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Mathematical Model of Spreading Oil Pollution in Coastal Marine Systems

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Abstract

Introduction. The negative consequences that may arise due to an accidental oil spill are difficult to account for, since they disrupt many natural processes and relationships within the ecosystem of the reservoir. After an oil spill, a dense layer of oil film forms on the water surface quite quickly, preventing access to air and light (after a spill of one ton of oil, an oil slick about 10 mm thick forms on the surface of the reservoir after 10 minutes). As a result, the fauna and flora of the reservoir suffer. If the accident occurred in the coastal zone near a populated area, then the toxic effect is enhanced, because petroleum products in combination with various pollutants of human origin can form dangerous compounds. For high-risk areas (the main routes of transportation of petroleum products, places of their bunkering and unloading, etc.), it is necessary to predict various scenarios for the spread and transformation of oil pollution, taking into account their multifractional composition, turbulent diffusion and advective transport, destruction under the influence of natural factors. The aim of the work is to build a linearized non-stationary spatially heterogeneous mathematical model of transport and transformation of oil pollution, taking into account the above factors.

Materials and Methods. The oil that has entered the aquatic environment is represented as a surface and suspended substance in the water column. Oil is subject to a variety of transformation processes: advection, gravitational spreading, emulsification, dispersion, dissolution, biodegradation, etc. The study of these processes and their forecasting, as a rule, requires the development of mathematical and software. In mathematical and numerical modeling, one should start from the system of Navier-Stokes equations and continuity equations, as well as introduce additional physical tolerances of the flow geometry, acceptable and justified in each case, as shown by world experience and objective analysis of the physical picture of processes. Mathematical modeling of the oil distribution process in coastal marine systems has been performed.

Results. Mathematical oil distribution model has been created, taking into account its multifractional composition. It is assumed that oil fractions can be in water in dissolved or undissolved states. The modeling takes into account such physical characteristics of particles as density, acceleration of gravity, molar mass, etc. After the linearization of the problem under consideration, difference schemes using extended uniform grids were constructed.

Discussion and Conclusion. Pollution caused by an oil spill in the aquatic environment occurs very quickly and is often very destructive. An important factor will be prompt response, which plays a crucial role in minimizing its negative consequences. Modeling of the oil spill process can be useful for determining the location and condition of oil at sea, conducting a risk analysis of the spread of the substance and developing measures to localize and eliminate pollution.

Keywords: coastal marine systems, emergency oil spill, oil slick, multi-fraction composition of oil, concentration of oil particles, mathematical modelling, continuous model approximation

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Научная статья

Математическая модель процесса распространения нефтяных загрязнений в прибрежных морских системах

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Аннотация

Введение. Негативные последствия, которые могут возникнуть по причине аварийного разлива нефти, носят, как правило, трудно учитываемый характер, поскольку нарушают многие естественные процессы и взаимосвязи внутри экосистемы водоёма. После разлива нефти на водной поверхности довольно быстро образуется плотный слой нефтяной пленки, препятствующий доступу воздуха и света (после разлива одной тонны нефти через 10 минут на поверхности водоёма образуется нефтяное пятно толщиной около 10 мм). Вследствие этого страдает животный и растительный мир водоема. Если авария произошла в прибрежной зоне неподалеку от населенного пункта, то токсический эффект усиливается, потому что нефть/нефтепродукты в сочетании с различными загрязнителями человеческого происхождения могут образовывать опасные соединения. Для территорий повышенного риска (основных маршрутов транспортировки нефтепродуктов, мест их бункеровки и выгрузки и др.) необходимо прогнозировать различные сценарии распространения и трансформации нефтяных загрязнений с учетом их многофракционного состава, турбулентной диффузии и адвективного переноса, деструкции под воздействием природных факторов и т. д. Целью работы является построение линеаризованной нестационарной пространственно-неоднородной математической модели транспорта и трансформации нефтяных загрязнений с учетом перечисленных выше факторов.

Материалы и методы. Попавшая в водную среду нефть представляется в виде поверхностной и взвешенной в водной толще субстанции. Нефть подвержена множеству трансформационных процессов: адвекции, гравитационному растеканию, эмульгированию, диспергированию, растворению, биодеградации и др. Исследование данных процессов и их прогнозирование, как правило, требует разработки математического и программного обеспечения. Как показывает мировой опыт и объективный анализ физической картины процессов, при математическом и численном моделировании следует отталкиваться от системы уравнений Навье-Стокса и уравнений неразрывности, а также вводить дополнительные физические допуски геометрии потока, приемлемые и обоснованные в каждом конкретном случае. С учетом данных соображений выполнено математическое моделирование процесса распространения нефти в прибрежных морских системах.

Результаты исследования. Создана математическая модель процесса распространения нефти, учитывающая её многофракционный состав. Предполагается, что фракции нефти могут находиться в воде в растворенном или нерастворенном состояниях. При моделировании учитываются такие физические характеристики частиц как плотность, ускорение свободного падения, молярная масса и др. После линеаризации рассматриваемой задачи были построены разностные схемы, использующие расширенные равномерные сетки.

Обсуждение и заключение. Загрязнение, вызванное разливом нефти в водной среде, происходит очень быстро и нередко является весьма разрушительным. В данной ситуации важным фактором будет оперативное реагирование, играющее решающую роль для минимизации его негативных последствий. Моделирование процесса разлива нефти может быть полезным для определения местоположения и состояния нефти в море, проведения риск-анализа распространения субстанции и разработке мер по локализации и ликвидации загрязнения.

Ключевые слова: прибрежные морские системы, аварийный разлив нефти, нефтяной слик, многофракционный состав нефти, концентрация частиц нефти, математическое моделирование, аппроксимация непрерывной модели

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Introduction. There is an increase in the volume of trade in oil and petroleum products all over the world, with a significant share in their transportation being occupied by maritime shipping. To ensure the environmental safety of waterways and nearby infrastructure, certain restrictions and measures are observed throughout the entire transportation of goods. Despite this, over the past 50 years, 5.86 million tons of oil spilled into the sea have been recorded in the world. Moreover, about 80 % of this oil is spilled at a distance of no more than 10 nautical miles from the coast [1]. The negative consequences of oil pollution of reservoirs can be significantly reduced with timely localization and elimination of pollution. For these purposes, a developed set of measures is needed for their use by rapid response services. This set of measures, among other things, should contain some apparatus that allows forecasting the distribution of oil pollution. These forecasts require the use of mathematical and numerical modelling methods [2–4].

Scientific research in this area is carried out in Russia and abroad by such scientific centers as the P.P. Shirshov Institute of Oceanology of the Russian Academy of Sciences (Russia), the Institute of Water Problems of the Russian Academy of Sciences (Russia), the State Hydrological Institute (Russia), the Chinese Petroleum University and the Institute of Oceanology of the Chinese Academy of Sciences in Qingdao (China), the universities of Tasmania and Macquarie (Australia), Memorial University of Newfoundland (Canada)In Russia and abroad, etc. [5–9]. The accumulation of new knowledge and experimental data encourages us to obtain new results on the problem we are interested in.

This paper presents a mathematical model of the distribution of oil pollution, taking into account the following physical parameters and processes: the multifractional composition of oil, turbulent diffusion and advective transfer, evaporation, destruction under the influence of microorganisms, etc. This mathematical model is integrated with the hydrodynamic model described, for example, in [10, 11]. For the initial boundary value problem modeling the processes under consideration, difference schemes on grids with uneven steps in boundary cells (near the boundary) are constructed.

Materials and Methods

Problem statement. We will use a rectangular Cartesian coordinate system *Oxyz*. Let $\Omega \subset R^3$ be the calculated area, $\Omega = \{0 < x < L_x, 0 < y < L_y, 0 < z < L_z\}$. We consider the case of an oil release within a short time interval (a single-stage release) into the area under consideration. The oil that has entered the area Ω forms a spot on the free surface Ω_0. The area of coverage of the initial unexploded oil slick is indicated by σ.

Note that in the initial boundary value problem modelling the spread of oil pollution, a number of processes are considered on the surface of a reservoir and therefore a two-dimensional formulation is used here. The process of oil distribution and transformation in the coastal zone is described by the following equations [12]:

– equations for the concentration of the fraction of the oil number α ocated in the surface layer:

$$\frac{\partial c_\alpha}{\partial t} + u\frac{\partial c_\alpha}{\partial x} + v\frac{\partial c_\alpha}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h^* \frac{\partial c_\alpha}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h^* \frac{\partial c_\alpha}{\partial y}\right) - \left(\frac{K_E P_\alpha}{R\theta} + K_D S_\alpha\right) X_\alpha m_\alpha - \frac{\omega_\alpha c_\alpha}{q\left(c_\alpha + K_s\right)} M, \quad (1)$$

$$c_\alpha\Big|_{t=0} = \begin{cases} 0, & (x,y) \notin \sigma, \\ c_{\alpha 0}, & (x,y) \in \sigma; \end{cases} \quad \frac{\partial c_\alpha}{\partial \vec{n}} = 0, \ (x,y) \in \gamma; \quad (2)$$

– equations for the concentration of microorganisms — destructors of oil:

$$\frac{\partial M}{\partial t} + u\frac{\partial M}{\partial x} + v\frac{\partial M}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h \frac{\partial M}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h \frac{\partial M}{\partial y}\right) + \frac{\omega_\alpha c_\alpha}{c_\alpha + K_s} M - \lambda M, \quad (3)$$

$$M\Big|_{t=0} = M_0, \quad \frac{\partial M}{\partial \vec{n}} = 0, \quad (x,y) \in \gamma; \quad (4)$$

– equations for the concentration of the fraction of the number α of oil in the dissolved state:

$$\frac{\partial \varphi_\alpha}{\partial t} + u\frac{\partial \varphi_\alpha}{\partial x} + v\frac{\partial \varphi_\alpha}{\partial y} + w\frac{\partial \varphi_\alpha}{\partial z} = \frac{\partial}{\partial x}\left(\mu_h \frac{\partial \varphi_\alpha}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h \frac{\partial \varphi_\alpha}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_v \frac{\partial \varphi_\alpha}{\partial z}\right), \quad (5)$$

$$\frac{\partial \varphi_\alpha}{\partial z} = K_D S_\alpha X_\alpha m_\alpha, \ (x,y,z) \in \Omega_0, \quad (6)$$

$$\frac{\partial \varphi_\alpha}{\partial \vec{n}} = 0, \quad (x,y,z) \in \Omega \setminus \Omega_0. \quad (7)$$

The following designations are used in equations (1)–(7): *u*, *v*, *w* are the components of the aqueous medium velocity vector; c_α is the concentration of the fraction of the oil number α located in the surface layer, $\alpha = \overline{1, A'}$; $\mu_h^* = \mu_h + (\rho_\alpha - \rho_w) g h^3 / \mu_h$ (μ_h is the coefficient of horizontal diffusion of particles, *g* is the acceleration of gravity, $\rho_\alpha \rho_w$ are the particle densities of the fraction α and water, respectively, *h* is the thickness of the oil film); K_E is the mass transfer coefficient for hydrocarbon, $K_E = 2{,}5 \cdot 10^{-3} U^{0.78}$ (*U* is the wind speed relative to water); P_α is the vapor pressure of the fraction particles α; *R* is the universal gas constant, *R* = 8.314; θ is the ambient temperature above the surface of the spot; K_D is the coefficient of mass transfer of dissolution; S_α is the solubility in water of the particles of the fraction α, $\alpha = \overline{A'+1, A}$; X_α is the molar fraction of fraction particles α; m_α is the value of the molar mass of the fraction particles α; q is the value of the proportionality coefficient between the number of microorganisms and the absorbed substrate; M is the concentration of microorganisms; ω_α is the value of the maximum growth rate of microorganisms when feeding on fraction particles α; K_S is the saturation coefficient value; λ is the rate of death of microorganisms; φ_α is the concentration of the fraction α of oil in the dissolved state; $\alpha = \overline{A'+1, A}$; μ_v is the coefficient of vertical diffusion; $\vec{n}$ is the vector of the external normal to the surface describing the boundary of the computational domain; γ is the area describing the surface layers of the reservoir.

Mathematical model of the spread of oil pollution is obtained using a superposition of the results of solving the problem (1)–(7) for each fraction.

Results

Linearization of the problem. A uniform grid with a step τ: $\omega_\tau = \{t_n = n\tau, n = 1,..., N; N\tau \equiv T\}$ is built on the time interval $0 < t \leq T$. The linearization of the tasks under consideration has been performed on the time grid ω_τ. The linearization was performed in such a way that in equation (1), which determines the concentration of the fraction on a given time layer, the concentrations of microorganisms on the previous time layer were used.

At each time step $n = 1,2,...,N$, $t_{n-1} < t \leq t_n$ let the solutions of equations (1)–(3) be the functions $\tilde{c}_\alpha^n$, $\tilde{M}^n$, $\tilde{\varphi}_\alpha^n$, $n = 1,2,..., N+1$ respectively. In this case, the linearized analogue of the problem under consideration for all intervals $t_{n-1} < t \leq t_n$, $n = 1,2,...,N$ will be written as:

$$\frac{\partial \tilde{c}_\alpha^n}{\partial t} + u^n \frac{\partial \tilde{c}_\alpha^n}{\partial x} + v^n \frac{\partial \tilde{c}_\alpha^n}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h^* \frac{\partial \tilde{c}_\alpha^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h^* \frac{\partial \tilde{c}_\alpha^n}{\partial y}\right) - \left(\frac{K_E P_\alpha}{R\theta} + K_D S_\alpha\right) X_\alpha m_\alpha - \frac{\mu_\alpha \tilde{c}_\alpha^n}{q\left(\tilde{c}_\alpha^n + K_s\right)} \tilde{M}^{n-1}, \tag{8}$$

$$\tilde{c}_\alpha^1\Big|_{t=0} = \begin{cases} 0, & (x,y) \notin \sigma, \\ c_{\alpha 0}, & (x,y) \in \sigma, \end{cases}$$
$$\tilde{c}_\alpha^n(x,y,t_{n-1}) = \tilde{c}_\alpha^{n-1}(x,y,t_{n-1}),\ n = 2,...,N,\ (x,y) \in \gamma, \tag{9}$$

$$\frac{\partial \tilde{c}_\alpha^n}{\partial \vec{n}} = 0,\ (x,y) \in \gamma; \tag{10}$$

$$\frac{\partial \tilde{M}^n}{\partial t} + u^n \frac{\partial \tilde{M}^n}{\partial x} + v^n \frac{\partial \tilde{M}^n}{\partial y} = \frac{\partial}{\partial x}\left(\mu_h \frac{\partial \tilde{M}^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h \frac{\partial \tilde{M}^n}{\partial y}\right) + \frac{\mu_\alpha \tilde{c}_\alpha^{n-1}}{\tilde{c}_\alpha^{n-1} + K_s} \tilde{M}^n - \lambda \tilde{M}^n, \tag{11}$$

$$\tilde{M}^1\Big|_{t=0} = M_0,$$
$$\tilde{M}^n(x,y,t_{n-1}) = \tilde{M}^n(x,y,t_{n-1}),\ n = 2,...,N,\ (x,y) \in \gamma, \tag{12}$$

$$\frac{\partial \tilde{M}^n}{\partial \vec{n}} = 0,\ (x,y) \in \gamma; \tag{13}$$

$$\frac{\partial \tilde{\varphi}_\alpha^n}{\partial t} + u^n \frac{\partial \tilde{\varphi}_\alpha^n}{\partial x} + v^n \frac{\partial \tilde{\varphi}_\alpha^n}{\partial y} + w^n \frac{\partial \tilde{\varphi}_\alpha^n}{\partial z} = \frac{\partial}{\partial x}\left(\mu_h \frac{\partial \tilde{\varphi}_\alpha^n}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_h \frac{\partial \tilde{\varphi}_\alpha^n}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_v \frac{\partial \tilde{\varphi}_\alpha^n}{\partial z}\right), \tag{14}$$

$$\frac{\partial \tilde{\varphi}_\alpha^n}{\partial z} = K_D S_\alpha X_\alpha m_\alpha,\ (x,y,z) \in \Omega_0, \tag{15}$$

$$\frac{\partial \tilde{\varphi}_\alpha^n}{\partial \vec{n}} = 0,\ (x,y,z) \in \Omega \setminus \Omega_0. \tag{16}$$

If $n = 1$, then it is sufficient to take the functions of the initial conditions from formulas (9) as $\tilde{c}_\alpha^1(x,y,0)$. If $n = 2$, then the function of the initial condition is taken from formulas (12) $\tilde{M}^1(x,y,0)$, it is substituted into equation (8) and then the solution of problems (8)–(10) and (14)–(16) is carried out in the interval $t_1 < t \leq t_2$, in the course of which the concentration values are found $\tilde{c}_\alpha^2(x,y,t_1)$, $\tilde{\varphi}_\alpha^2(x,y,t_1)$. In turn, equation (11), which contains a function $\tilde{c}_\alpha^1(x,y,0)$, in the right part, has a solution $\tilde{M}^2(x,y,t_1)$. When continuing this process for cases $n = 3,...,N$ we will adhere to the described logic. Functions $\tilde{c}_\alpha^n(x,y,t_{n-1}) = \tilde{c}_\alpha^{n-1}(x,y,t_{n-1})$ and $\tilde{\varphi}_\alpha^n(x,y,z,t_{n-1}) = \tilde{\varphi}_\alpha^{n-1}(x,y,z,t_{n-1})$ are determined when solving problems (8)–(10) and (14)–(16) in the interval $t_{n-1} < t \leq t_{n-2}$, $n = 3,...,N$ assuming that the known functions are $\tilde{M}^{n-1}(x,y,t_{n-1})$ for the previous time period $t_{n-2} < t \leq t_{n-1}$.

Difference scheme for linearized problem. The terms describing the convective transport of particles from equations (8), (11) and (14) have the form in symmetric form [13]:

$$\frac{1}{2}\left[u\frac{\partial\tilde{c}_\alpha^n}{\partial x}+v\frac{\partial\tilde{c}_\alpha^n}{\partial y}+\frac{\partial\left(u\tilde{c}_\alpha^n\right)}{\partial x}+\frac{\partial\left(v\tilde{c}_\alpha^n\right)}{\partial y}\right],$$

$$\frac{1}{2}\left[u\frac{\partial\tilde{M}^{n-1}}{\partial x}+v\frac{\partial\tilde{M}^{n-1}}{\partial y}+\frac{\partial\left(u\tilde{M}^{n-1}\right)}{\partial x}+\frac{\partial\left(v\tilde{M}^{n-1}\right)}{\partial y}\right],$$

$$\frac{1}{2}\left[u\frac{\partial\tilde{\varphi}_\alpha^n}{\partial x}+v\frac{\partial\tilde{\varphi}_\alpha^n}{\partial y}+w\frac{\partial\tilde{\varphi}_\alpha^n}{\partial z}+\frac{\partial\left(u\tilde{\varphi}_\alpha^n\right)}{\partial x}+\frac{\partial\left(v\tilde{\varphi}_\alpha^n\right)}{\partial y}+\frac{\partial\left(w\tilde{\varphi}_\alpha^n\right)}{\partial z}\right],$$

this makes it possible, as a result of discretization, to construct a difference advective transfer operator with the property of skew symmetry [14, 15].

In the domain $\overline{G}$ we will construct a connected grid $\overline{\omega}_h$, $\overline{\omega}_h=\overline{\omega}_x\times\overline{\omega}_y\times\overline{\omega}_z$ where $\overline{\omega}_x=\{x_i:x_i=ih_x;\ i=0,1,...,N_x;N_xh_x\equiv L_x\}$, $\overline{\omega}_y=\{y_j:y_j=jh_x;j=0,1,...,N_y;N_yh_y\equiv L_y\}$, $\overline{\omega}_z=\{z_k:z_k=kh_x;\ \ k=0,1,...,N_y;N_zh_z\equiv L\}$. The set of internal nodes of the grids $\overline{\omega}_h,\overline{\omega}_x,\overline{\omega}_y,\overline{\omega}_z$ will be denoted, respectively, as $\omega_h\omega_x\omega_y\omega_z$. On the space-time grid $\omega_{\tau h}=\omega_\tau\times\omega_h$ we approximate the problem (8)–(16) with the task in nodes shifted by half the grid step speeds and in the corresponding coordinate direction.

Next, the "–" symbol is above the functions c_α^n, c_α^{n-1}, φ_α^n, φ_α^{n-1} and M^n, M^{n-1} will indicate that they belong to the class of grid functions. The functions $\tilde{c}_\alpha^n$, $\tilde{\varphi}_\alpha^n$, $\tilde{M}^n$ are considered as sufficiently smooth functions of continuous variables.

After approximation in the inner nodes of the grid $\overline{\omega}_h$ the equations (8), (11) and (14) will take the form:

$$\begin{aligned}&\frac{\overline{c}_\alpha^n-\overline{c}_\alpha^{n-1}}{\tau}+\frac{1}{2h_x}\left(u^n\left(x_i+0.5h_x,y_j\right)\overline{c}_\alpha^n\left(x_i+h_x,y_j\right)-u^n\left(x_i-0.5h_x,y_j\right)\overline{c}_\alpha^n\left(x_i-h_x,y_j\right)\right)+\\&+\frac{1}{2h_y}\left(v^n\left(x_i,y_j+0.5h_y\right)\overline{c}_\alpha^n\left(x_i,y_j+h_y\right)-v^n\left(x_i,y_j-0.5h_y\right)\overline{c}_\alpha^n\left(x_i,y_j-h_y\right)\right)=\\&=\frac{1}{h_x^2}\left(\mu_h^*\left(x_i+0.5h_x,y_j\right)\left(\overline{c}_\alpha^n\left(x_i+h_x,y_j\right)-\overline{c}_\alpha^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i-0.5h_x,y_j\right)\left(\overline{c}_\alpha^n\left(x_i,y_j\right)-\overline{c}_\alpha^n\left(x_i+h_x,y_j\right)\right)\right)+\\&+\frac{1}{h_y^2}\left(\mu_h^*\left(x_i,y_j+0.5h_y\right)\left(\overline{c}_\alpha^n\left(x_i,y_j+h_y\right)-\overline{c}_\alpha^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i,y_j-0.5h_y\right)\left(\overline{c}_\alpha^n\left(x_i,y_j\right)-\overline{c}_\alpha^n\left(x_i,y_j-h_y\right)\right)\right)-\\&-\left(\frac{K_EP_\alpha}{R\theta}+K_DS_\alpha\right)X_\alpha m_\alpha-\frac{\omega_\alpha\overline{c}_\alpha^n\left(x_i,y_j\right)}{q\left(\overline{c}_\alpha^n\left(x_i,y_j\right)+K_s\right)}\overline{M}^{n-1}\left(x_i,y_j\right);\end{aligned}\tag{17}$$

$$\begin{aligned}&\frac{\overline{M}^n-\overline{M}^{n-1}}{\tau}+\frac{1}{2h_x}\left(u^n\left(x_i+0.5h_x,y_j\right)\overline{M}^n\left(x_i+h_x,y_j\right)-u^n\left(x_i-0.5h_x,y_j\right)\overline{M}^n\left(x_i-h_x,y_j\right)\right)+\\&+\frac{1}{2h_y}\left(v^n\left(x_i,y_j+0.5h_y\right)\overline{M}^n\left(x_i,y_j+h_y\right)-v^n\left(x_i,y_j-0.5h_y\right)\overline{M}^n\left(x_i,y_j-h_y\right)\right)=\frac{1}{h_x^2}\left(\mu_h^*\left(x_i+0.5h_x,y_j\right)\cdot\right.\\&\left.\cdot\left(\overline{M}^n\left(x_i+h_x,y_j\right)-\overline{M}^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i-0.5h_x,y_j\right)\left(\overline{M}^n\left(x_i,y_j\right)-\overline{M}^n\left(x_i+h_x,y_j\right)\right)\right)+\\&+\frac{1}{h_y^2}\left(\mu_h^*\left(x_i,y_j+0.5h_y\right)\left(\overline{M}^n\left(x_i,y_j+h_y\right)-\overline{M}^n\left(x_i,y_j\right)\right)-\mu_h^*\left(x_i,y_j-0.5h_y\right)\cdot\right.\\&\left.\cdot\left(\overline{M}^n\left(x_i,y_j,0\right)-\overline{M}^n\left(x_i,y_j-h_y\right)\right)\right)+\frac{\omega_\alpha\overline{c}_\alpha^{n-1}\left(x_i,y_j\right)}{\overline{c}_\alpha^{n-1}\left(x_i,y_j\right)+K_s}\overline{M}^n\left(x_i,y_j\right)-\lambda\overline{M}^n\left(x_i,y_j\right);\end{aligned}\tag{18}$$

$$\begin{aligned}&\frac{\overline{\varphi}_\alpha^n-\overline{\varphi}_\alpha^{n-1}}{\tau}+\frac{1}{2h_x}\left(u^n\left(x_i+0.5h_x,y_j,z_k\right)\overline{\varphi}_\alpha^n\left(x_i+h_x,y_j,z_k\right)-u^n\left(x_i-0.5h_x,y_j,z_k\right)\overline{\varphi}_\alpha^n\left(x_i-h_x,y_j,z_k\right)\right)+\\&+\frac{1}{2h_y}\left(v^n\left(x_i,y_j+0.5h_y,z_k\right)\overline{\varphi}_\alpha^n\left(x_i,y_j+h_y,z_k\right)-v^n\left(x_i,y_j-0.5h_y,z_k\right)\overline{\varphi}_\alpha^n\left(x_i,y_j-h_y,z_k\right)\right)+\\&+\frac{1}{2h_z}\left(w^n\left(x_i,y_j,z_k+0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_i,y_j,z_k+h_z\right)-w^n\left(x_i,y_j,z_k-0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_i,y_j,z_k-h_z\right)=\right.\end{aligned}$$

$$= \frac{1}{h_x^2}\Big(\mu_h \left(x_i + 0.5h_x, y_j, z_k\right)\left(\overline{\varphi}_\alpha^n\left(x_i + h_x, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right)\right) - \mu_h \left(x_i - 0.5h_x, y_j, z_k\right)\cdot \tag{19}$$

$$\left(x_i, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i + h_x, y_j, z_k\right)\Big)\Big) + \frac{1}{h_y^2}\Big(\mu_h \left(x_i, y_j + 0.5h_y, z_k\right)\left(\overline{\varphi}_\alpha^n\left(x_i, y_j + h_y, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right)\right) -$$

$$, y_j - 0.5h_y, z_k\Big)\left(\overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j - h_y, z_k\right)\right)\Big) + \frac{1}{h_z^2}\Big(\mu_v\left(x_i, y_j, z_k + 0.5h_z\right)\Big(\overline{\varphi}_\alpha^n\left(x_i, y_j, z_k + h_z\right) -$$

$$- \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right)\Big) - \mu_v\left(x_i, y_j, z_k - 0.5h_z\right)\left(\overline{\varphi}_\alpha^n\left(x_i, y_j, z_k\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, z_k - h_z\right)\right)\Big).$$

To the difference equations (17)–(19), it is necessary to add the initial conditions for $(x, y, z) \in \omega_h$ as well as the approximation of the boundary conditions.

To set the boundary conditions, it is convenient to introduce an extended grid:

$$\overline{\omega}^* = \Big\{\left(x_i, y_j, z_k\right), i = -1,0,\dots, N_x + 1;\ j = -1,0,\dots, N_y + 1;\ k = -1,0,\dots, N_z + 1;$$
$$x_i = ih_x;\ y_j = jh_j;\ z_k = kh_z;\ N_x h_x = L_x;\ N_y h_y = L_y;\ N_z h_z = L_z\Big\}.$$

We will consider the known values of the components of the velocity vector of the aquatic medium at the nodes of the grid $\overline{\omega}^* \setminus \overline{\omega}_h$ with fractional index values, for example, $u^n\ (-0{,}5h_x, y_j, z_k)$, $u^n\ (L_x + 0{,}5h_x, y_j, z_k)$, $v^n\ (x_i, -0{,}5\ h_y, z_k)$, $v^n\ (x_i, L_y + 0{,}5\ h_y, z_k)$, $w^n\ (x_i, y_j, -0{,}5\ h_z)$, $w^n\ (x_i, y_j, L_z + 0{,}5\ h_z)$, etc.

We will approximate the boundary conditions using the example of condition (15). The arguments for boundary conditions (10), (13) and (16) are carried out in a similar way.

We will assume that $\overline{\varphi}_\alpha^n(x, y, z) = 0$, if $(x, y, z) \in \overline{\omega}^* \setminus \overline{\omega}_h$. For those grid nodes $\overline{\omega}^* \setminus \overline{\omega}_h$, that are outside the calculated area, the value of the components of the velocity vector of the aquatic medium is assumed to be zero.

Let's formally write down the expression:

$$\mathrm{C}_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} = \frac{1}{2h_z}\Big(w^n\left(x_i, y_j, 0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_j, y_j, h_z\right) - w^n\left(x_i, y_j, -0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right)\Big), \tag{17}$$

which can be considered as a difference approximation of the convective term at $z = 0$.

Along with (17), it is possible to write the equality for the boundary condition (15):

$$\frac{\overline{\varphi}_\alpha^n\left(x_j, y_j, h_z\right) - \overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right)}{2h_z} = K_D S_\alpha X_\alpha m_\alpha,$$

from which we obtain:

$$\overline{\varphi}_\alpha^n\left(x_j, y_j, h_z\right) = \overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right) + 2h_z K_D S_\alpha X_\alpha m_\alpha, \tag{18}$$

From expressions (17) and (18) we obtain:

$$\mathrm{C}_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{2h_z}\Big(w^n\left(x_i, y_j, 0.5h_z\right)\left(\overline{\varphi}_\alpha^n\left(x_i, y_j, -h_z\right) + 2h_z K_D S_\alpha X_\alpha m_\alpha\right) - w^n\left(x_i, y_j, -0.5h_z\right)\overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right)\Big). \tag{19}$$

Next, let us formally consider the equality on an extended grid $\overline{\omega}^*$

$$\mathrm{D}_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{h_z}\left(\mu_v\left(x_i, y_j, 0{,}5h_z\right)\frac{\overline{\varphi}_\alpha^n\left(x_i, y_j, h_z\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right)}{h_z} - \mu_v\left(x_i, y_j, -0{,}5h_z\right)\frac{\overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, -h_z\right)}{h_z}\right). \tag{20}$$

Since there is no turbulent diffusion on the free undisturbed surface of the reservoir, we can assume that $\mu_v\ (x_i, y_j, -0{,}5\ h_z) \equiv 0$. With this in mind, from the expression (20) we get

$$\mathrm{D}_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{h_z^2}\mu_v\left(x_i, y_j, 0{,}5h_z\right)\left(\overline{\varphi}_\alpha^n\left(x_i, y_j, h_z\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right)\right).$$

From (18) and (21) we find

$$D_z\left(\overline{\varphi}_\alpha^n\right)\Big|_{z=0} \equiv \frac{1}{h_z^2}\mu_v\left(x_i, y_j, 0.5h_z\right)\left(\overline{\varphi}_\alpha^n\left(x_j, y_j, -h_z\right) - \overline{\varphi}_\alpha^n\left(x_i, y_j, 0\right) + 2h_z K_D S_\alpha X_\alpha m_\alpha\right).$$

Discussion and Conclusion. The paper presents a mathematical model of the process of spreading and transformation of oil pollution in coastal marine systems. This model takes into account the multifractional composition of oil pollution, turbulent diffusion and advective transport, destruction of oil particles under the influence of microorganisms, etc. The approximation of the proposed model is performed with the second order of accuracy relative to the steps of the spatial grid. The issues related to the study of the monotony of the constructed difference scheme and its convergence to the solution of the initial initial boundary value problem are the subject of further research by the author.

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