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SPILLMOD – A CFD MODEL FOR INFORMATION SUPPORT OF MARINE OIL SPILL RESPONSE

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A mathematical model of the evolution of marine oil spills with taking into account the processes of spreading and weathering, has been implemented as a software package called SPILLMOD. In doing so, a new Eulerian-Lagrangian method for Computational Fluid Dynamics (CFD) has been developed in the context of solving shallow-water-type equations with the capability to handle the situation where advancing/vanishing layer of the light fluid (oil) only partially covers the heavy (water) in a domain with an arbitrary configuration of the coastline shape. When calculating the evaporation of high-viscosity oil types, the effect of reduction the evaporation rate due to molecular diffusion of lighter oil fractions within the oil layer is taken into account. Simulation of the natural dispersion of oil layer is carried out considering multiple factors, such as: sea surface conditions, experimental data on oil film crushing in the wave mixing layer, turbulent diffusion in the upper layer, as well as changes of physical and chemical properties of oil over time. An additional module in the model is designed to estimate domain boundaries of possible spill detection for different sources of uncertainties during oil spill modeling. Modeling examples of application in realistic configuration of port-water areas for an actually occurred emergency situation of oil spill demonstrate the declared qualities of the model as a tool for supporting emergency response operations.

Keywords: SPILLMOD, CFD, oil spill model, oil spill response, oil evaporation, oil dispersion, particle-in-cell numerical method, spatial uncertainty

1. Introduction

The purpose of mathematical modeling of oil spills in the sea should be considered in the conjunction with operational support for Oil Spill Response (OSR). To be able to accomplish this goal, mathematical models should adequately, with a high degree of reliability, describe the behavior of oil in the sea and provide the simulated data. Based on this information, it is possible to select OSR strategy for a specific situation at the stage of developing OSR plans, or during the incident. Although OSR operations are usually carried out within the first few days after an accident, in many cases accounting for evaporation and dispersion processes may play a key role in assessing the amount of oil on the surface, as well as in the estimation of potential impact on vulnerable sites. The article presents the basic principles underlying the development of the SPILLMOD marine oil spill model. In the introduction,

we provide the necessary aspects to be taken into account when creating an oil spill model for OSR informational support.

This article is organized as follows:

Sec. 2 defines the requirements for building oil spill models for offshore conditions;

In Sec. 3.1. presents the formulation of the problem of gravitational spreading of oil as a light liquid over the surface of a heavier one, taking into account the lateral boundaries (coastline, port facilities, booms), as well as changes of oil properties and its amount on the surface over time due to weathering processes;

Secs. 3.2–3.3 outlines the algorithms to simulate processes affecting oil spill evolution due to evaporation and natural dispersion;

Sec. 4 is describes to the numerical method used by the authors to solve the formulated mathematical problem;

Sec. 5 briefly describes the module for assessing the uncertainty in determining the position of an oil slick in forecasting;

Sec. 6 provides various examples of practical oil spill simulations with the model.

1.1. Oil spill transformation processes on the sea

The outcome of oil spills in the aquatic environment and their impact on vulnerable resources is strikingly diverse. The reason lies in the variety in physical and chemical characteristics of oil, the meteorological conditions, and oil spill source characteristics. The evolution of an oil spill in open water is accompanied by transport under the influence of wind, sea currents, and surface waves. The area of an oil spill on the water surface is formed as the result of spreading and is accompanied by weathering processes. Because of evaporation and dispersion by waves, a significant part of the oil is removed from the sea surface. Evaporation, emulsification, dissolution into water column, and photooxidation change the composition and physical characteristics of the oil residue on the sea surface. At first, there is an increase in the density and viscosity of oil on the sea surface. On one hand, this change in the density leads to slowdown of spreading. On the other, to a decrease in the rate of surfacing of droplets of dispersed oil, which leads to an intensification of the natural dispersion process. Furthermore, an increase in the viscosity of oil leads to a decrease of dispersion of the oil film into droplets due to the formation of larger diameter droplets. The interrelationships between the processes and somewhat competing factors make it necessary to simultaneously take into account the oil film thickness and weathering processes. Oil transport due to wind and currents depends on vertical mixing of dispersed oil in the upper ocean layer (Röhrs et al., 2018). With varying degrees of detail, the main factors of the evolution of oil spills at sea are described in a number of scientific articles and technical documents (ITOPF, 2014; Spaulding, 2017; Keramea et al., 2021; Zatsepa et al., 2018a).

1.2. Evolution of mathematical modeling of oil spills at sea. Brief history

A comprehensive review of the current trends, perspectives and problems in the field of offshore oil spill modeling (Keramea et al., 2021) compares 18 European and American models. The review contains a significant number, over two hundred, of references for publications in the field of oil spill modeling. The list of references can be extended by adding other works not mentioned in there, e.g. (Stanovoy et al., 2012; Semanov et al., 2017; Zatsepa et al., 2018a, 2020; Korotenko, 2018).

Note that the term 'oil spill model' is interpreted very broadly. It may refer to a model that simulates a floating oil plume from subsea source, a model of sea surface oil spill, a 3D sea circulation model, and a wind-wave model for the area of interest. It is understandable that oil transformation processes at sea cannot be properly simulated without an area-specific calculation of wind and current fields. In practice, marine circulation models require some adaptation for each individual water area, which is often a tedious job. On the other hand, in such cases, modelers focus too much on marine circulation models, at the expense of leaving behind the description of weathering and dispersion processes. To date, it seems generally accepted that the uncertainty in the oil slick position is related to the inaccuracy of weather forecasts. However, uncertainty assessment should also be accompanied by oil slick predictions, including estimates of the amount of oil that has evaporated and that has penetrated into the water column as droplets. Even contemporary oil spill models often use parameterisations of spreading and weathering processes based on a small number of laboratory experiments from the 1980s (Fay, 1971; Hoult, 1972; Mackay et al., 1980; Delvigne and Sweney, 1988), while new experimental data and theoretical understanding of the process of natural and chemical dispersion of oil have been obtained during the last decade (Brandvik et al., 2014; Li et al., 2017; Zatsepa et al., 2018a, b). In order to increase the level of confidence modeling, there is a need to refine the understanding of the behaviour of oil in the marine environment and to design models that adequately describe the processes.

Within the first 24 hours after an incident, spreading is the most important of the transformation processes of an oil spill on the sea surface. It is the process which is responsible for changing the area and shape of the oil slick. The area, the physical and chemical properties of the oil determine the amount of oil that evaporates into the atmosphere and disperses into the water column. Factors that influence the fate of oil at sea also include environmental conditions such as sea temperature and sea state, wind speed and proximity to the shore, type of oil, volume of discharge and its location (sea surface or seabed) and many others. The mathematical model of an oil spill is a set of mathematical equations and relationships that describe the evolution of an oil spill after it enters the marine environment. Some oil spill transformation processes, such as spreading or evaporation, can be described in great detail; others, such as dispersion or sedimentation, can be described at a phenomenological level.

The initial attempts to describe the spreading process of a light liquid on the surface of a heavier one were purely phenomenological. Mathematical models of this process were formulated as the time dependence of the size of a spot or lens of a lighter fluid (DiPietro, Cox, 1979). To describe the spreading of an oil spill on the sea surface, the method of analogy was

utilized. Thus, Blokker (1964) proposed a model of oil spreading, suggesting that the radius of an axisymmetric oil slick increases as it would be in the case of propagation of shock wave front in a two-dimensional gas, while the volume of oil decreases due to evaporation, while oil itself was assumed to be a homogeneous single-component liquid.

James A. Fay (Fay, 1969) was the first who analyzed a balance of the forces acting in case of symmetric spill on the calm water. Fay's three-regime spreading theory suggested that the forces that cause oil to spread are the forces of gravity and surface tension, and the forces that slow down the process of spreading are the forces of inertia and viscous friction in the boundary layer of water under the oil layer. The oil spreading was presented in the form of successive stages. At the first stage, the gravitational force is balanced by the inertia force (gravitation-inertial stage), at the second stage (gravitational-viscous stage) – by the viscous friction force, and at the third stage, the surface tension forces are balanced by viscous forces (Fay, 1969; Fay, 1971). The first article was entitled "The spread of oil slicks on a calm sea" (Fay, 1969), the second – "Physical processes in the spread of oil on a water surface" (Fay, 1971). In spite of presence word "oil" in both titles, the model describes idealized conditions excluding "…*The physically most important assumption underlying our analysis, which is most likely to be violated in any real incident of a spill, is the absence of any effects of wind, tidal currents and waves…*" (Fay, 1971). Moreover, the weathering processes including evaporation, dispersion and emulsification were out of consideration. The oil weathering problem was brought to the attention of Donald Mackay (Mackay et al., 1980). As a result of research Mackay and his colleagues developed the first relatively complete model of oil transformation on the sea surface, which included a description of the spreading process, accompanied by the processes of oil weathering (evaporation and dispersion), leading to changes in the physical properties of the spreading substance. Crucially, thanks to McKay's research, it became clear that the process of oil spreading across the sea surface is largely determined by the type of oil or petroleum product. Fay's relations (Fay, 1971) were confirmed by a number of laboratory experiments, however, these experiments had spatial scales of the order of tens of centimeters or first meters, and temporal scales of the order of several minutes or tens of minutes. A disadvantage of Fay's relations is the use of assumption that friction at the oil-water interface can be derived from the laminar boundary layer approximation, which is more consistent with the laboratory experiments and less with the turbulent conditions of the open sea. These papers, like most oil spill models, virtually ignore the effect of oil viscosity on the spreading process. It is not true for all cases, in particular, for very viscous types of oil in the initial period of spreading. In (Ahn, 1978) and later (DiPietro, Cox, 1979), spreading regimes in a wide range of viscosity ratios were investigated and self-similarity relationships and limits of their applicability for these regimes were obtained.

1.3. Oil spill response and oil spill models

Understanding how physical processes changes the dynamics, chemical composition, and behavior of oil over time is important for an oil spill response. For example, in some cases it can be predicted with certainty that oil will not reach sensitive natural resources due

to natural dispersion, so that clean-up operations will not be required. If an active response to a spill is required, however, the choice of the most effective response will depend on the type of oil and its likely behaviour (ITOPF, 2014).

Mathematical models are created to solve a variety of problems in order to find answers to practical questions. To model spills for the information support for OSR operations should take into account the oil spill transformation processes that are most important in the first hours and days after an oil spill is released at sea. The key questions are: where will be the oil spill located, what is the area of oil contamination and the volume of oil on the sea surface, and what strategies can be used to contain the spill? For this reason, oil component dissolution can be neglected when modelling spills to support OSR operations because, according to McAuliffe (McAuliffe, 1987) the mass of hydrocarbons dissolved into the water column is generally less than 1 % of the oil slick, and, according to Riazi (Riazi, 1996), the dissolution rate of oil on the sea surface is less than about 0.1 % of the evaporation rate of oil. The description of oil sedimentation can also be neglected, as sedimentation occurs as a result of the 'continuation' of the oil dispersion process. To predict the environmental impacts of oil spills the description of oil dissolution in water, aggregation and seabed deposition of oil, and biodegradation need to be 'added' into the consideration. The assessment of the impact of an oil spill to the marine environment is based on detailed information about the hydrological, hydrochemical and hydrobiological characteristics of the incident area (Barker et al., 2020). It is not always possible to obtain this information with the necessary accuracy from marine circulation modeling results.

Operational meteorological forecasts are used to provide information support for OSR, while environmental tasks require assessment of consequences of an accident that has already occurred and, as a rule, the results of atmospheric and marine reanalysis are used. When solving environmental tasks, requirements to promptness of calculations are reduced, there is an opportunity to use oil spill models that take into account a larger number of processes, and models of marine dynamics with a more detailed spatial resolution.

2. Specifics of marine oil spills

The differences between the spills in laboratory experiments and spills that occur in natural marine environment are:

1) Sea water is almost always in motion. Fay's theory for the spreading phenomenon assumes that the movement of water under the oil layer is initiated by the movement of oil, which is reflected in the titles of the relevant works "... *quiescent water surface*, *calm sea»* However, in the upper layer of the sea, wave motions and turbulence are the main physical mechanism of the energy and matter exchange between interacting media. Jacques Nihoul (Nihoul, 1984) was the first who highlighted the need of the friction model to be changed. Based on the results of field observations in the cited paper it was proposed linear form of the friction stress $\tau = k\left(\overline{\mathbf{u}}_o - \mathbf{u}_w\right)$, where the coefficient $k = 0.003\ kg\ m^{-2}s^{-1}$, $\overline{\mathbf{u}}_o$ is the

average horizontal velocity in the oil layer, $\mathbf{u}_w$ is the water current under the oil layer. In the environmental hydromechanics a quadratic dependence of the friction stress is often used $\tau = C_u \rho_w \left(\Delta u\right)^2 \mathrm{Re}^{-1/2}$ in a laminar flow and $\tau = C_u \rho_w \left(\Delta u\right)^2 \mathrm{Re}^{-1/5}$ in a turbulent flow, where C_u is the drag coefficient, ρ_w is the density of water, i.e., friction is proportional to the square of the local difference in the velocities $\left(\Delta u\right)^2$ of interacting media and the Re is Reynolds number. When estimating the Reynolds number in (Fannelop, 1971; Hoult, 1972), which studied the flow of oil *on a calm surface* of water, the changing size of the spill was chosen as a characteristic length scale, while for currents in the upper layer of the ocean under the oil patch, this size can be either the size of eddies or convective cells, but in any case, the characteristic scale of dynamic processes in the upper sea layer is not determined by the movement of oil and can be considered constant at any point of a sufficiently large oil slick. For large oil spills, the following friction model is more realistic:

$$\left|\tau_{ow}\right| / \rho_w = \beta \left|\Delta \mathbf{u}\right|^2, \ \Delta \mathbf{u} = \mathbf{u}_o(x, y, t) - \mathbf{u}_w(x, y, 0, t), \tag{2.1}$$

where β is the friction coefficient, $\mathbf{u}_w(x, y, 0, t)$ – water velocity at sea surface.

An important consequence of (2.1) is that friction at the lower boundary of the oil slick can both inhibit and accelerate movement in the oil layer, and at the later stages of formation of the oil contamination field, the oil layer thickness distribution will be determined by divergence of the current field in the upper sea layer. Thus, the task of oil spill dynamics on the sea surface turns out to be directly related to the dynamical processes in the upper sea layer. An example of this kind of interaction between an oil spill and mesoscale processes in the upper ocean layer is given in (Korotenko, 2018), when the formation of large-scale sea surface pollution is associated with the convergence of currents in anticyclonic eddies of the Black Sea.

2) The scale of "oil" spills in the laboratory and in full-scale conditions differs by several orders of magnitude-from tens of centimeters and the first meters in laboratory basins and up to hundreds of meters and kilometers in full-scale conditions. In the case of large spills, the contaminated area is reached tens of thousands of square kilometers. The time scales of laboratory experiments were limited from tens of seconds to minutes; spills last for days and months in natural conditions (for example the Deep Water Horizon accident in the Gulf of Mexico). Spill volumes in the laboratory are limited to units or tens of cubic centimeters, while in the field, spills of many thousands of tons of oil occur.

3) Spills in natural conditions are neither instantaneous nor occur with a constant outflux rate.

4) Spills occurring close to shore or in port areas are limited by a number of contact boundaries – jetties, ship hulls and other technical structures – which limit the free spreading of spills and must be taken into account when assessing spill characteristics. A speculative experiment is sufficient to demonstrate this by considering the simplest case of a spill at the 'wall' and in open water. In the number of oil spill models the oil spill area is described by a power dependence in the form $A(t) = aV^{\alpha} t^{\beta}$, where a is a coefficient, V is the oil volume, t is the time, α, β are constants depend on the choice of the oil-water friction model.

Such dependencies, are usually, obtained from self-similar solutions for oil spills of constant volume or occurring with constant intensity.

For reasons of symmetry, it is clear that the spill area in open water should be the same on both sides of a straight line (axis OY) passing through the center of the spill, as shown in Figure 1a and the areas of Area 1 and Area 2 are equal.

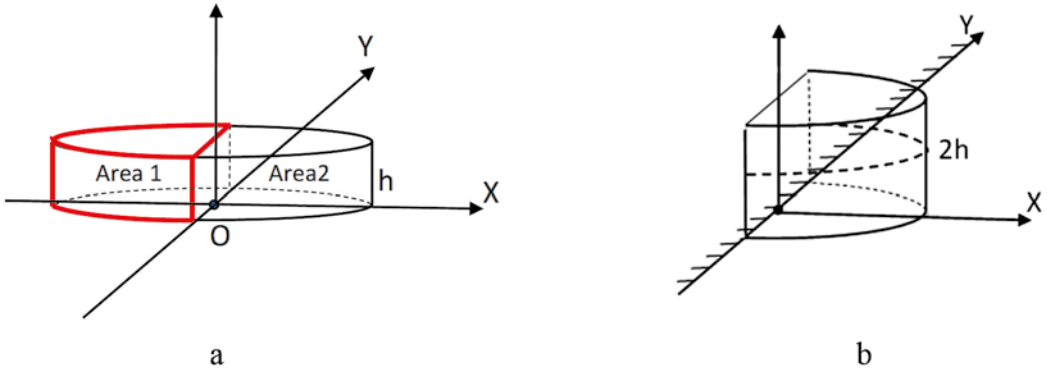


Figure 1 – Sketches of oil spill spreading: (**a**) in open water and (**b**) at the contact boundary

Let's suggest that the entire volume of an oil spill V is concentrated on one side of the conventional OY line. Fill this configuration to a full circle, as shown in Figure 1a, and, thus, the area of the spill with the addition is $A(t) = a(2V)^{\alpha} t^{\beta}$, and, accordingly, the half of the spot of interest to us $A(t) = a(2V)^{\alpha} t^{\beta} / 2$. The area of the spot A_{φ} bounded by two straight lines, the angle between which φ is defined as:

$$A_{\varphi}(t) = \varphi / 2\pi \, a(2\pi V/\varphi)^{\alpha} t^{\beta}. \tag{2.2}$$

As a result, the ratio of areas $A_{2\pi}$ and A_{φ} spills of equal volume, one of which spreads without the influence of contact boundaries, and the other in a segment with an angle φ is

$$A_{\varphi} / A_{2\pi} = \varphi / (2\pi)(2\pi/\varphi)^{\alpha} = \varphi^{1-\alpha} / (2\pi)^{1-\alpha}. \tag{2.3}$$

For axisymmetric spreading with the friction model used in the spreading parameterization (Fay, 1971), the exponent α is equal to the 2/3, and thus, for example, the ratio of the area of the stage and the spill in semi-infinite space (at the "wall") to the area of the spill in open water is $A_{\varphi} / A_{2\pi} = (1/2)^{1/3} = 0.79$.

These simple considerations show that the area of the spreading liquid depends on the configuration of the lateral boundaries of the region, in which the oil propagates. For the cases considered above, self-similar solutions exist, and they can be used to verify computational procedures that are generally suitable for more complex arbitrary boundaries.

5) A realistic-case spill may occur in all possible weather conditions, not always in still water corresponding to the laboratory one. Thus, there is a need to develop models accounting winds, sea currents, and surface waves.

6) As noted in (Mackay et al., 1980), oil weathering occurring in situ conditions can make it impossible to apply observational data obtained from specific experiments, even under controlled conditions, to other situations. Comparisons of observations of oil spills have shown that simple relationships are unlikely to be good due to the wide variety of petrol products and its properties (i.e., density, viscosity and interface tension) significantly changing while weathering in progress. Thus, to construct the model of oil spill fate on the sea it's necessary to "collect" in the complex model a number of simply models of individual physicochemical processes.

The oil spill model SPILLMOD presented in current work was developed for support OSR operations in the sea. The time length of the oil spill forecast is bounded by for some days after accident. The description of the model presented below.

3. Oil spill model for marine conditions SPILLMOD

3.1. Basic equations

An oil spill on the sea surface is described by a system of partial differential equations of the "shallow-water" type. The equations are applicable within the area covered by oil floating on the sea surface, with boundary conditions specified at the free (the line separating oil-covered and free of oil surface) and the solid contact (coastlines, piers at port, oil spill containment boom, etc) boundaries (Zatsepa et al., 1992, 2015, 2018a; Ovsienko et al., 1999):

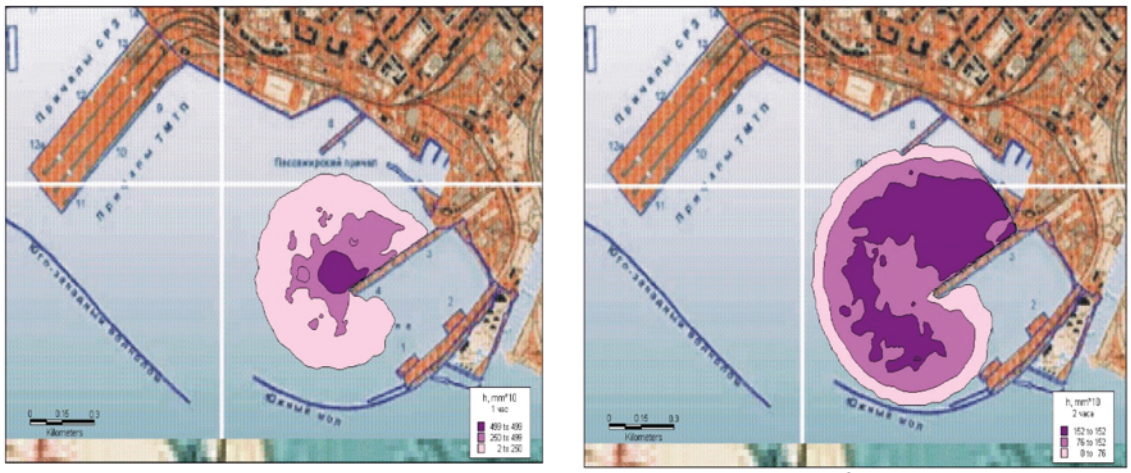
$$\rho_{oil}\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\nabla\mathbf{u}\right)=-\rho_{oil}g'\nabla h-\frac{\beta\cdot\rho_w}{h}\left|\mathbf{u}-\mathbf{u}_d-\mathbf{u}_c\right|\left(\mathbf{u}-\mathbf{u}_d-\mathbf{u}_c\right)+\frac{1}{h}\nabla.\mathbf{T}\,, \qquad (3.1)$$

$$\rho_{oil}\left(\frac{\partial h}{\partial t}+\nabla.\left(h\mathbf{u}\right)\right)=Q_o-Q_e-Q_d\,, \qquad (3.2)$$

where (x,y) are Cartesian coordinates t is time, h is the thickness of the oil layer, $\mathbf{u}$ is the oil velocity, (u,v) are it's components, $g'=g\left(\rho_w-\rho_{oil}\right)/\rho_w$ is the reduced gravity acceleration, ρ_{oil}, ρ_w are densities of oil and water respectively, $\mathbf{u}_d$ is the parameterized wind drift, $\mathbf{u}_c$ is the velocity of wind-driven current at the sea surface, obtained from a hydrodynamical model or from measurements, β is the friction coefficient, Q_0 are all sources and loss of oil except for evaporation Q_e and dispersion by wind waves Q_d, $\mathbf{T}$ is the lateral viscous stress tensor within the oil layer, the components of which are represented as (Ovsienko et al., 1999):

$$\begin{aligned} T_{xx}&=\mu_{oil}h\left(4\frac{\partial u}{\partial x}+2\frac{\partial v}{\partial y}\right), \quad T_{xy}=\mu_{oil}h\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right),\\ T_{yx}&=\mu_{oil}h\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right), \quad T_{yy}=\mu_{oil}h\left(2\frac{\partial u}{\partial x}+4\frac{\partial v}{\partial y}\right). \end{aligned} \qquad (3.3)$$

On the OXY plane, we consider a two-dimensional region $\Omega(x,y)$ with the boundary $d\Omega$. Oil or petroleum product occupies a subdomain $\Omega' \in \Omega$. Figure 2 shows as an example the water area of the port of Tuapse, which corresponds to the domain $\Omega(x,y)$, the domain $\Omega' \in \Omega$ – the area occupied by the spill, and its border $d\Omega'$ is partly free, and partly contact and coincide with the boundaries of port facilities.



a b

Figure 2 – Two phases (or snapshots) of an oil spill evolving in a port:
(**a**) 1 hour, (**b**) 2 hours after the (spill) release

3.2. Boundary conditions on the free and contact boundary

We assume that the modeling object (oil slick) is – the area $\Omega'(x,y,t)$ is delineated by a boundary line $R(x,y,t)=0$, either stationary or moving, that separates it from another environment.

At the free boundary, kinematic and dynamic conditions are set, which follow from the conditions of the absence of mass flux through the boundary of the region and the continuity of the momentum flux, respectively.

If the domain boundary $\Omega'(x,y,t)$ is $R(x,y,t)$ and $R = L_1(x,y,t) \cup L_2(x,y,t)$, where L_1 is the free boundary and L_2 is the contact (solid) boundary, the system of equations (3.1)–(3.2) must be supplemented with the following boundary conditions:

kinematic:

$$L_1: R_t + \mathbf{u}\nabla R = 0, \tag{3.4}$$

and the dynamic condition is the stress continuity condition:

$$L_1: \; h(x,y,t) \; = \; 0, \; \frac{\partial u_\tau}{\partial n} = 0. \tag{3.5}$$

On the solid/contact fixed boundary L_2, the condition of non-flux must be met:

$$L_2: u_n = 0, \tag{3.6}$$

where u_n is the orthogonal to the boundary L_2 component of **u**.

The complexity of the problem is associated with the possibility of changing the boundary conditions on the solid contour to the kinematic condition, if under the action of external factors, the oil slick moves away from the wall. Conversely, the part of the oil slick boundary which was movable becomes fixed when it comes into contact with the solid contour and a no-flux condition is set on it. A similar problem was considered in (Ovsienko, Efroimson, 1983). Correlation (3.4) is valid when the boundary displacement is due to dynamic factors. In some cases, the boundary of the area may change due to removal of oil from the surface both by natural factors – by evaporation and natural dispersion – and as outcomes of OSR.

At the initial time, the thickness distribution $h(x, y, 0)$, velocity field $\mathbf{u}(x, y, 0)$, and area $\Omega'(0)$ are assumed to be known. Its required to determine $h(x, y, t)$, $\mathbf{u}(x, y, t)$ and $\Omega'(t)$ when $t > 0$.

An important difference SPILLMOD model from the many others consists in the direct solution of hydrodynamic equations describing the flow of a light fluid on the heavier one in simulation region with free and contact boundary. These properties make it possible to calculate the surface oil thickness distribution. That is important to evaluate the geometric characteristics of the oil spill, and, subsequently, the required amount of resources required for OSR.

3.3. Parametrization of natural dispersion of oil spill

The process of dispersing an oil film by waves is seen as a combination of three processes: transition of the film from the sea surface into the water column by wave breaking, crushing of the oil film into droplets in the wave mixing layer and vertical turbulent diffusion, accompanied by droplets floating to the surface due to positive buoyancy (Zatsepa et al., 2018a; Zatsepa et al., 2018b).

To calculate the oil flux due to wind-wave dispersion a system we use

$$Q_d = \begin{cases} \rho_{oil} TOR \cdot h_{oil} \cdot F_{up}\left(d_{50}^N\right) \cdot F_m\left(d_{\max},\, v_d\right), & h_{oil} \geq h_T, \\ \rho_{oil} TOR \cdot h_T, & h_{oil} < h_T, \end{cases} \tag{3.7}$$

where d_{50}^N is the median oil droplets size, h_{oil} is the surface oil thickness, ρ_{oil} is the oil density, h_T is the threshold thickness of oil on the sea surface, $TOR \approx 1.4 * 10^{-2} u_*^3 g c_T^{-4}$, c_T is the threshold wave phase velocity at which overturn commences, u_* is the dynamic velocity in the atmospheric boundary layer under sea surface, F_{up} is the function determining the efficiency of oil transfer from the surface to the water column, F_m is the amount of oil droplet volume not resurfacing after wave turnover and depending on vertical mixing.

The median of the lognormal distribution of the number of oil droplets versus size on the physical parameters of oil, the thickness of the oil slick, and wind speed:

$$d_{50}^N = A \frac{h_{oil}^{0.4} \sigma_{ow}^{0.6}}{\rho_{oil}^{0.6}} \frac{1 + 0.02\left(\mu_{oil} W_{10} / \sigma\right)^{0.6}}{0.57 \cdot W_{10}^{1.2}}, \tag{3.8}$$

where S is the variance of the lognormal distribution, σ_{ow} is the oil-water surface tension coefficient, A is the constant.

The correction factor in the ratio (3.7) $F_{up}(d_{50}^N)$ denotes the proportion of oil returning to the surface between successive wave overturning events:

$$F_{up}\left(d_{50}^N\right)=\left(1-1/w_{cr}\cdot K_{up}k_{St}\left(d_{50}^N\right)^2\right), \tag{3.9}$$

where $K_{up}=\exp\left(3S^2\right)\int_0^{\exp\left(3\left(S-S^2\right)\right)}\zeta^2 f_{norm}\left(1,\ S,\ \zeta\right)d\zeta$, $f_{norm}\left(1,\ S,\ d\right)$ is the lognormal distribution for droplet sizes, normalized by d_{50}^V is the median diameter of the oil volume distribution over droplet sizes, $k_{St}=g'/18v_w$ is the coefficient.

The multiplier $F_m(d_{\max},\ v_d)$ denotes the fraction of droplets that do not return to the surface due to turbulent diffusion:

$$F_m\left(d_{\max},\ v_d\right)=v_d\int_0^{d_{\max}}\frac{f_V\left(d'\right)}{w_d+v_d}dd',\ \ d_{\max}=d_{50}^N\cdot e^{3S}, \tag{3.10}$$

where w_d is the ascent velocity oil droplets a diameter d in the water, $v_d=0.14v_w^*$, v_w is the dynamic velocity in water, the maximum size of drops when dispersed by waves is given by formula $d_{\max}^N=d_{50}^N\cdot e^{3S}$, $f_V(\zeta)$ is the probability density function of the oil volume depending of the oil drop size ζ. To parameterize the vertical turbulent exchange coefficient $K(z)$ in the upper sea layer the model (Nakamura, Hayakawa, 1991) is chosen:

$$K(z)=\kappa v_w^* z\cdot \mathrm{Pr}^{-1}\cdot e^{-k_d z}f(Ri), \tag{3.11}$$

where κ is the von Karman constant, v_w^* is the dynamic velocity in water, z is the depth, Pr is the turbulent Prandtl number, k_d is the attenuation coefficient of turbulent stresses with depth, $f(Ri)=(1+\alpha Ri^{\gamma})^{-\beta}$, where Ri is the Richardson number – the ratio of density stratification and vertical shear of velocity in the water column close to the surface, $Ri=N^2(\partial u_w/\partial z)^{-2}$, $N^2=\frac{g}{\rho_w}\frac{\partial\rho_w}{\partial z}$, $N-$ is the Brunt-Vaisala frequency, $u_w\equiv u_w(x,y,z,t)$ – horizontal velocity of water.

The parametrization of the oil natural dispersion from the surface film to the water column depends on meteorological conditions (wind waves, water density) and on the characteristics of sea surface pollution (oil layer thickness, viscosity, surface tension, density). This approach presented allows us to take into account the use of chemical dispersants also through their influence on the surface tension and viscosity of oil.

3.4. Parametrization of oil evaporation

Since the mid-70s of the last century, the treatment of oil evaporation from a spill is based on the representation of oil as a mixture of fractions or “pseudo-components” with known physical and chemical properties. The oil mass flux due to evaporation Q_e from the sea surface is represented as the sum of fluxes of pseudo-components:

$$Q_e=\sum_i Q_{ei}=k_m\sum_i\left(M_iP_iX_i\right)/\left(RT_{wK}\right)=\sum_i k_iX_i, \tag{3.12}$$

where Q_{ei} is the flux of the *i*-th component, k_m is the empirical mass transfer coefficient depending on the wind velocity, P_i is the saturated vapor pressure of the oil fraction, M_i is

the molecular weight of the fraction, X_i is the molar fraction of the fraction at the interface, *R is* the universal gas constant, T_{wK} and is the temperature of the underlying surface (water temperature) [°K].

In equation (3.12), we can change variable from the molar to the volume concentration:

$$k_i X_i = \underbrace{k_i \cdot 1/\rho_{oil} \cdot M_0/M_i}_{\tilde{k}_i} C_i = \tilde{k}_i C_i \,, \tag{3.13}$$

where ρ_{oil} is the oil density, M_0 is the average molecular weight of the mixture (oil).

The shallow water equations for the oil layer on the sea surface are a good approximation describing the spill dynamics. However, if we consider a multicomponent mixture with a wide range of saturated vapor pressure of these components, then the molecular diffusion of oil fractions in the oil layer may limit the evaporation flux to the atmosphere.

Oil evaporation models are formulated in terms of layer-averaged concentrations of oil components, however, it reality only a thin sublayer located near the liquid-gas interface is in equilibrium with the gas phase. When oil evaporation begins, an individual concentration of a component decreases in just a small near-surface sublayer while its gradient of near the oil-to-air interface is approximated by the equation (3.14), as shown in Figure 3a (Zatsepa et al., 2020):

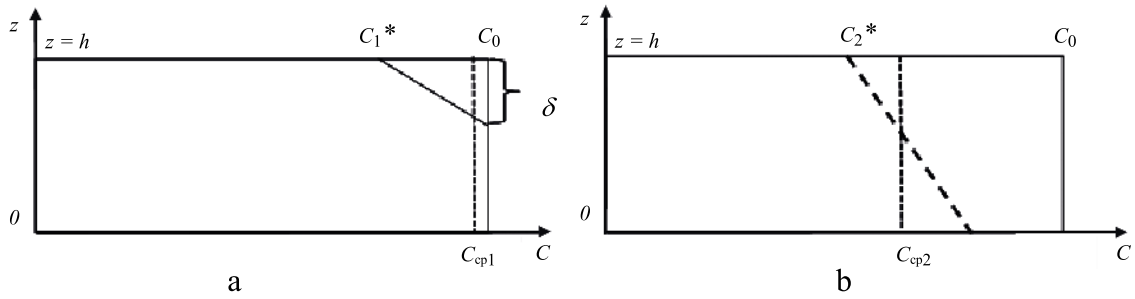


Figure 3 – Schematic of change in the concentration of the component in the oil layer over time: (**a**) at $t < h^2/D_i$ (**b**) and at $t > h^2/D_i$

$$\frac{\partial C_i}{\partial z} \approx -\left(C_{i0} - C_i^*\right)/\delta = -\left(C_{i0} - C_i^*\right)/\sqrt{D_i t} \,, \tag{3.14}$$

where C_{i0} is the initial oil component concentration, $\delta = \sqrt{D_i t}$ is the diffusion layer thickness, D_i is the *i*-th fraction molecular diffusion coefficient, *t* is the time, *h* is the layer thickness.

The relationship between the initial oil component concentration C_{i0}, the average in the layer $\overline{C}_i = \overline{C}_i(t)$ and the concentration at the interface C_i^* can be written as (see Figure 3a):

$$C_i^*/\overline{C}_i = C_{i0}/\overline{C}_i + \left(1 - C_{i0}/\overline{C}_i\right) 2h/\sqrt{D_i t} = \alpha_{i1} \,. \tag{3.15}$$

On large time scales $\hat{T}_i = h^2/D_i$ a quasi-stationary regime is established, thus the relationship between the volume concentration of the oil component at the interface C^* and the average concentration in the layer $\overline{C}$ is defined as (dashed line in Figure 3b):

$$\overline{C}_i = C_i^* + C_i^* \tilde{k}_i h/(2D_i) = C_i^* \left(1 + \tilde{k}_i h/(2D_i)\right), \tag{3.16}$$

or:

$$C_i^* = \overline{C}_i \Big/ \left(1 + \tilde{k}_i h/(2D_i)\right) = \alpha_{i2} \overline{C}_i, \tag{3.17}$$

$$\alpha_{i2} = \frac{1}{1 + \tilde{k}_i h/(2D_i)}. \tag{3.18}$$

Due to the linear relationship between the volume and molar concentrations, the basic formula for calculating the mass flux of oil due to evaporation can be written as:

$$Q_{ei} = \begin{cases} \alpha_{i1} k_i \overline{X}_i, \text{ if } 0 < t \le \hat{T}_i \\ \alpha_{i2} k_i \overline{X}_i, \text{ if } t > \hat{T}_i \end{cases}, \tag{3.19}$$

where α_{i1}, α_{i2} are determined by the equations (3.15) and (3.18).

Table 1 shows the numerical values of the dimensionless parameter $\tilde{k}_i h/(2D_i)$, calculated for a wind velocity of 10 m/s and allows to distinguish conditions of significant effect on evaporation of molecular diffusion.

Table 1. Numerical values of the parameter $\tilde{k}_i h/(2D_i)$ calculated in the evaporation model including diffusion in the liquid phase

No	D, m²/s		1E-7	1E-7	1E-7	1E-7	1E-9	1E-9	1E-9	1E-9
	h_{oil}, mm		1	5	10	20	1	5	10	20
1	Boiling temperature T_{bi}, °C	50	0.075	0.37	0.75	1.51	7.59	37.97	75.95	151.90
2		100	0.0077	0.038	0.077	0.15	0.77	3.89	7.79	15.59
3		150	0.00058	0.0029	0.0058	0.011	0.058	0.29198	0.58	1.16
4		200	3.12E-5	0.00015	0.00031	0.00062	0.0031	0.01562	0.031	0.062
5		250	1.16E-6	5.79E-6	1.16E-5	2.31E-5	0.00011	0.00057	0.0011	0.0023
6		300	2.84E-8	1.42E-7	2.84E-7	5.69E-7	2.84E-6	1.42E-5	2.84E-5	5.69E-5
7		350	4.39E-10	2.19E-9	4.39E-9	8.78E-9	4.39E-8	2.19E-7	4.39E-7	8.78E-7
8		400	3.95E-12	1.98E-11	3.95E-11	7.9E-11	3.95E-10	1.98E-9	3.95E-9	7.9E-9
9		450	1.89E-14	9.47E-14	1.89E-13	3.79E-13	1.89E-12	9.47E-12	1.89E-11	3.79E-11
10		500	4.3E-17	2.15E-16	4.3E-16	8.59E-16	4.3E-15	2.15E-14	4.3E-14	8.59E-14

The Table 1 includes the data with a typical oil film thickness of about 1 mm (10^{-3} m) and a "normal" diffusion coefficient of about 10^{-7}m²/s (Stronach, Hospital, 2014), molecular diffusion in the film practically does not affect the evaporation processes, since $\tilde{k}_i h/(2D_i) << 1$ a decrease in the diffusion coefficient to 10^{-9} can lead to a decrease in the only the evaporation of highly volatile components with boiling points up to 100 °C can be "slowed down". However, with an oil film thickness below 10 mm, diffusion becomes a limiting evaporation factor. Figure 4 shows the results of calculations of type "A" oil evaporation[1] with fraction flux correction due to molecular diffusion in the liquid phase

[1] Artificial fractional composition with uniform mass concentration distribution of petrol components in the boiling temperature range from 50 °C till 500 °C.

(Equation 3.19) for oil film thicknesses from 1 to 20 mm and diffusion coefficients in the range from 10^{-7}–10^{-10} m^2/s. Figure 4 also shows the results of calculations using the SPILLCALC model (Stronach, Hospital, 2014). With a decrease in the diffusion coefficient and an increase in the layer thickness of the evaporating oil product, the evaporation rate (mm/day) stabilizes to an almost constant value. The result of calculations based on Equation (3.12), taking into account Equation (3.19), corresponds to calculations based on the SPILLCALC numerical model and conclusions from (Shuplyak, 2013), which showed that the evaporation rate of a rather "thick" layer of a multicomponent mixture stabilizes over time, while for a layer of oil products of finite thickness, the evaporation rate decreases exponentially.

The layer can be attributed to "thick" if condition $\sqrt{D_i t} < h$ is valid. In this case, it follows from equation 3.15 that the flux of evaporating components is determined only by the properties of the component, the initial concentration C_{i0}, and the diffusion coefficient D_i:

$$Q_{ei} \approx \frac{\tilde{k}_i \sqrt{D_i / t}}{(\tilde{k}_i + \sqrt{D_i / t})} C_{i0}. \qquad (3.20)$$

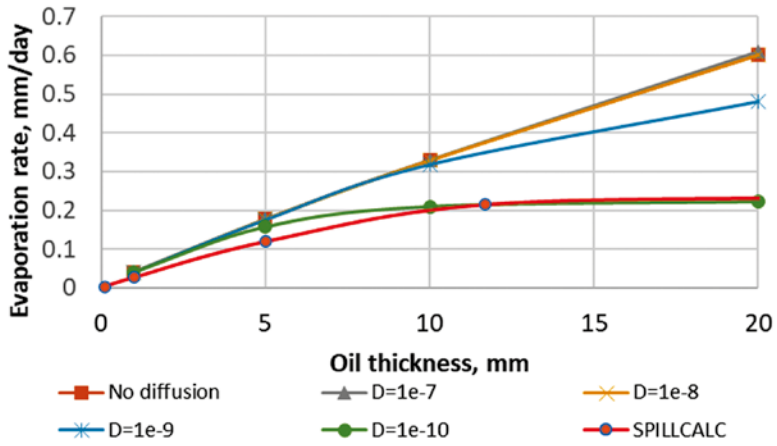


Figure 4 – Dependence of the evaporation rate from oil films of different thickness at different diffusion coefficients

At the initial time when $\sqrt{D_i / t}) >> \tilde{k}_i$ the component flux is equal $Q_{ei} \approx \tilde{k} C_{i0}$. If the condition $\sqrt{D_i / t} << \tilde{k}_i$ and $t < h^2 / D_i$ from (3.22) is satisfied, it follows that $Q_{ei} \approx \sqrt{D_i / t} C_{i0}$. On the contrary, for large times, when $t > h^2 / D_i$ the relation (3.18) is valid, which for values $\tilde{k}_i h / (2D_i) >> 1$ leads to the expression for the *i*-th oil fraction flux:

$$Q_{ei} \approx \frac{2D_i k_i}{h\tilde{k}_i} \bar{X}_i = \rho_{oil} \frac{2D_i M_i}{h M_0} \bar{X}_i. \qquad (3.21)$$

However, if $\tilde{k}_i h / (2D_i) << 1$ the effect of diffusion processes on the evaporation rate from the oil film can be ignored.

Oil, as a mixture of individual components with different properties, can be considered as a dispersed system and the Einstein formula $D \sim 1/\mu$ is valid for it. The consequent substitution of diffusion coefficient into the equation 3.21 leads to:

$$Q_{ei}\big|_{T=T} = \frac{2D_i k_i}{h\tilde{k}_i}\bar{X}_i = \rho_{oil}\frac{\mu_0}{\mu_T}\frac{2D_i M_i}{hM_0}\bar{X}_i, \tag{3.22}$$

where μ_0, μ_T is the viscosity of the oil at temperature T_0, and the ambient temperature T, respectively. It should be noted that the weathering processes, on the one hand, depend on the density and viscosity of the spreading substance, and, on the other hand, both the density and viscosity of oil change due to changes in the fractional composition of oil due to evaporation.

The change in the fractional composition due to evaporation significantly depends on the thickness of the oil layer (Zatsepa et al., 2020). Thin layers of oil or petroleum products change their properties much faster than relatively thick layers. Natural dispersion leads to a decrease in the surface oil thickness and, as a result, the processes of changing the content of fractions are accelerated, leading to an increase in the density of weathered oil.

3.5. Oil viscosity and density evolution parameterization

The density and viscosity of oil significantly increase during volatile oil fractions evaporation. The "water in oil" emulsion formation is a reason of oil density and viscosity changes. That processes depend on the ambient temperature especially important when considering oil spills in the Arctic.

To calculate changes in the density and viscosity of oil, the following relations are used:

$$\rho_{oil} = F_{em}\rho_w + \rho_{oil}^{(0)}\left(1-F_{em}\right)\left(1+c_{ev}F_{ev}\right)\left[1-c_T\left(T_{wK}-T_{0K}\right)\right]. \tag{3.23}$$

Change of the oil viscosity due to temperature is evaluated by the formula:

$$\mu_{oil} = \mu_{oil}^{(0)}\exp\left[a_T\left(1/T_{wK}-1/T_{oK}\right)\right]. \tag{3.24}$$

Change of the oil viscosity while evaporation is in the following form:

$$\mu_{oil} = \mu_{oil}^{(0)}\exp\left(a_{ev}F_{ev}\right). \tag{3.25}$$

Change of the oil viscosity depends on emulsification:

$$\mu_{em} = \mu_{oil}^{(0)}\exp\left(\frac{a_1 F_{em}}{1-a_2 F_{em}}\right), \tag{3.26}$$

where $\rho_{oil}^{(0)}$ is the initial density of oil $\mu_{oil}^{(0)}$ is the initial viscosity of oil, T°K is the reference water temperature, F_{ev} is the evaporated oil mass fraction, F_{em} is the volume fraction of water in the emulsion, $c_{ev}, c_T, a_{ev}, a_T, a_1, a_2$ are empirical coefficients. According to the data given in (Nelson-Smith, 1972), the coefficient $c_{ev} = 0.14 \div 0.25$. The article (Belore and Buist, 1994) presented the results for 13 crude oil types and it was founded the coefficient a_T to be in the range from 1085 to 17838, the coefficient a_{ev} varies in the range from 2.8 to 16.95, $c_T = 7\cdot10^{-4}$ °C^{-1}.

The SPILLMOD model uses the *Mackay* parameterization water-in-oil content (Mackay et al., 1980). To calculate the change of the oil density due to evaporation not only an engineering approach equation 3.23 can be used. The oil density can be recalculated on the base of narrow fractions density and their mass concentrations. The formula to calculate oil density have the following form $\rho_{oil}(t) = 1 \Big/ \sum_{i=1}^{N_f} \left(C_i / \rho_i \right)$, where ρ_i, C_i are an oil component density and an oil component mass concentration.

4. Numerical method

Among the above-mentioned features of marine oil spills, we will highlight changes in spatial scales during the spreading of oil and petroleum products on the sea surface from the first meters at the beginning of the accident to kilometers a several days after. When the scale of the oil spill is measured about kilometers, a local change in characteristics on a scale of several meters, as can happen when, for example, a relatively small obstacle in the form of a vessel or a boom, on the one hand, does not matter much for changing the parameters of the entire spill. On the other hand, the need to consider local deformations of the oil spill when interacting with fixed boundaries (vessel hull, mooring wall, shoreline) makes the use of self-similar solutions unacceptable. The numerical method developed to solve this problem uses a discrete representation of the oil spill (2-D continuum) in the form of a set of Lagrangian elements (particles). Coastline and other elements that prevent the movement of the spill, for example, booms, are given as a piecewise linear function of arbitrary shape. To solve two-dimensional equations with free boundaries describing the dynamic transformation of an oil spill, the use of traditional Eulerian techniques is problematic. The boundaries of the solution area itself are unknown and are determined from the process of solving the problem. The scale of this area can vary by several orders of magnitude, which excludes the use of numerical schemes with constant spatial resolution. To solve the system of equations, a new Eulerian-Lagrangian numerical method has been created and used, using adaptive Eulerian grids, with dimensions changing by orders of magnitude during the solution of the problem.

The modeling object (oil spill) is represented by an ensemble of Lagrangian particles, each having a set of variables, in this case, such as spatial coordinates $\{x_i, y_i\}$, velocity $\{u_i, v_i\}$ and mass $\{m_i\}$ associated with it. The initial state is specified if all the variables of the particles are known: $\{x_i, y_i\}_{t=0}$, $\{u_i, v_i\}_{t=0}$, $\{x_i, y_i\}_{t=0} \in \Omega_0$, where Ω_0 – the initial configuration of the oil spill. The number of particles N_p can be variable, sufficient to determine the initial configuration of the region Ω_0, and subsequently its time evolution $\Omega(t)$. A rectangular Eulerian grid is overlaid over the ensemble, so that all the particles are contained inside the grid region, as shown in Figure 5.

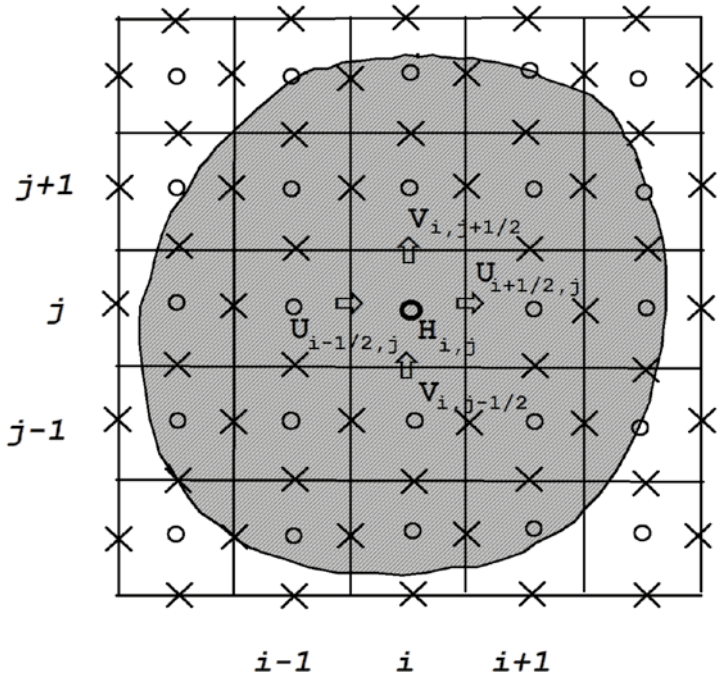


Figure 5 – Schematized view of the Eulerian grid for calculating oil spreading
(the shaded area is occupied by the simulated medium)

After that, the velocity of movement in the oil layer $\mathbf{u}(x, y, t)$ and the thickness of the oil $h(x, y, t)$ are determined in the Eulerian representation. The method uses a grid "C" according to the Arakawa classification in which the values of the thickness of the oil layer are assigned to the centers of the cells, and the velocities are calculated on its faces. The components of the velocity along the X axis are defined in the middle of the left and right cell interfaces, as $u_{i-1/2,j}$ and $u_{i+1/2,j}$, while the components along Y-axis of in the middle of the upper and lower sides, as $v_{i,j+1/2}$ and $v_{i,j-1/2}$. The separation of grid functions in the coordinate space makes it possible to interpret each cell as an element of the volume of the medium, which is characterized by the pressure (thickness) calculated at its center. Knowing the normal component of the velocity at the cell boundaries allows one to directly calculate the impulse and mass flux through this boundary. The computational grid used in this technology is not purely Eulerian, since it is reconstructed at each time step depending on the configuration of particles and differs from the traditional Eulerian representation of fixed points in space. The thickness $h_{i,j}$ is calculated using the sum of the masses of individual particles related to the area of the cell occupied by the particles:

$$h_{i,j} = \frac{1}{\rho_o} \frac{1}{\gamma \Delta x \Delta y} \sum_{k}^{N_{ij}} m_k , \tag{4.1}$$

where γ – the part of the cell area occupied by particles, m_k – the mass of the k-th particle, N_{ij} – the number of particles in (i, j) cell, $\Delta x, \Delta y$ – the size of the cell in two horizontal coordinates, respectively. As a method of the velocity reduction from particles to the grid, SPILLMOD uses linear regression, which has a higher order of accuracy in contrast to the "nearest node" method used in the original method PIC (Harlow, 1964). The number of

particles N_p in a cell must be greater than the number of cells in the computational grid along one of the coordinates. Typically, a grid of $N_x \cdot N_y = 2000$ is used. In this case, the total number of particles is on the order of 200,000.

The solution procedure can be considered as a variant of the method of splitting into physical processes of the system (3.1) – (3.2). The original system of equations is replaced by three auxiliary ones. The first system describes the change in the amount of movement caused by the work of pressure forces and external forces:

$$\frac{\partial \tilde{\mathbf{u}}}{\partial t} = -g'\nabla h - \frac{\beta \rho_w / \rho_{oil}}{h}\left|\tilde{\mathbf{u}} - \mathbf{u}_d - \mathbf{u}_c\right|\left(\tilde{\mathbf{u}} - \mathbf{u}_d - \mathbf{u}_c\right) + \frac{1}{\rho_{oil} h}\nabla.\mathbf{T}, \tag{4.2a}$$

$$\frac{\partial \tilde{h}}{\partial t} = 0. \tag{4.3a}$$

The second system describes the advection processes:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\nabla\mathbf{u} = 0, \tag{4.2b}$$

$$\frac{\partial h}{\partial t} + \nabla.\left(h\mathbf{u}\right) = 0. \tag{4.3b}$$

The third system describes the change in the momentum and thickness of the oil layer under the influence of weathering processes:

$$\frac{\partial \mathbf{u}}{\partial t} = 0, \tag{4.2c}$$

$$\frac{\partial h}{\partial t} = -\frac{1}{\rho_{oil}}(Q_e + Q_d). \tag{4.3c}$$

After the grid functions are defined, the whole computational cycle can be represented as a sequence of several steps.

Step I. Calculation of intermediate values with equations (4.2*a*) – (4.3*a*), where we neglect all the effects associated with the motion of the medium. At this step, all the necessary characteristics of the medium are known in the Eulerian representation.

Step II. Interpolation of intermediate velocity values from grid nodes to particle locations. All known values of the velocities in the nodes of the Eulerian grid, the velocity is transferred to the particles by linear interpolation:

$$\hat{u}_k = \tilde{u}_{i-1/2,j}(1-\hat{x}_k) + \tilde{u}_{i+1/2,j}\hat{x}_k, \quad \hat{v}_k = \tilde{v}_{i,j-1/2}(1-\hat{y}_k) + \tilde{v}_{i,j+1/2}\hat{y}_k, \tag{4.4}$$

where $\hat{u}_k, \hat{x}_k$ – velocity and coordinate ($0 \le \hat{x}_k \le 1$) *k*-th a Lagrangian particle in the *i, j*-th cell.

The velocity interpolation from nodes to particles and reinterpolation is carried out independently along the *x* and *y* coordinates, i.e., the position of the particles is considered only along one of the coordinates.

After interpolating the velocity from the grid nodes to the particles, the particles along with their attributes are moved to their new positions according to the transfer algorithm:

$$\hat{x}_i(t+\Delta t) = \hat{x}_i(t) + \hat{u}_i(t)\Delta t\,, \quad \hat{y}_i(t+\Delta t) = \hat{y}_i(t) + \hat{v}_i(t)\Delta t\,. \tag{4.5}$$

The second step of the computational cycle is a discrete approximation of the system (4.2b) – (4.3b) (Ovsienko, Efroimson, 1983). Numerical stability of these schemes generally requires that the time step be limited by a Courant–Friedrichs–Lewy condition of the form $Max|\mathbf{u}|\cdot\Delta t/\Delta x<1$. The interpolation and reinterpolation of velocity procedures have the important property that in a situation where the velocity field changes slightly, for example, at small time steps, repeated implementation of these procedures does not lead to a non-physical change in velocity.

At this step, the calculation of mass fluxes due to evaporation and dispersion processes is performed in accordance with the equations (3.8) – (3.27) and the calculation of new values of the mass of the *k*-th particle in accordance with:

$$m_k(t+\Delta t) = m_k(t) - \Delta t(Q_e + Q_d)S_k\,, \tag{4.6}$$

where $S_k = \gamma\Delta x\Delta y/N_{i,j}$.

At the end of this step, all the characteristics of the medium are fully defined in the Lagrangian representation. If the trajectory of the particle crosses a shoreline, a special procedure is used to determine the new position of the particle, and the mass of the particle decreases, simulating its deposition on the shoreline.

Step III. Determining a new position of the particles after their transfer, forming a new Eulerian grid and the transfer of particle properties to determine new values of the thickness of the oil layer h_{ij} and velocities $\mathbf{u}_{ij}$ on the "Eulerian" grid, built taking into account the new configuration of particles.

The numerical scheme, due to the use of the least squares method when transferring the velocity values of the medium from particles to grid, is characterized by a low scheme viscosity.

The method of splitting by physical processes makes it easy to include new parameterizations of weathering processes into the overall algorithm. As stated above the boundaries of the area in which the solution of the problem is being sought are not fixed. Under certain conditions, the part of the boundary of the area that was considered as contact can become mobile (free). For example, when oil moves away from the shore under the influence of wind. And, conversely, the kinematic condition that is stated on the free boundary, when approaching the shore or the boom, is transformed into an impermeability condition. Since the area of the problem solution itself is the desired value, the actual boundary condition is determined at the Lagrangian stage of the computational scheme. In such a way, both the non-flux condition and the kinematic condition can be realized on the same site of the oil spill boundary, depending on the direction of oil spill propagation. Unlike traditional parameterizations of the spreading process based on the use of various

self-similar solutions for individual stages of the spreading process, the computational technique developed here allows calculating the thickness distribution in the interior of the oil slick in areas with a complex geometry of contact boundaries and with arbitrary oil source distribution.

5. Assessment of the area of probable detection of oil spill on the sea

The movement of an oil slick across the sea surface is caused by the action of wind, currents and waves. Calculating instantaneous values of meteorological fields is a virtually unsolvable mathematical problem. For this reason, all models calculate the most probable trajectory of the oil slick movement accompanied by an estimate of uncertainty of the spill location. The location uncertainty is described by a distribution function for deviations of the actual oil spill position from the calculated location.

Some models (Sebastião, Soares, 2006; 2007) present ensembles of oil spill propagation trajectories with perturbation of forcing inputs around to their average values. The ensemble of trajectories covers the area on the map, which is then interpreted as the uncertainty in oil spill position.

Consider the original approach that uses a probability density function of oil spill coordinates as the measure of the uncertainty. Let's assume that the probability density is known $f(x,y,t)$, here (x,y) are coordinates, t is the time.

The following functional is to be constructed:

$$F(f_l,t)=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y,t)\theta\left(f(x,y,t)-f_l\right)dydx,\ \theta(z)=\begin{cases}0, z<0\\ 1, z\geq 0\end{cases}, \tag{5.1}$$

here θ is the Heaviside function, f_l is the probability density level of the probability density function. It is clear the function $F(f_l,t)$ is a non-increasing function with respect f_l, and it is possible to construct the inverse function F^{-1} with respect to F:

$$f_l = F^{-1}(f,t), \tag{5.2}$$

or more generally:

$$f_l(F_l,t)=\min(f)\big|_{F(f,t)\geq F_l}. \tag{5.2a}$$

In fact, the region of space in which the probability density exceeds the value f_l corresponds to the probability of detecting a spill with a probability value F_l within this region.

Let us now consider a particular case of the oil spill position uncertainty, which is caused by the uncertainty of the wind speed setting. The oil spill coordinates probability density function evolution is then described by the advection-diffusion equation:

$$\frac{\partial f}{\partial t}+\frac{\partial f u_i}{\partial x_i}=\frac{\partial}{\partial x_i}K\frac{\partial f}{\partial x_j}. \tag{5.3}$$

In (Zatsepa et al., 2014), the following formulation of the dispersion coefficient in equation (5.3) is proposed:

$$K(t) = (\alpha \cdot \sigma_W)^2 T_u \left(1 - \exp\left(-t/T_u\right)\right), \tag{5.4}$$

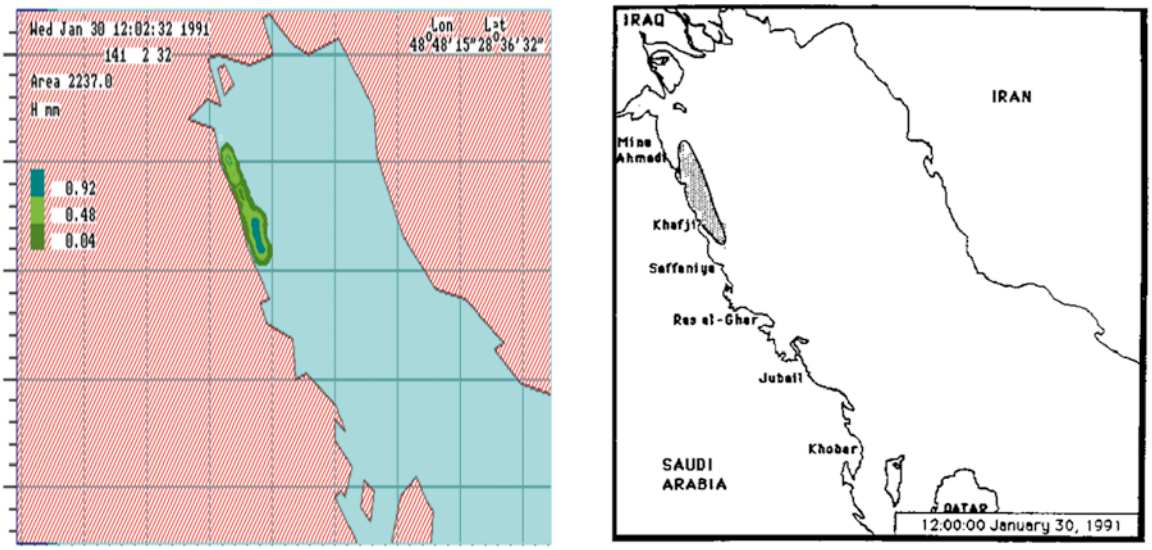
where σ_W is the standard deviation of the measured and simulated wind speeds (approximately equal to 2.9 m/s), T_u is the time correlation scale between the wind speed pulsation rates (approximately equal to 11 hour), α is the wind drift coefficient. The above equation for the probability density function of the distribution of spill coordinates corresponds to the equation for the tracer concentration in the marine environment with two features. First, the integral f over the entire space is equal to 1, and second, the variance coefficient K depends on time in a special way. The above equations are numerically solved by the discrete cloud method. A detailed description of the numerical method for the case of instantaneous and continuous cases can be found in (Solbakov et al., 2016). The values of the probability density function for the distribution of spill coordinates decrease over time and cannot be directly used as a stable estimate of uncertainty, in contrast to the functional introduced above. Note that this approach can be used to estimate domain boundaries of possible spill detection for other sources of uncertainties during oil spill modelling caused different factors such as sea current inaccuracy or wind waves, or initial oil spill position and time and etc.

6. Examples of model implementation

6.1. Experience in operational forecasting of oil spill spreading

The first experience of using the mathematical model presented above was the prediction of the spread of a large-scale oil spill which occurred shortly after the start of the Gulf War in January 1991. At that time, besides the general news reports, there was very limited information about the exact time, place, and the amount of oil released. Nor it was possible to determine the exact location of the point of release on the coastline (thereafter in became known from the media that there were several such points). Therefore, for our calculations we choose to set up a single source located in the Gulf of Kuwait (close to north-western corner of Persian Gulf). The total amount of oil released was specified as 6 million barrels and the duration of the release between 3 to 4 days (again, these estimates are based on data from the media). What make this case extraordinary is an unusually large amount of oil released into the sea during an extended interval of time under relatively calm meteorological conditions. Wind speed in the relevant area (Gulf of Kuwait) during the period of oil release was within the range of 2 to 5 m/s. The initial time for our simulation was set to noon of 24 January 1991. Although this was the very first version of the model, the calculations were carried out on a low-power PC, and with very limited data support, the outcome results showed a high degree of correspondence with the observational data. Later that year, the authors had an opportunity to compare the results of operational calculations with satellite observations in the Persian Gulf region. Figure 6 shows a comparison of the results of calculations (a)

and schematic representation the oil spill position at two instances in time obtained using satellite imagery (b). Current time, time from the beginning of spill, and the coordinates of the geometric center of the spill are shown. The color scale refers to the thickness of the oil slick on the sea surface.



a b

Figure 6 – Results (**a**) of operational simulation and (**b**) results of satellite survey of the position of the oil spill in the Persian Gulf

In the mid-90s, the model was implemented into the simulator PISCES[1], designed to train personnel to act in incidents related to oil spills at sea, developed by TRANSAS MARINE, Ltd (UK). Later, the model was designed as an independent software product integrated with Mapinfo GIS (in the desktop version), and as a server application designed to work as part of an information system for environmental monitoring. The features of the model implementation make it possible to use it for calculations in a wide range of spill parameters, in various geographical and meteorological conditions, in areas of complex geometry taking into account the use of OSR technical means.

6.2. Oil spill in a tidal sea

Figure 7 shows the oil spill configuration 72 hours after the start of oil discharge in conditions of strong tidal dynamics on the shelf of the Sea of Okhotsk adjacent to the northeastern tip of Sakhalin Island during a prolonged emergency oil spill. It should be noted that calculations of a rather complex oil spill configuration were carried out using the original Eulerian-Lagrangian numerical technology, briefly presented in section 4.

[1] https://www.marinelink.com/article/naval-architecture/oilguard-designed-minimize-damage-644

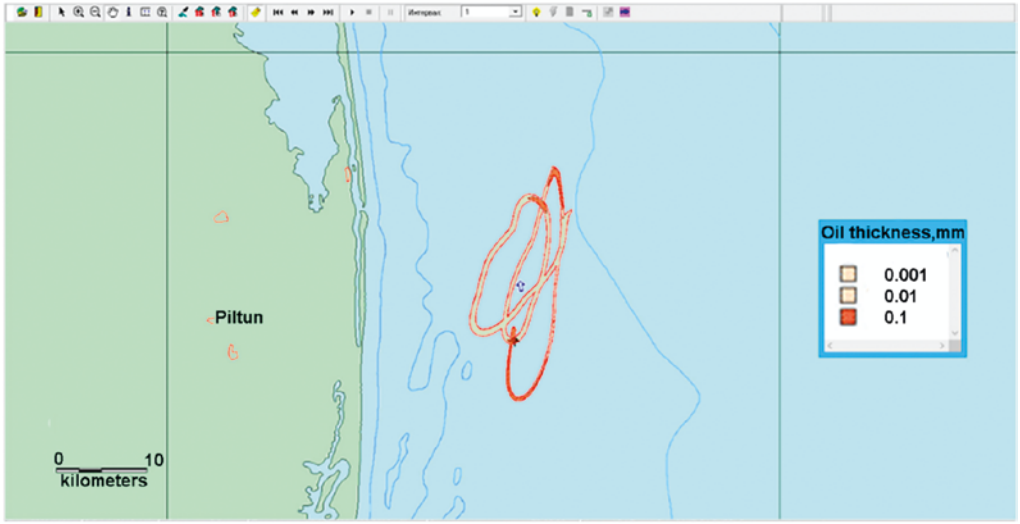
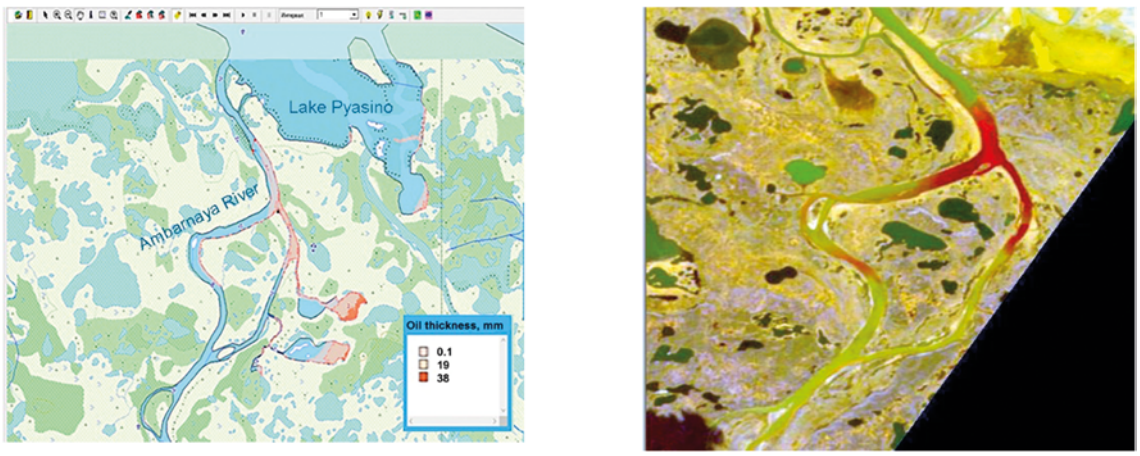


Figure 7 – Oil spill configuration 72 hours after the beginning of an ongoing spill on an offshore stationary platform

6.3. Diesel fuel spill under limited spreading conditions

A feature of the SPILLMOD model is the ability to calculate the spread and weathering of oil spill in areas of complex geometry, in the presence of contact boundaries. The model was used in the reconstruction of a diesel fuel spill on May 29, 2020, in Norilsk (see Figure 8). During the incident, approximately 30,000 tons of diesel fuel leaked into the river network and began to spread towards Lake Pyasino. Restricted by the banks of a small river, and subsequently by a system of booms, until it was finally contained, the diesel fuel spill had an area an order of magnitude smaller than it could have been with the free spread of the spill in open water. For this reason, the evaporation of diesel fuel in this incident was an order of magnitude less than with free spreading. This result was confirmed when collecting fuel in the next few weeks after the spill.



a b

Figure 8 – Spread of diesel fuel spill on June 1:
(**a**) model calculations, (**b**) satellite image 01.06.2020 Sentinel-2

Calculations of the movement of the spill along the Ambarnaya River were confirmed in satellite survey materials (Troshko et al., 2020).

6.4. Change in area of the fast-evaporating oil product

When spreading oil or oil products with large quantities of volatile fractions such as petrol, the oil slick should be expected to disappear from the sea surface fairly quickly. Figure 9a shows the results of calculations of evaporation 10 t of various types of oil and petroleum products with free spreading on the water surface. It is clear that oil and petroleum product weathering processes have a significant impact on the size of the pollution area on the sea surface, as shown in Figure 9b.

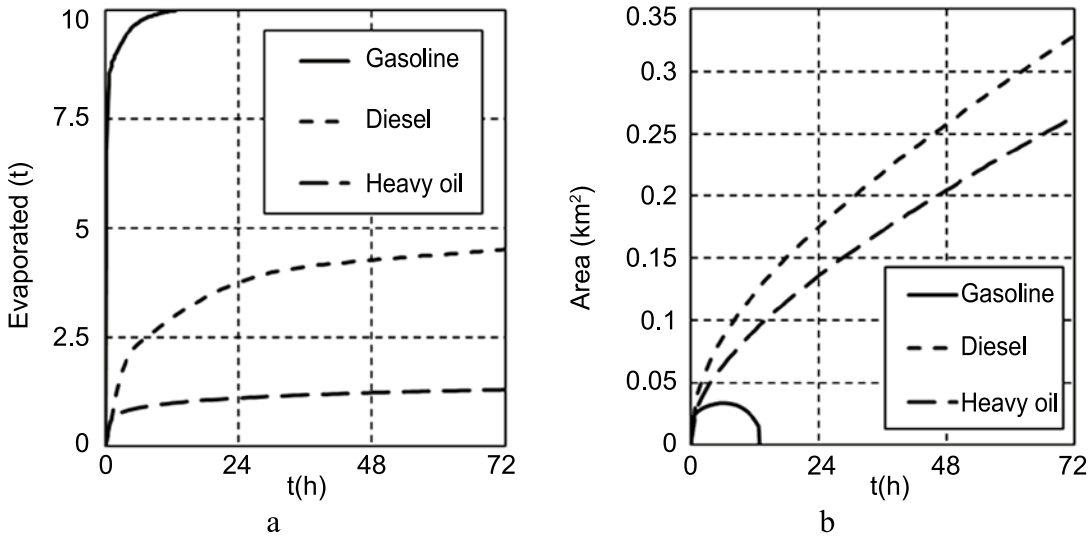


Figure 9. Evaporation losses and spill area for various types of petroleum products

Figure 10 shows a schematized image of an oil spill, where the red outline indicates areas with different thicknesses of the oil film. The SPILLMOD model makes it possible to calculate not only the total area of the oil spill, but also the distribution of the layer thickness inside this area, the length *L*1, *L*2, *L*3 and width *W*1, *W*2, *W*3 of the oil pollution area, where the thickness of the oil film exceeds 1 microns (*T*1), 10 microns (*T*2) and 100 microns (*T*3), respectively.

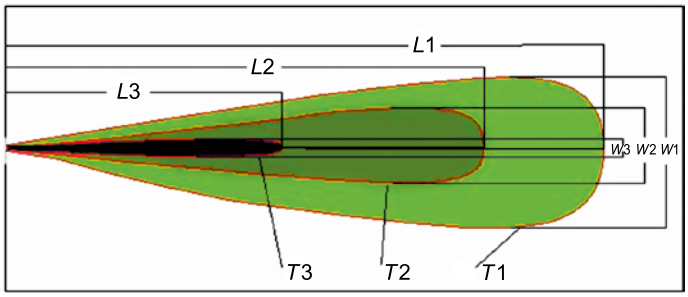


Figure 10 – Schematic image of a continuous oil spill with the allocation of areas with different film thicknesses

Figure 11 shows the change in the areas of subdomains, within which the thickness of the oil product film exceeds the threshold values of 1, 10 and 100 microns, for the spill of 10 tons of diesel fuel in calm conditions.

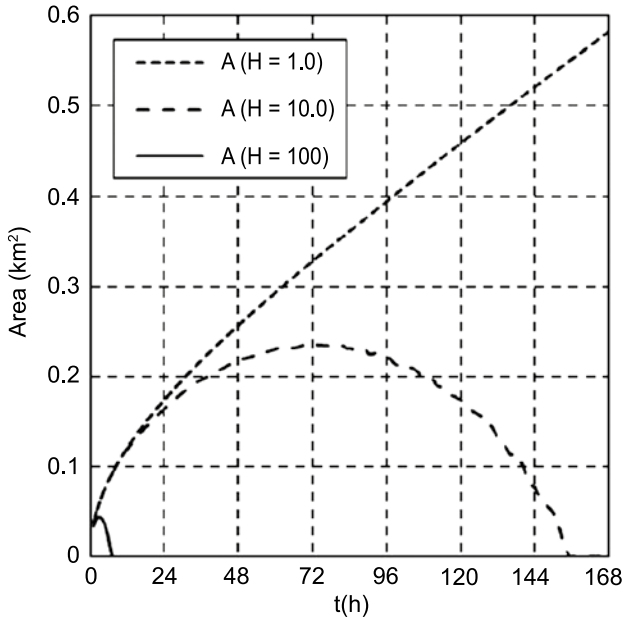


Figure 11 – Changing the areas of subregions for the batch spill of diesel fuel during calm

These estimates are for reference and may be useful for planning the effort and resources required to respond to a spill with given parameters. Nevertheless, it is these estimates that clearly show that, depending on the type of oil or oil product, the size of an oil spill and the size of sub-areas within which the oil film thickness exceeds a given thickness can vary by an order of magnitude or more.

6.5. Evaporation of oil with a high pour point

Oil viscosity increases exponentially as temperature decrease, approaching the pour point. An increase in viscosity leads to a decrease in diffusion in the oil layer. This gives a reason to believe that the new oil evaporation model proposed here allows more accurate evaporation calculation compared to traditionally used ones. The importance of this possibility is especially great in conditions of Arctic seas. From the authors' point of view, the proposed oil evaporation model is more user-friendly than the model previously described in the SPILLCALC literature (Stronach, Hospital, 2014). New method for calculating evaporation from oil layer takes into account the limiting factor due to diffusion of volatile components in liquid phase, which in its turn allows to explain results of the first experiments in 1975–1977, which study behaviour of oil spills at sea (Cormack, 1989). In these experiments, spills of Ekofisk and Beatrix oil, which were almost similar in distillation data, but had different pour point temperatures. Evaporation of Beatrix oil was much less than in the Ekofisk spill. This is explained by high paraffin content (pour point 20 °C) of Beatrix oil, causing it quickly form encapsulated lumps on the sea surface at water temperatures of 6–10 °C.

6.6. Estimation of probable oil spill detection area

As an example of an estimate of the area of probable oil spill detection, the results of calculations performed for the Barents Sea (Solbakov et al., 2016).

The spill detection probability fields for the preliminary forecast time of 24 and 48 hours with a spill duration of 1 hour (Figure 12a, Figure 12b) and 48 hours (Figure 12c, Figure 12d) are shown in Figure 12.

The fields of probability distribution for instantaneous spill could be seen to have the expressed symmetry (Figure 12a, Figure 12b), with the fields of the probability for the continuous spill extending in the drift direction (Figure 12c, Figure 12d). Approaching the coast, both spills become deformed to some extent (Figure 12b, Figure 12d) because of the proximity of the coast affecting the current velocities. The area sizes with probability of 95% for the oil detection reached 50 km at the end of the second day from the beginning of the spill (Figure 12b, Figure 12d).

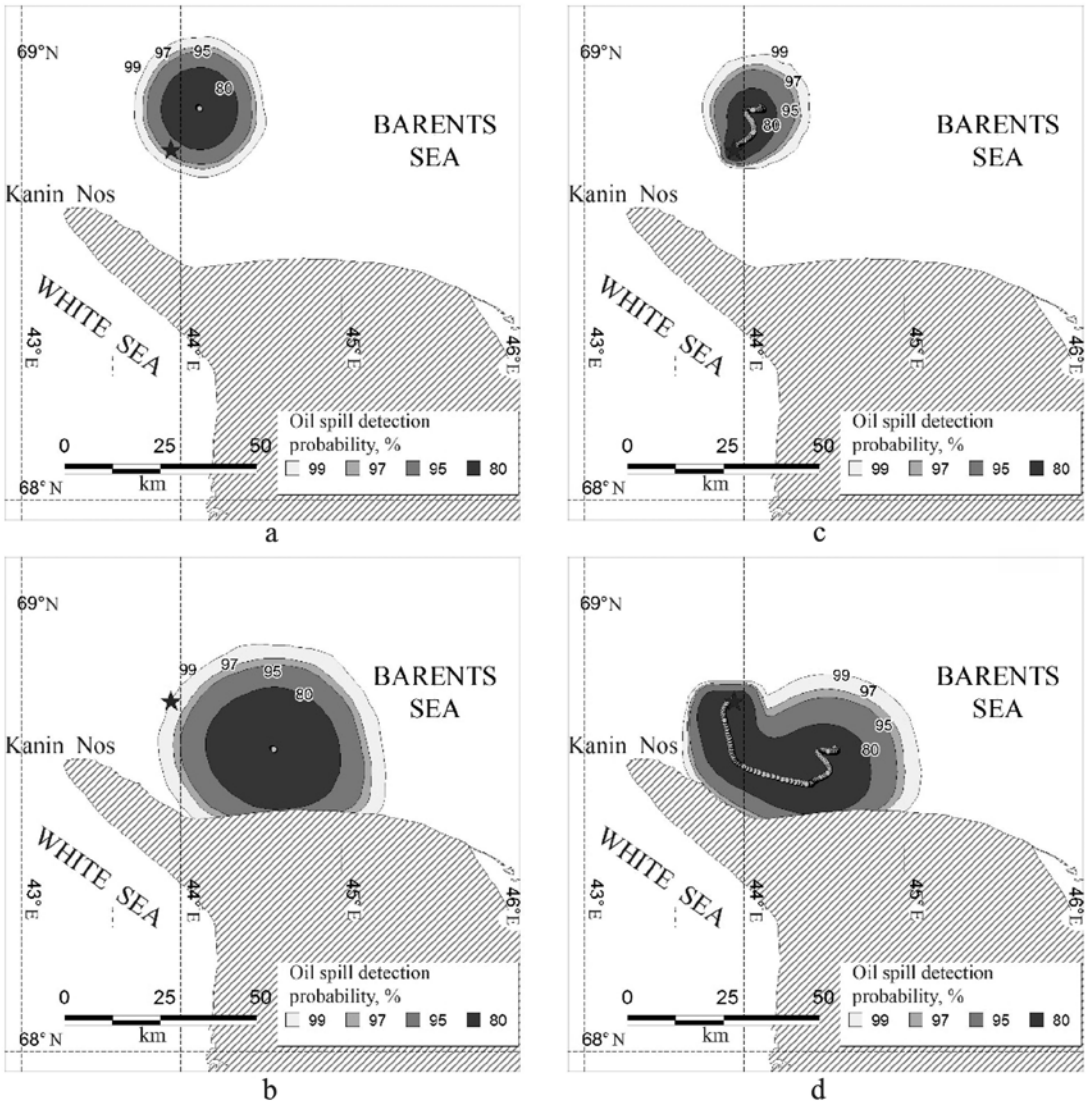


Figure 12 – The fields of the spill detection probability: (**a**, **b**) instantaneous spill; (**c**, **d**) continuous spill; (**a**, **c**) 24 hours after spill start; (**b**, **d**) 48 hours after spill start

7. Conclusion

Mathematical modeling is one of the support tools for oil spill response in the sea and selection of a response strategy depending on the available OSR facilities and meteorological conditions. Models should provide information about the location and condition of the spill, calculate the area and configuration of the oil slick. The SPILLMOD model of oil spill on the sea surface is based on the use of vertically averaged equations of motion of a thin layer of light liquid on the surface of a denser substrate. The SPILLMOD model makes it possible to (i) calculate the configuration of an oil spill on the high seas and in a port area. The model includes (ii) modern parametrization of the processes of oil dispersion by wind waves and (iii) evaporation, taking into account the restrictions on the transport of volatile components of the hydrocarbon mixture to the oil-air interface due to molecular diffusion. The model can be implemented using the Euler-Lagrangian technique developed by the authors to solve the problem of oil spreading over the sea surface in the framework of the shallow water theory, taking into account free and contact boundaries that limit spreading. The emphasis on a more accurate calculation of the oil spill area gives an advantage over many models of oil distribution in the sea, since the oil evaporation rate, the thickness of the oil slick and the natural dispersion rate directly depend on the calculation of slick area. The final viscosity of oil on the sea surface depends on the amount of oil evaporated, which must be taken into account when choosing a method to deal with a spill. It should be emphasized that in order to predict the behavior of marine spills of oil and oil products, it is extremely important to determine the spatially inhomogeneous current velocities in the upper layer of the ocean. The uniqueness of each oil spill that have already occurred and those that will occur in future is determined not only by the volume and type of oil spilled, but also by regional meterological conditions. The experience of using the model in a situation where the distribution of oil products is limited by river banks and booms (the Norilsk diesel oil spill) has shown the advantage of SPILLMOD compared to other models used for information support of OSR operations. The simulation results presented in the article as an illustration demonstrate the possibilities of using the SPILLMOD model as an information support tool for oil spill response operations in various water bodies.

Acknowledgments. Research on the behavior of oil spills at sea, oil spill prevention and emergency response are interdisciplinary issues. Progress in this area is ensured by the joint efforts of oceanographers and ecologists, offshore oil spill response specialists and oil spill response specialists. The authors are grateful to their colleagues from the N. N. Zubov's State Oceanographic Institute, Roshydromet, the Marine Rescue Service of the Russian Federation and the World Wildlife Fund (Russia), whose experience and knowledge allow us to focus on solving urgent problems of ensuring the environmental safety of Russian offshore projects. An additional impetus for the preparation of the article was the participation of the authors in a seminar1 on modeling oil spills at sea at the University of Anchorage, Alaska, in December

[1] https://crrc.unh.edu/AMSM_Arctic_Modeling

2019, traditionally organized by Professor Nancy Kinner (University of New Hampshire, USA) As a result of the discussion of the state of the art in offshore oil spill modeling, the need to revise many “traditional” computational algorithms, some of which were proposed more than half a century ago, was recognized. The authors also express special gratitude to the referees for their correspondence and some controversy, which helped to correct some inaccuracies in the text and improve its structure and clarity.

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SPILLMOD – МОДЕЛЬ ГИДРОДИНАМИЧЕСКОГО ТИПА ДЛЯ ИНФОРМАЦИОННОЙ ПОДДЕРЖКИ РЕАГИРОВАНИЯ НА РАЗЛИВЫ НЕФТИ В МОРЕ

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SPILLMOD представляет собой реализованную в виде программного комплекса математическую модель эволюции морских разливов нефти. Для решения системы уравнений типа мелкой воды в области со свободными и контактными границами произвольной конфигурации был создан новый Эйлерово-Лагранжев вычислительный метод. Отличительной чертой модели является возможность рассчитывать поле толщины нефтяного загрязнения при наличии контактных границ с учетом процессов растекания и выветривания. При расчете испарения высоковязких типов нефти учитывается фактор демпфирования скорости испарения за счет молекулярной диффузии компонент нефти в жидкой фазе. Расчет естественного диспергирования слоя нефти проводится с учетом состояния поверхности моря, экспериментальных данных о дроблении пленки нефти в слое волнового перемешивания и турбулентной диффузии в верхнем слое океана, учетом физико-химических свойств поверхностного загрязнения. Дополнительный модуль в модели разработан для оценки зон возможного обнаружения разлива. Приведенные примеры использования модели в условиях реальной конфигурации портовых акваторий и для реально произошедших аварийных разливов демонстрируют заявленные качества модели как инструмента информационной поддержки работ по ликвидации аварийных разливов нефти на поверхности моря и других водных объектов.

Ключевые слова: SPILLMOD, вычислительная гидродинамика, модель нефтяного разлива, реагирование на нефтяные разливы, испарение нефти, диспергирование нефти, метод частиц в ячейках, пространственная неопределенность

Благодарности: Исследования поведения разливов нефти в море, предотвращение разливов нефти и реагирование на чрезвычайные ситуации являются междисциплинарными вопросами. Прогресс в этой области обеспечивается совместными усилиями океанографов и экологов, специалистов по ЛРН на шельфе и специалистов по подготовке к ЛРН. Авторы выражают благодарность своим коллегам из Государственного океанографического института им. Н. Н. Зубова, Росгидромета, Морской спасательной службы Российской Федерации и Всемирного фонда дикой природы (Россия), чей опыт и знания позволяют сосредоточить внимание на решении актуальных задач по обеспечению экологической безопасности российских шельфовых проектов. Дополнительным импульсом для подготовки статьи было участие авторов в семинаре[1] по моделированию разливов нефти в море в Университете Анкориджа,

[1] https://crrc.unh.edu/AMSM_Arctic_Modeling

штат Аляска, в декабре 2019 года, традиционно организуемом профессором Нэнси Киннер (Университет Нью-Гемпшира, США). В результате обсуждения современного состояния моделирования разливов нефти в море была признана необходимость ревизии многих «традиционных» расчетных алгоритмов, некоторые из которых были предложены более полувека назад. Авторы также выражают особую благодарность рецензентам за их переписку и некоторую полемику, которые помогли исправить неточности в тексте и улучшить его структуру и ясность.

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