sum \), \( u_n \) is normal in relation to \( \sum \) the water flow velocity vector component.

The boundary conditions for sistem (22) are as follows:

\[
\varphi_k = 0 \text{ at } \sigma, \text{ if } u_n < 0; \quad \frac{\partial \varphi_k}{\partial n} = 0 \text{ at } \sigma, \text{ if } u_n \geq 0; \quad \frac{\partial \varphi_k}{\partial z} = 0, \quad \text{if } k \neq S_j; \quad \frac{\partial S_j}{\partial z}(x, z, t) = \psi(S_j) \text{ at } \sum_0;
\]

\[
\frac{\partial \varphi_k}{\partial z} = -\xi_k \varphi_k \text{ at } \sum_\nu, \quad k \in \{F_1, F_2, B, S_j, Z, M_1, M_2\},
\]

where \( \xi_k \) are non-negative constants; \( \xi_1, \xi_2 \) take into account the algae sinking to the bottom and their flooding; \( \xi_2 \) takes into account the zooplankton elimination and its sinking to the bottom; \( \xi_1 \) take into account the nutrients absorption, pollutants and metabolites of green and blue-green algae by bottom sediments.

5. The model discretization

Discrete analogues of the diffusion and convective transfers operators are obtained from the diffusion-convection equation [16, 17], to which each of the equations of system (22) can be reduced by the linearization field:

\[
\frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} + w \frac{\partial S}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial z} \left( \nu \frac{\partial S}{\partial z} \right) + f \tag{24}
\]

under boundary conditions

\[
\frac{\partial S}{\partial n}(x, z, t) = \alpha_n S + \beta_n, \tag{25}
\]

where \( u, w \) are the velocity vector components, \( \mu, \nu \) are coefficients of turbulent exchange, \( f(x, z) \) is a function describing the intensity and distribution of matter sources, \( S \) – pollutant concentration.

To build a discrete air movement model, we consider the computational domain, which is inscribed in a rectangle. We cover the area with a uniform rectangular computational mesh \( \omega = \omega_x \times \omega_y \times \omega_z \):

\[
\omega_x = \{x_i = ih_x, \quad 0 \leq i \leq N_x - 1, \quad l_x = h_x (N_x - 1)\},
\]

\[
\omega_y = \{y_j = jh_y, \quad 0 \leq j \leq N_y - 1, \quad l_y = h_y (N_y - 1)\},
\]

\[
\omega_z = \{z_k = kh_z, \quad 0 \leq k \leq N_z - 1, \quad l_z = h_z (N_z - 1)\},
\]

where \( n, i, j \) are variables in time and space indices, \( \tau, h_i, h_j \) are steps on temporal and spatial variables, \( l_x, l_y, l_z \) are typical computational domain dimensions, \( N_x, N_y, N_z \) are nodes numbers of variables in time and space. To describe the computational domain geometry, the coefficients \( q_0, q_1, q_2, q_3, q_4 \) are introduced, which describe the control regions filling degree lying in the cell vicinity. Value \( q_0 \) characterizes the area fullness \( D_0: x \in (x_{i-1/2}, x_{i+1/2}), z \in (z_{j-1/2}, z_{j+1/2}) \), \( q_1 \) – \( D_1: x \in (x_{i-1/2}, x_{i+1/2}), z \in (z_{j-1/2}, z_{j+1/2}) \), \( q_2 \) – \( D_2: x \in (x_{i-1/2}, x_{i+1/2}), z \in (z_{j-1/2}, z_{j+1/2}) \), \( q_3 \) – \( D_3: x \in (x_{i-1/2}, x_{i+1/2}), z \in (z_{j-1/2}, z_{j+1/2}) \), \( q_4 \) – \( D_4: x \in (x_{i-1/2}, x_{i+1/2}), z \in (z_{j-1/2}, z_{j+1/2}) \).

To approximate problem (24), (25), we will take into account the cells filling. The diffusion-convection equation approximation in time is written in the form:
\[
\frac{\dot{S} - S}{h_x} + u \frac{\partial S}{\partial x} + w \frac{\partial S}{\partial z} = \frac{\partial}{\partial x} \left( \mu \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial S}{\partial z} \right) + f.
\]

\[
(q_0)_{i,j} \left( \frac{\dot{S}_{i,j} - S_{i,j}}{h_x} + \left( q_1 \right)_{i,j} u_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{2h_x} + \left( q_2 \right)_{i,j} \mu_{i-1/2,j} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{2h_x} \right) +
\]

\[
+ \left( q_3 \right)_{i,j} w_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{2h_z} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{2h_z} + \left( q_4 \right)_{i,j} v_{i,j-1/2} \frac{\overline{S}_{i,j} - \overline{S}_{i,j-1}}{h_z} \frac{\overline{S}_{i,j} - \overline{S}_{i,j-1}}{h_z} = (26)
\]

\[
= \left( (q_1)_{i,j} \mu_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{h_x} - (q_2)_{i,j} \mu_{i-1/2,j} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{h_x} \right) \left( q_1 \right)_{i,j} - \left( q_2 \right)_{i,j} \mu_{i,j} \left( \alpha \frac{\overline{S}_{i,j}}{h_x} + \beta \right) \frac{h_x}{h_x} +
\]

\[
+ \left( (q_3)_{i,j} v_{i,j-1/2} \frac{\overline{S}_{i,j} - \overline{S}_{i,j-1}}{h_z} - \left( q_4 \right)_{i,j} v_{i,j-1/2} \frac{\overline{S}_{i,j} - \overline{S}_{i,j-1}}{h_z} \right) \left( q_1 \right)_{i,j} - \left( q_2 \right)_{i,j} \left( q_1 \right)_{i,j} \left( q_4 \right)_{i,j} f_{i,j}.
\]

We divide the obtained equality (28) by the cell area \( h_x h_z \), as a result of which we obtain the diffusion-convection-reaction equation (26) discrete analogue.

\[
(q_0)_{i,j} \left( \frac{\dot{S}_{i,j} - S_{i,j}}{h_x} + \left( q_1 \right)_{i,j} u_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{2h_x} + \left( q_2 \right)_{i,j} \mu_{i-1/2,j} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{2h_x} \right) +
\]

\[
+ \left( q_3 \right)_{i,j} w_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{2h_z} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{2h_z} + \left( q_4 \right)_{i,j} v_{i,j-1/2} \frac{\overline{S}_{i,j} - \overline{S}_{i,j-1}}{h_z} \frac{\overline{S}_{i,j} - \overline{S}_{i,j-1}}{h_z} = (29)
\]

Here \( \dot{S} \) is the pollutant concentration on the new time layer. Thus, we have obtained discrete analogues of the operators of convective and diffusion transfers in the partial cells filling case

\[
(q_0)_{i,j} \frac{\partial S}{\partial x} \approx (q_1)_{i,j} u_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{2h_x} + \left( q_2 \right)_{i,j} \mu_{i-1/2,j} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{2h_x},
\]

\[
(q_0)_{i,j} \frac{\partial S}{\partial x} \approx (q_1)_{i,j} u_{i+1/2,j} \frac{\overline{S}_{i+1,j} - \overline{S}_{i,j}}{2h_x} + \left( q_2 \right)_{i,j} \mu_{i-1/2,j} \frac{\overline{S}_{i,j} - \overline{S}_{i-1,j}}{2h_x} - \left( q_1 \right)_{i,j} - \left( q_2 \right)_{i,j} \mu_{i,j} \left( \alpha \frac{\overline{S}_{i,j}}{h_x} + \beta \right) \frac{h_x}{h_x},
\]

\[
\text{were } \overline{S} = \sigma \dot{S} + (1 - \sigma) S, \sigma \in [0,1], \sigma \text{ is scheme weight, } q_l \text{ is coefficients of filling } l = 1, 4.
\]

6. Results of the Experimental Studies

In the summer of 2018, a research expedition was carried out by SFedU staff together with specialists from Rospotrebnadzor in the Rostov Region to study areas of Taganrog that are dangerous from the viewpoint of the pollutants spread, including the coastal zone. Table 2 presents data on the composition and concentration of the main pollutants obtained in the course of expeditionary research. These data were used to calibrate and verify the developed models.
Table 2. Pollutants composition and concentration of 2018.

| Major pollutants                                | Maximum one-time | Maximum average daily | Hazard class |
|-------------------------------------------------|------------------|-----------------------|--------------|
| 1. The nitrogen dioxide - 0.2                   | 0.085            | 0.04                  | II           |
| 2. Sulfur dioxide - 0.2                         | 0.5              | 0.05                  | III          |
| 3. benzene - 0.2                                | 1.5              | 0.1                   | II           |
| 4. benzo(a)pyrene - 0.015                       | -                | 0.01                  | I            |

st. Babushkina - st. Shchadenko (influence zone of metallurgical enterprise "Tagmet" and vehicle emissions), mg / l

| Major pollutants                                | Maximum one-time | Maximum average daily | Hazard class |
|-------------------------------------------------|------------------|-----------------------|--------------|
| 1. Manganese - 0.2                              | 0.01             | 0.001                 | II           |
| 2. Nitrogen dioxide - 0.2                       | 0.085            | 0.04                  | II           |
| 3. Sulfur dioxide - 0.2                         | 0.5              | 0.05                  | III          |

st. Shevchenko - per. Obryvnoy (influence zone of JSC "TSTP" (Taganrog sea trade port), shipyard)

| Major pollutants                                | Maximum one-time | Maximum average daily | Hazard class |
|-------------------------------------------------|------------------|-----------------------|--------------|
| 1. Inorganic dust SiO$_2$ 70-20% - 0.051         | 0.3              | 0.5                   | III          |
| 2. Nitrogen dioskid - 0.051                      | 0.085            | 0.04                  | II           |
| 3. Sulfur dioxide - 0.051                        | 0.5              | 0.05                  | III          |
| 4. The carbon oxide - 0.051                      | 0.15             | 0.05                  | IV           |

Figures 2–7 show the data of FGU «Azovmorinformcenter»: average annual nitrites values, dissolved oxygen and basic heavy metals in the Taganrog Bay of the Azov Sea.

Figure 2. Average annual nitrites values dynamics

Figure 3. Dissolved oxygen dynamics

Figure 4. Iron concentration dynamics, comparison with MPC (mg/m$^3$)

Figure 5. Iron concentration dynamics in water and bottom sediments (mg/g)
Studies have shown that the most polluted the Sea of Azov waters are: the the river Don mouth (mouth of the hands Kuterma, Perevoloka), r. Maly Elanchik, r. Mius, mouth r. Valovaya (Taganrog); the eastern part of the Taganrog Bay (Pivotny buoy of the Azov-Don Sea Canal (ADMK), near the dump of sea soil (Taganrog); port, Central beach, Primorsky beach, Petrushino beach, release area (Taganrog) [18].

On the developed software module basis, which numerically implements the mathematical pollutant transport model, numerical experiments were carried out taking into account the field expedition data. Figures 9 – 16 show the results of pollutant transport process numerical modelling at different convective transfer intensities, vector modulus values V and impurities types for given intervals.

The OZ axis is directed vertically upward.

Simulation parameters:
- dimensions of the computational domain in coordinates x and z: \( N_x = 80, N_z = 80 \) respectively;
- time intervals used in the calculation: \( T = 10 \text{ s}, 20 \text{ s}, 80 \text{ s} \);
- time step: \( \tau = 0.001 \);
- steps in horizontal and vertical coordinates \( x : h_x = 1 \) and \( z : h_z = 1 \);
- boundary conditions: \( \alpha = 0, \beta = 0, \alpha_z = 0, \beta_z = 0 \);
- calculation error for grid equations: \( \varepsilon = 0.0000001 \).

Scenario 1. There is no convective transfer. Constant uneven function of the pollution source on the area surface. Impurity type: heavy uneven, this is how heavy metals behave: aluminum, molybdenum, lead and antimony, which are contained in the exhaust gases that are emitted by internal combustion engines (Figure 8, 9).

**Figure 6.** Dynamics of aluminum concentration in water (mg/dm³)

**Figure 7.** Dynamics of molybdenum concentration in water (mg/dm³)

**Figure 8.** Pollutants concentration distribution. \( t = 6; \) pollution source \( f = 1 \) and \( f = 0.5 \). Coefficient values: \( \mu = 0.005; w = 0.1 \).

**Figure 9.** Pollutants concentration distribution. \( t = 80; \) pollution source \( f = 1 \) and \( f = 0.5 \). Coefficient values: \( \mu = 0.005; w = 0.1 \)
Scenario 2. There is no convective transfer. Constant uniform function of the pollution source on the area surface. Impurity type: conservative uneven, it can be nitrogen dioxide, sulfur dioxide, the pollution source can be industrial enterprises, as well as vehicles (Figure 10, 11).

![Figure 10. Pollutants concentration distribution. $t = 6$; pollution source $f = 20$. Coefficient values: $\mu = 0.01; w = 0.1$.](image10)

![Figure 11. Pollutants concentration distribution. $t = 80$; pollution source $f = 20$. Coefficient values: $\mu = 0.01; w = 0.1$.](image11)

Scenario 3. Convective transport is present, the admixture propagates only due to diffusion, the flow is from west to east. Constant uneven function of the source of pollution on the area surface. Impenetrable border on the right. Impurity type: heavy uniform. This is how a substance such as manganese behaves, mining and processing enterprises can act as a pollution source. (figure. 12, 13).

![Figure 12. Pollutants concentration distribution. $t = 6$; pollution source $f = 20$. Coefficient values: $\mu = 0.01; w = 0.1; V=5$ m/s.](image12)

![Figure 13. Pollutants concentration distribution. $t = 80$; pollution source $f = 20$. Coefficient values: $\mu = 0.01; w = 0.1; V=5$ m/s.](image13)

Scenario 4. Convective transport is present, flow from east to west. Constant uneven function of the pollution source on the area surface. Permeable border on the left. Impurity type: conservative non-uniform such as inorganic dust, benzapyrene found in smoke, for example, as a result of burning organic matter (figure 14,15)
Conclusion

Complex of interconnected models of aerohydrodynamics is proposed, which allows studying the various pollutions types propagation processes from the reservoir surface, taking into account their settling to the bottom. The considered impurities propagation processes mathematical models in the in the water layer bordering on atmosphere are intended for the analysis and prediction of the water quality environment. Continuous and discrete a multicomponent air medium motion mathematical models, which take into account such factors as the water transition from a liquid to a gaseous state, turbulent exchange, matter sedimentation, heat transfer between liquid and gaseous states, and variable density and temperature, more accurately describe these processes compared to other well-known models is offered. To calculate the pressure field, an equation is obtained that takes into account the compressibility of the medium, thermal expansion, matter sources associated with the water transition from a liquid to a gaseous state and vice versa, as well as a multicomponent air medium turbulent mixing. A distinctive feature of the developed mathematical model is the inclusion of turbulent mixing in the equation for calculating the medium density. The model discretization was based on the method of calculation cells partial filling, which made it possible to improve the accuracy of calculations for presented air-to-water transport scenarios in the system. Numerical experiments on the study of the input parameters influence confirmed the results validity of the program module. The developed software and algorithmic tools can be used to develop schemes for optimal environmental management, assessing the aquatic ecosystems state.

Acknowledgments

The reported study was funded by RFBR, project number 19-31-51017.

References

[1] Andre J C et al. 1978 Modeling the 24-hour evolution of the mean and turbulent structures of the planetary boundary layer. *J. Atmos. Sci.* 35 pp 1861-1883
[2] Berselli L C, Iliescu T and Layton W J 2006 Mathematics of Large Eddy Simulation of Turbulent Flows. *Springer. Series: Scientific Computation.* XVIII p 348
[3] Germano M, Piomelli U, Moin P. and Cabot W H 1991 A dynamic subgrid-scale eddy viscosity model *Phys. Fluids.* A 3, pp 1760-1765
[4] Ghosal S 1996 An analysis of numerical errors in large-eddy simulations of turbulence. *J. Comput. Phys.*, 125, 187-206
[5] Glazunov A V and Lykossov V N 2003 Large-eddy simulation of interaction of ocean and atmospheric boundary layers. - Russ. *J. Numer. Anal. Math. Modelling*, 18 pp 279-295
[6] Lund T S and Kaltenbach H-J 1995 Experiments with explicit filtering for LES using a finite-difference method. Center for Turbulence Research, Annual Research Briefs pp 91-105

[7] Sukhinov A I, Khachunts D S and Chistyakov A E 2015 A mathematical model of pollutant propagation in near-ground atmospheric layer of a coastal region and its software implementation. Computational Mathematics and Mathematical Physics, 55 (7) pp 1216-1231

[8] Meneveau C and Katz J 1999 Dynamic testing of subgrid models in LES based on the Germano identity. Phys. Fluids, 11 pp 245-47

[9] Monin A S and Yaglom A M 1963. On the laws of small-scale turbulent flow of liquids and gases (in Russian), Russian Mathematical Surveys, vol. 18, no. 5 (113) pp 93-114

[10] Marchuk G I 1982 Mathematical modeling in environmental issues, (in Russian). (Moscow: Nauka).

[11] Sukhinov A I, Chistyakov A E, Shishenya A V and Timofeeva E F 2013 Mathematical model for calculating coastal wave processes, Math. Models and Comp. Simulations. Vol. 5, No. 5 P 122-129

[12] Sukhinov A I, Chistyakov A E, Shishenya A V and Timofeeva E F 2013 Predictive modeling of coastal hydrophysical processes in multiple-processor systems based on explicit schemes. Mathematical Models and Computer Simulations. Vol. 10, No. 5 P 648-658

[13] Sukhinov A I, Chistakov A E et al. 2016 Modelling of oil spill spread. Proceedings of the 5th International Conference on Informatics, Electronics and Vision (ICIEV 2016) pp 1134-1139

[14] Aloyan A E 2002 Dynamics and kinetics of trace gases and aerosols in the atmosphere, Lectures, (in Russian). Moscow: IVM RAN

[15] Sukhinov A I, Chistyakov A E, Protsenko E A, Sidoryakina V V and Protsenko S V 2020 Accounting method of filling cells for the solution of hydrodynamics problems with a complex geometry of the computational domain, Mathematical Models and Computer Simulations, 12 (2) pp 232-245

[16] Sukhinov A I, Nikitina A V, Semenyakina A A and Chistyakov A E 2016 Complex of models, explicit regularized schemes of high-order of accuracy and applications for predictive modeling of after-math of emergency oil spill, CEUR Workshop Proceedings, 1576 pp 308-319

[17] Voevodin V V and Gergel V P 2010 Supercomputer Education: The third component of supercomputer technologies (in Russian), J. Computational Methods and Programming, vol. 11, no. 2 pp 117-122

[18] Gushchin V A, Sukhinov A I, Chistyakov, A E, Nikitina A V, Semenyakina A A 2018 A Model of transport and transformation of biogenic elements in the coastal system and its numerical implementation. Computational Mathematics and Mathematical Physics, 58 (8) pp 1316-1333