

Complex of parallel programs for modeling oil products transport in coastal systems

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Abstract. This paper covers the model of oil products transport in view the evaporation of light, neutral and no-evaporating pseudofractions of oil slick, dissolution of oil slick and biodegradation. Approximation of diffusion-convection problem was performed on the basis of schemes of high-order of accuracy. Experimental software was designed for mathematical modelling of possible scenarios of development of ecosystems of shallow waters for oil spills on the example of the Azov-Black Sea basin, based on multiprocessor computer systems. Decomposition methods of grid domains have been used for computationally laborious diffusion-convection tasks in parallel implementation. Maximum acceleration was equal to 228.36 times on 512 computational nodes.

1 Introduction

The influence of oil pollution on the water is manifested in the next: the deterioration of the physical properties of the water (turbidity, change in color, taste, smell); the dissolution of toxic substances in water; the formation of oil surface film and sludge at the bottom of the reservoir, which decreased the oxygen in the water.

Characteristic smell and taste appear at a concentration of oil and oil products in the water 0.5 mg/dm³, and naphthenic acids – 0.01 mg/dm³. Significant changes in chemical parameters of water occurs when the content of oil and oil products more than 100-500 mg/dm³. The oil film on the surface of water basin worse the gas exchange with the atmosphere and slow the rate of aeration and removal of carbon dioxide, formed by oxidation of the oil. When the oil film is equaled to 4.1 mm and the oil concentration in water is equaled to 17 mg/dm³, the amount of dissolved oxygen is reduced by 40% per 20-25 days.

Analysis of the numerical solution of the model problem of transport materials showed that time costs are reduced for the explicit scheme at the increasing of grid dimension. Modification of the explicit scheme is the introduction of the second-order derivative of the difference with the factor - regularizater - can significantly ease restrictions on the permissible value of the time step [1]. In addition, explicit regularized schemes showed real-time cost advantages (10-15 times and more), compared to the previously used conventional implicit and no-regularized explicit schemes [2].

A variant of the finite volumes method in the case of account of filling control domains was proposed in [3]. Algorithm of calculation in view the partial «fill» cells

without flows associated with a stepwise boundary of representation on a rectangular grid. The proposed method was applied to solve three-dimensional hydrodynamic problems [4]. Flow fields, which are used to calculate the transport of oil products, have been calculated on the basis of this model.

Schemes of high-order of accuracy are used in solving the problem of oil products transport. It should be noted that in solution the problem of diffusion model was able to increase the accuracy in 66.7 times, and for convection-diffusion problems – in 48.7 times [5].

2 Mathematical model of hydrodynamics

The input data of the problem of transport of oil products are fields of the speed vector of the water flow, which required for mathematical modelling of water environment. The initial equations of hydrodynamics of shallow waters are [4]:

– motion equation (the Navier – Stokes equation)

$$\begin{aligned}
 u'_t + uu'_x + vu'_y + wu'_z &= -p'_x / \rho + (\mu u'_x)'_x + \\
 &+ (\mu u'_y)'_y + (v u'_z)'_z + 2\Omega(v \sin \theta - w \cos \theta), \\
 v'_t + uv'_x + vv'_y + wv'_z &= -p'_y / \rho + (\mu v'_x)'_x + \\
 &+ (\mu v'_y)'_y + (v v'_z)'_z - 2\Omega u \sin \theta, \\
 w'_t + uw'_x + vw'_y + ww'_z &= -p'_z / \rho + (\mu w'_x)'_x + \\
 &+ (\mu w'_y)'_y + (v w'_z)'_z + 2\Omega u \cos \theta + g(\rho_0 / \rho - 1);
 \end{aligned}
 \tag{1}$$

– continuity equation in the case of variable density can be written as follows:

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$$\rho'_t + (\rho u)'_x + (\rho v)'_y + (\rho w)'_z = 0, \quad (2)$$

where $\bar{u} = \{u, v, w\}$ are components of the speed vector; p is the overpressure on the hydrostatic pressure of the unperturbed liquid, ρ is a density; Ω is the angular velocity of the earth's rotation, θ is the angle between the vertical and angular velocity; μ, ν are horizontal and vertical components of the turbulent exchange coefficient.

The system of equations (1)-(2) is considered in the following boundary conditions:

– at the entrance (the mouth of the Don and Kuban rivers):

$$u(x, y, z, t) = u(t), v(x, y, z, t) = v(t),$$

$$p'_n(x, y, z, t) = 0, \bar{u}'_n(x, y, z, t) = 0,$$

– the lateral boundary (the bank and the bottom):

$$\rho_v \mu(u')_n(x, y, z, t) = -\tau_x(t), \rho_v \mu(v')_n(x, y, z, t) = -\tau_y(t),$$

$$\bar{u}'_n(x, y, z, t) = 0, p'_n(x, y, z, t) = 0,$$

– the upper boundary:

$$\rho \mu(u')_n(x, y, z, t) = -\tau_x(t), \rho \mu(v')_n(x, y, z, t) = -\tau_y(t),$$

$$w(x, y, t) = -\omega - p'_t / \rho g, p'_n(x, y, t) = 0, \quad (3)$$

– output (Kerch Strait):

$$p'_n(x, y, z, t) = 0, \bar{u}'_n(x, y, z, t) = 0,$$

where ω is the rate of evaporation of the liquid, τ_x, τ_y are tangential stress components (Van Dorn law), ρ_v is the density suspension.

The components of the tangential stress for the free surface:

$$\tau_x = \rho_a C_p (|\bar{w}|) w_x |\bar{w}|, \tau_y = \rho_a C_p (|\bar{w}|) w_y |\bar{w}|,$$

where \bar{w} is the wind speed vector relatively of the water; ρ_a is the density of atmosphere; $C_p(x)$ is the dimensionless coefficient.

Components of the tangential stress for the bottom based on this notation can be written as follows:

$$\tau_x = \rho C_p (|\bar{u}|) u |\bar{u}|, \tau_y = \rho C_p (|\bar{u}|) v |\bar{u}|.$$

On the basis of the measured speed fluctuations the discussed below approximation is required to the developing the coefficient of vertical turbulent exchange, heterogeneous by the depth [6]:

$$\nu = C_s^2 \Delta^2 \frac{1}{2} \sqrt{\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2}, \quad (4)$$

where Δ is the characteristic scale of the grid; C_s is the dimensionless empirical constant, whose value is generally determined based on the calculation of the decay of homogeneous isotropic turbulence.

The grid method is used to solve (1)-(3) problem [7]. The approximation of equations by the time variable is determined on the basis of splitting schemes by physical processes [8] in the form of an amendment method of pressure.

3 Mathematical model of oil products transport

The system of equations was used to describe the process of oil products transport, subject to the evaporation of light, neutral and no-evaporating pseudofractions of oil spot, dissolution of oil spot and biodegradation [9]:

$$\begin{aligned} (c_i)'_t + u(c_i)'_x + v(c_i)'_y = & \left(\mu^*(c_i)'_x \right)'_x + \left(\mu^*(c_i)'_y \right)'_y - \\ & - \left(\frac{K_E P_i}{RT} + K_D S_i \right) X_i M_i^m - \frac{1}{q} \frac{\mu_m c_i}{c_i + K_s} M, \quad (c_i)'_n \Big|_{(x,y) \in \Gamma} = 0, \\ M'_t + uM'_x + vM'_y = & \left(\mu M'_x \right)'_x + \left(\mu M'_y \right)'_y + \\ & + \frac{\mu_m c_i}{c_i + K_s} M - \lambda M, \quad M'_n \Big|_{(x,y) \in \Gamma} = 0, \end{aligned} \quad (5)$$

$$\begin{aligned} (\varphi_i)'_t + u(\varphi_i)'_x + v(\varphi_i)'_y + w(\varphi_i)'_z = & \left(\mu(\varphi_i)'_x \right)'_x + \\ & + \left(\mu(\varphi_i)'_y \right)'_y + \left(\mu(\varphi_i)'_z \right)'_z, \\ (\varphi_i)'_n \Big|_{(x,y,z) \in \Gamma \setminus (z=0)} = 0, \quad (\varphi_i)'_z \Big|_{z=0} = & K_D S_i X_i M_i^m, \end{aligned}$$

where c_i is the concentration of the i -th oil fractions; ρ_w, ρ are the water and oil density respectively; $\mu^* = \mu + (\rho - \rho_w)gh^3 / \mu$ is the function describing the process of pollutant decomposition; μ is the diffusion coefficient; g is the acceleration; $h = \sum_1^l c_i$ is the width

of oil slick; $i = \overline{1, k}$; $M_i^{(m)}$ is the molar mass of i -th component, [kg/mol]; $K_E = 2,5 \cdot 10^{-3} U^{0.78}$ is the mass transport coefficient for hydrocarbon, [m/s]; U is the wind speed, relatively to the water, [m/s]; X_i is the mole fraction of the component with the number i , equaled to $v_i / \sum v_i$; v_i is an amount of substance i -th components, [mol]; P_i is the vapor pressure of the i -th component, [Pa]; $R = 8,314$ J/mol; K is the universal gas constant; T is an ambient temperature over the surface of the spot, $K, K_D = kK_{D0}$ is the coefficient of mass transport of dissolution; K_{D0} is the initial value of the mass transport coefficient of dissolution; k is the coefficient, depending on the sea state; S_i is the dissolubility of i -th component in water, [kg/m³]; A is the area of the oil spill, [m²]; M is the concentration of microorganisms; μ_m is the maximum speed of the growth of microorganisms; K_s is the coefficient of saturation; λ is the rate of cell death; q is the proportion coefficient between the amount of bacteria and the absorbed substrate.

Changes of the oil initial solubility are described by the equation:

$$S = S_0 e^{-0,1t},$$

where S_0 is an initial oil solubility; t is the time, [day].

The coefficient of horizontal turbulent diffusion depends on the hydrodynamic and climatic conditions in

which the process takes place. The coefficient of horizontal turbulent diffusion will be subject to the law of the «four thirds» by Richardson for difficult hydrodynamic and climatic conditions of the Azov-Black Sea area [10]:

$$\mu \approx \varepsilon^{1/3} L^{4/3}, \quad (6)$$

where L is the characteristic size of diffusing spots; ε is the rate of dissipation of turbulent energy. It is equaled to the order of $1 \cdot 10^{-1} \text{ cm}^2/\text{s}^3$ at the surface and decreased at the average with depth to values of the order of $10^{-3} \cdot 10^{-4} \text{ cm}^2/\text{s}^3$.

Boundary and initial conditions for the one-shot volley oil spill were determined for solving the above systems of equations:

$$c|_{t=0, (x,y) \in S_0} = c_0, \quad c|_{t=0, (x,y) \notin S_0} = 0,$$

where S_0 is an area, covered by the spot; c_0 is the oil concentration in the considered area.

4 Approximation problem of oil products transport

A two-dimensional convection-diffusion problem is considered for implementation the oil products transport model in the form:

$$c'_t + uc'_x + vc'_y = (\mu c'_x)'_x + (\mu c'_y)'_y + f \quad (7)$$

with the boundary conditions: $c'_n(x, y, t) = \alpha_n c + \beta_n$,

where u, v are the velocity components, μ is the coefficient of turbulent exchange, f is a function, describing the intensity and distribution of sources.

We introduced a uniform rectangular grid:

$$w_h = \{t^n = n\tau, x_i = ih_x, y_j = jh_y; n = \overline{0..N_t}, i = \overline{0..N_x},$$

$$j = \overline{0..N_y}; N_t\tau = T, N_x h_x = l_x, N_y h_y = l_y\}$$

where τ is the time step; h_x, h_y are spatial steps; N_x, N_y are the spatial boundary; N_t is the upper time boundary.

B.N. Chetverushkin have been proposed the idea of use of regularized schemes to increase the safety factor of explicit schemes [1]. A modified equation is used to construct the explicit regularized scheme for the equation (7):

$$c'_t + \frac{\tau^*}{2} c''_t + uc'_x + vc'_y = (\mu c'_x)'_x + (\mu c'_y)'_y + f, \quad (8)$$

where $\tau^* \approx h/c^*$ is the regularization parameter; h is the grid step; c^* is the speed of sound in water. Adding the regularize-term (the second derivative of the time difference with the factor τ^*), the restriction on the time step variable is $\tau \leq O(h^{3/2})$ is sufficient for the stability of the explicit scheme. This condition is less rigid in comparison with the condition for explicit no-regularized scheme is $\tau \leq O(h^2)$.

We conducted the discretization of convective and diffusive transport operators of the second order of approximation error in the case of partially filled cells as follows:

$$\begin{aligned} (q_0)_{i,j} uc'_x &\approx (q_1)_{i,j} u_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{2h_x} + (q_2)_{i,j} u_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{2h_x}, \\ (q_0)_{i,j} (\mu c'_x)'_x &\approx (q_1)_{i,j} \mu_{i+1/2,j} \frac{c_{i+1,j} - c_{i,j}}{h_x^2} - \\ &- (q_2)_{i,j} \mu_{i-1/2,j} \frac{c_{i,j} - c_{i-1,j}}{h_x^2} - \left| (q_1)_{i,j} - (q_2)_{i,j} \right| \mu_{i,j} \frac{\alpha_x c_{i,j} + \beta_x}{h_x}, \end{aligned} \quad (9)$$

where q_i is the coefficient, describing the occupancy of computing domains [11].

The approximation of convective transport operator uc' by the difference scheme, which has the fourth order of accuracy, is given by [12]:

$$\begin{aligned} (q_0)_i L(c) &= -(q_1)_i \frac{u_{i+1/2}}{12h} \left(\frac{q_1}{q_0} \right)_{i+1} c_{i+2} - \left(-(q_1)_i \frac{u_{i+1/2}}{12h} \left(2 + \frac{(q_1)_i}{(q_0)_i} \right) + \right. \\ &+ (q_2)_i \frac{u_{i-1/2}}{12h} \left(\frac{q_1}{q_0} \right)_i + (q_1)_i \left(-\frac{u_{i+1/2}}{2h} + k_i^{(1)} + k_i^{(2)} \right) \left. \right) c_{i+1} + \\ &+ \left(-(q_1)_i \frac{u_{i+1/2}}{12h} \left(2 + \frac{(q_2)_{i+1}}{(q_0)_{i+1}} \right) + (q_2)_i \frac{u_{i-1/2}}{12h} \left(2 + \frac{(q_1)_{i-1}}{(q_0)_{i-1}} \right) + \right. \\ &+ (q_2)_i \frac{u_{i-1/2}}{2h} - (q_1)_i \frac{u_{i+1/2}}{2h} - \left. \left((q_2)_i - (q_1)_i \right) k_i^{(1)} + \right. \\ &+ \left. \left((q_2)_i + (q_1)_i \right) k_i^{(2)} \right) c_i - \left(-(q_1)_i \frac{u_{i+1/2}}{12h} \left(\frac{q_2}{q_0} \right)_i + \right. \\ &+ (q_2)_i \frac{u_{i-1/2}}{12h} \left(2 + \frac{(q_2)_i}{(q_0)_i} \right) + (q_2)_i \left(\frac{u_{i-1/2}}{2h} + k_i^{(2)} - k_i^{(1)} \right) \left. \right) c_{i-1} - \\ &- \left(-(q_2)_i \frac{u_{i-1/2}}{12h} \left(\frac{q_2}{q_0} \right)_{i-1} \right) c_{i-2}, \end{aligned} \quad (10)$$

where $k_i^{(1)} = \left(\frac{(q_1)_i}{(q_0)_i} (u_{i+1} - u_i) - \frac{(q_2)_i}{(q_0)_i} (u_i - u_{i-1}) \right) / (8h)$,

$$k_i^{(2)} = \frac{(q_1)_i}{(q_0)_i} \frac{u_{i+1} - u_i}{8h} + \frac{(q_2)_i}{(q_0)_i} \frac{u_i - u_{i-1}}{8h}.$$

The approximation of diffusive transport operator by the difference $(\mu c)'$ schemes, which has the fourth order of accuracy, is given by:

$$\begin{aligned} (q_0)_i (L(c)) &\approx -(q_1)_i \frac{\mu_{i+1}}{12h^2} \left(\frac{q_1}{q_0} \right)_{i+1} c_{i+2} + \left((q_1)_i \frac{\mu_{i+1/2}}{h^2} c_{i+1} + \right. \\ &+ (q_1)_i \frac{\mu_{i+1}}{12h^2} \left(\frac{(q_1)_i}{(q_0)_i} + 2 \right) + (q_2)_i \frac{\mu_{i-1}}{12h^2} \left(\frac{q_1}{q_0} \right)_i - \left. \left((q_1)_i \frac{\mu_{i+1/2}}{h^2} + \right. \right. \\ &+ (q_2)_i \frac{\mu_{i-1/2}}{h^2} + (q_1)_i \frac{\mu_{i+1}}{12h^2} \left(\frac{(q_2)_{i+1}}{(q_0)_{i+1}} + 2 \right) + \left. \right) c_{i+1} \\ &+ (q_2)_i \frac{\mu_{i-1}}{12h^2} \left(\frac{(q_1)_{i-1}}{(q_0)_{i-1}} + 2 \right) + (q_2)_i \left(\frac{\mu''_i - \mu''_{i-1}}{12} - k_i \right) - \\ &- (q_1)_i \left(\frac{\mu''_{i+1} - \mu''_i}{12} + k_i \right) \left. \right) c_i + \left((q_2)_i \frac{\mu_{i-1/2}}{h^2} c_{i-1} + \right. \end{aligned} \quad (11)$$

$$\begin{aligned}
 & + (q_1)_i \frac{\mu_{i+1}}{12h^2} \left(\frac{q_2}{q_0} \right)_i + (q_2)_i \frac{\mu_{i-1}}{12h^2} \left(\frac{q_2}{q_0} \right)_i + 2 \left(\frac{q_2}{q_0} \right)_i + \\
 & + (q_2)_i \left(\frac{\mu_i'' - \mu_{i-1}'' - k_i}{12} \right) c_{i-1} - (q_2)_i \frac{\mu_{i-1}}{12h^2} \left(\frac{q_2}{q_0} \right)_{i-1} c_{i-2},
 \end{aligned}$$

where $\mu_i'' = \left(\frac{(q_1)_i}{(q_0)_i} c_{i+1} - 2c_i + \frac{(q_2)_i}{(q_0)_i} c_{i-1} \right) / h^2$,

$$k_i = \frac{(q_1)_i}{(q_0)_i} \frac{\mu_{i+1} - \mu_i}{4h^2} - \frac{(q_2)_i}{(q_0)_i} \frac{\mu_i - \mu_{i-1}}{4h^2}.$$

5 Parallel implementation

Decomposition methods of grid domains are used for computationally laborious convection-diffusion tasks in parallel implementation, which are considered parameters of architecture and multiprocessor systems. The maximum performance of multiprocessor computer system (MCS) is equaled to 18.8 teraflops. 128 single-type of 16-core Blade-servers HP ProLiant BL685c were used as computational nodes, each of which has the four quad-core AMD Opteron processor 8356 of 2.3GHz and memory, equaled to 32 GB.

The time costs, which are required for the one time layer on various grids, acceleration and effectiveness values for different numbers of MCS cores are given in the Table 1.

Table 1. Acceleration and Efficiency of the Number of Processors

		100x100	500x500	1000x1000	5000x5000
1	Time	0.000271	0.00846	0.03608	1.633
	Speed-up	1	1	1	1
	Efficiency	1	1	1	1
4	Time	0.000052	0.00341	0.00978	0.533
	Speed-up	5.212	2.481	3.689	3.064
	Efficiency	1.303	0.62	0.922	0.766
16	Time	0.000025	0.00054	0.00628	0.142
	Speed-up	10.84	15.667	5.745	11.5
	Efficiency	0.677	0.979	0.359	0.719
64	Time	0.000125	0.00016	0.00110	0.044
	Speed-up	2.168	52.875	32.8	37.114
	Efficiency	0.034	0.826	0.513	0.58
128	Time	-	0.00040	0.00048	0.017
	Speed-up	-	21.15	75.167	96.059
	Efficiency	-	0.165	0.587	0.75
512	Time	-	-	0.00129	0.0072
	Speed-up	-	-	27.883	228.36
	Efficiency	-	-	0.054	0.446

6 Software description

The experimental software was developed on the basis of MCS, which is intended for mathematical modelling of possible scenarios of ecosystems of shallow waters on the example of the Azov-Black Sea basin. The software «Azov3d» was designed for construction of operational flow forecasts turbulence of the water environment - the speed field of water environment on grids with high resolution. This complex is used to calculate the three-dimensional speed vector of water environment of the Azov Sea. The complex takes into account such physical parameters as the Coriolis force, the turbulent exchange, the complex geometry of the bottom surface and coastline, evaporation, river flows, wind-surges, wind currents and friction bottom, and provides the following functions: the calculation of the speed field without pressure; the calculation of hydrostatic pressure (used as an initial approximation for the hydrodynamic pressure); the calculation of hydrodynamic pressure; the calculation of three-dimensional velocity field of water flow.

The output parameters of this software are the next: steps by spatial coordinates, error of calculation of grid equations, the grid dimension, the time interval, the evaporation intensity, the initial distribution of the components of the speed vector of water environment and pressure.

We can add new calculation functions to the developed complex. Particularly, program modules were designed and integrated to this complex for calculation the oil products transport in view the evaporation of light, neutral and no-evaporating pseudofractions of oil spot, dissolution oil spot and biodegradation. The water flow fields, calculated on the basis of the mathematical model (1)-(4), are included to the input data for the oil products model (5).

Results of natural experiments for researching the destruction of crude oil in seawater are given in [10]. The experimental results are shown that only 3-15% of the original amount of crude oil subject to oxidation, biodegradation, photochemical reactions, while from 10 to 40% of substance is evaporated. The peak of its solubility is occurred on the 10th day of exposure (Fig. 1).

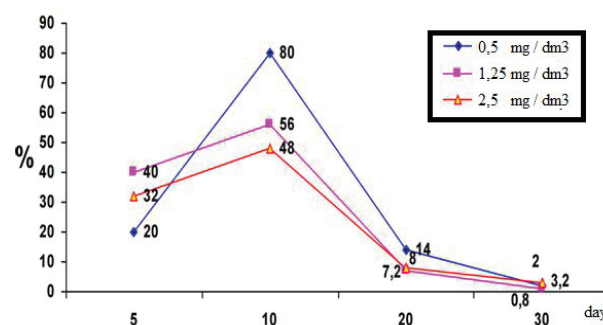


Fig. 1. Dynamics of crude oil destruction

According to [11], upon receiving a message about the oil and oil products spill, the containment time should not exceed 4 hours at spill in the area, and 6 hours – at spill on the ground since the discovery of the oil and oil products spill or from the providing the information about the spill. We considered the case where measures are not taken to localize oil spills. The results of natural experiments are shown that the calculated time interval must be equal to 20-30 days.

The wind speed in the range of 3-8 m/s is an ideal for the localization of oil pollution: in this case, the slicks appear as dark spots on the bright (rough) surface of the sea (see Fig. 2).

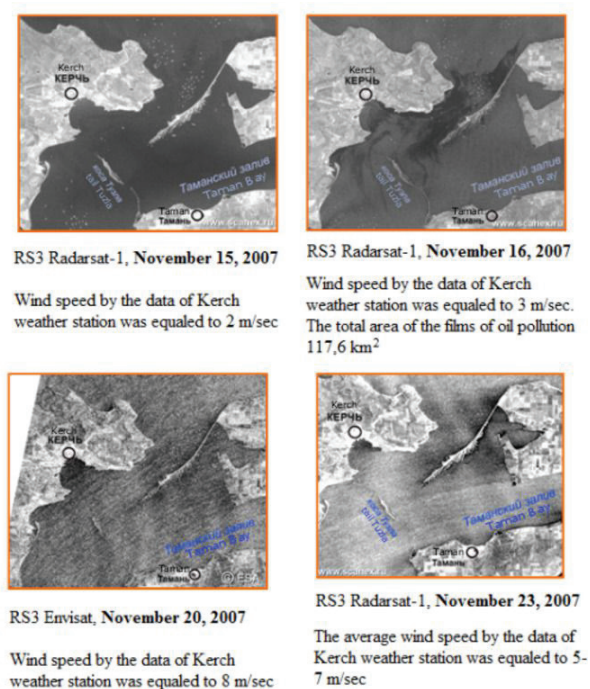


Fig. 2. The radar image of area during the catastrophic oil spill

The data about the wind speed and direction during the extreme storm, occurred in November 2007, is given in Fig. 3. The highest wind speed was fixed in November 11th, 2007 in Kerch Strait and amounted to 24 m/s according to the Gismeteo [12].

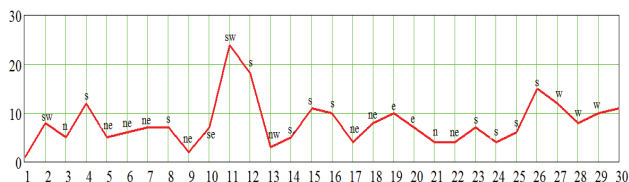


Fig. 3. The wind speed in the Kerch Strait in November, 2007

Results of numerical experiments of modelling the light oil transport in the Kerch Strait on November 16th, 2007 are given in Fig. 4. The calculation was performed on the basis of the developed software. The results was used to test the efficiency of this complex.

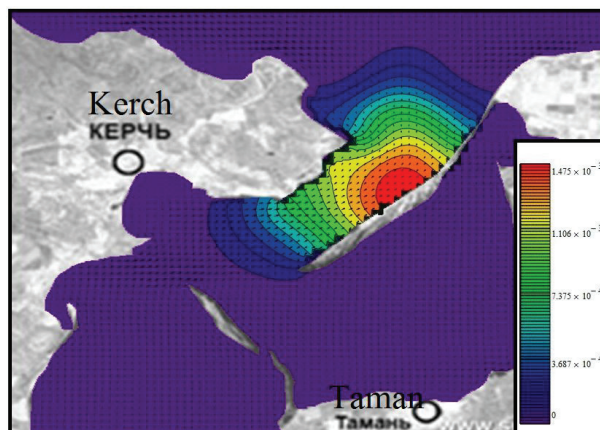


Fig. 4. The concentration field of light oil products

Further, we schedule to develop a model for calculation the transport of bottom materials [13, 14], as well as for calculation the transport of dissolved substances and oil vapor. The three-dimensional mathematical model of surface aerodynamics is required to develop a model of transportation of oil vapor. In the modelling of oil spills it is also important to consider the influence of the dissolved oil to the nature and course of hydrobiological processes in the water [15, 16]. Comparing the calculation results of the concentration of light oil products, which are given in Fig. 4, with the results of radar images, where a catastrophic oil spill (Fig. 2) was occurred, we can see their qualitative conformance. The forecast time was equaled to 4 days after the spill.

7 Conclusion

The three different models for describing the oil products transport in view of evaporation of light, neutral and no-evaporating pseudofractions of oil spot, dissolution of oil spot and biodegradation were developed in [9]. The developed model was presented in this paper that describes all of the above processes. The usage of regularized schemes [1] for increasing the safety factor of explicit schemes has been proposed by B.N. Chetverushkin. The approximation of convection-diffusion problem was performed on the basis of schemes of high-order of accuracy. The experimental software was developed on the basis of multiprocessor computer system for mathematical modeling of possible scenarios of ecosystems of shallow waters on the example of Azov-Black Sea basin in oil spills. The decomposition methods of grid domains are used for computationally laborious convection-diffusion problems in parallel implementation, which are considered parameters of architecture and multiprocessor systems. The maximum acceleration was equaled to 228.36 times on 512 computational nodes. The advantages of the developed software is also the use of hydrodynamic models, included the motion equation for the three coordinate directions.

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