Model for oil spill simulation in the Black Sea

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1. Introduction

The growing concern over the impact of the accidental spill in the new oil transport routes from the Eastern to Western Black Sea is a motivating factor for the development and implementation of the decision support tools to evaluate the oil spill response strategies, to provide the environmental impact assessment, and to use in contingency planning and training. Over the past 30 years a number of models that describe the fate and transport of oil spilled in water were developed (see state-of-art reviews [1-2]). The transport and fate of spilled oil are governed by set of interrelated processes: the advection by wind and currents, surface slick spreading due to both turbulent diffusion and to the gravitational and surface tension forces, mass transfer and changes in physicochemical properties due to the weathering processes, interaction of oil with suspended and bottom sediments and shoreline. The results of laboratory and field experiments have advanced understanding of oil transport and fate processes and formed the basis for the model development. However, the model parameterizations are strongly dependent on the marine and atmospheric environment parameters. Irrespective of complexity of oil spill model the availability of marine and atmospheric environment data close to spill site places a serious constraint on the accuracy of spill model [3]. Experience of many oil spill response actions worldwide, including the recent "Prestige" accident, demonstrates importance of forecasts of weather and sea state to predict movement and fate of oil spill. Now, increasing computational resources allow coupling of oil spill models to models of weather, circulation and wave forecast.

This paper presents recent development of the modelling system for simulation of the accidental oil spill. The system includes 3D oil spill and fate model OILTOX, circulation and sediment transport model THREETOX and wave forecast model WAVEWATCH III coupled with the weather forecast model MM5. This paper is organized as follows. The oil spill model is briefly described in Section 2, implementation of weather, circulation and wave forecasting model for the Black Sea is described in Section 3. Section 4 describes the modeling system design and options. Section 5 presents the results of two applications of model. Future development of model and conclusions are given in Section 6.

2. The oil spill model

OILTOX is a Lagrangian model for simulating oil transport and fate. It is being developed by IMMSP and UCEWP to support response on oil spill in the Black and Azov seas and large river reservoirs in the Ukraine. The model describes the main transport and weathering

processes in five interactive "phases": oil-on-surface, oil-in-water, oil-on-suspended sediments, oil-on-bottom and oil-at-shoreline.

Oil-on-surface phase.

The model of oil on surface describes the spreading due to gravity and surface tension force, advection by wind and surface currents, evaporation, oil-shore interaction, entrainment of oil in the water by breaking waves and resurfacing entrained droplets. The oil spill models mainly use classical self-similar solutions for instantaneous release in the calm sea [4], which do not describe realistic variability of slick thickness, observed non-symmetrical spreading of oil slick caused by wind and currents and dependence of spreading rate on release conditions [2]. Here we use model [5] that is able reproduce these features. The governing equations for oil slick spreading velocity \vec{u}_a and thickness h are

$$\frac{\partial \vec{u}_o}{\partial t} + \vec{u}_o \nabla_H \vec{u}_o = \vec{F} \left(h, \chi_1, \overrightarrow{W} \right) + \frac{C_w \rho_w}{\rho_o h} \sqrt{\nu_w \left| \Delta \vec{u} \right| / L} \Delta \vec{u}, \tag{1}$$

$$\frac{\partial h}{\partial t} + \vec{u}_o \nabla_H h = Q^{(h)}. \tag{2}$$

Here

$$\vec{F}\left(h,\chi_{1},\vec{W}\right) = \frac{C_{a}\left|\vec{W}\right|\vec{W}}{\rho_{0}h} - \nabla_{H}h\left(g' + \frac{C_{\sigma}\chi_{1}}{\rho_{w}h}\right),\tag{3}$$

 $\Delta \vec{u} = \vec{u}_o - \vec{u}_w^{(s)}$, $\vec{u}_w^{(s)}$ is the water velocity at surface, ρ_w , v_w are water density and viscosity, respectively; ρ_o is oil density; $g' = g(\rho_w - \rho_o)/\rho_w$; \overrightarrow{W} is wind velocity at 10 m height, χ_1 is the surface tension parameter, $\chi_1 = \min\left(\chi, \sigma_0/h_{\max}\right)$; σ_0 is surface tension coefficient, h_{\max} is the maximal thickness in the slick, in the thin slick $\chi = \text{const}$, $C_a = 1.75 \cdot 10^{-6}$, $C_w = 0.5$, $C_\sigma = 0.3$ are constants [5], L is the linear horizontal scale in the oil-water friction law, ∇_H is horizontal operator. The surface oil slick mass is changed due to flux in water and atmosphere

$$Q^{(h)} = -Q^{(dis)} + Q^{(res)} - Q^{(eva)}, (4)$$

where $Q^{(dis)}$ is mass flux—caused by breakup the surface slick by breaking waves into small droplets and entrainment of these droplets into water column by turbulence, $Q^{(res)}$ is flux of oil by resurfacing of dispersed droplets, $Q^{(eva)}$ is evaporation rate. The beaching and refloating from shoreline can also change oil mass in the slick. The right side of equation (1) represents effects of wind drift, advection by currents, gravitational spreading and surface tension. The self-similar solutions (1)-(2) for viscous-gravitational and surface tension stages [3] were obtained as particular cases in [5].

The pseudo-component method for calculation of evaporation is considered as most reliable [2]. However, the computational intensity and high data requirements justifies simplistic empirical approaches. Following [6] we assume that fraction of oil evaporated depends only on temperature, time and oil properties. Experiments [6] show that oils with greater than 7

components evaporating in one time can be modelled with logarithmic equation and those with 3 to 7 components, with square root equation. The volume fraction evaporated F_e is

$$F_e = (C_1 + C_2 T) \ln(t), \text{ or } F_e = (C_1 + C_2 T) \sqrt{t},$$
 (5)

where T – temperature in ${}^{o}C$; t is time in minutes after release, C_1 , C_2 are dependent on oil properties constants. Then $Q^{(eva)}$ can be approximated as

$$Q^{(eva)} = \frac{h(C_1 + C_2 T)}{1 - F} \exp\left(-\frac{F}{C_1 + C_2 T}\right) \text{ or } Q^{(eva)} = \frac{h(C_1 + C_2 T)^2}{2F(1 - F)}.$$
 (6)

To simulate process of emulsification we used the model [7]. The change in viscosity and density caused by evaporation and emulsification was calculated according [8].

In the Lagrangian approach a surface slick is modelled as a collection of N_p Gaussian "spillets", which have spatially distributed mass [9]. The changes in mass of at the cost of continuous release, evaporation and change of phase are simulated by born or death of spillets. Distribution of the slick thickness in the spillet is approximated by Gaussian as

$$h_i(x, y) = \frac{m_i}{2\pi\rho_o w_x w_y} \exp\left(-\frac{(x - x_i)^2}{2\lambda_x^2} - \frac{(y - y_i)^2}{2\lambda_y^2}\right),\tag{7}$$

where $\vec{x} = (x, y)$ are Cartesian coordinates, λ_x, λ_y are horizontal scales of spillet. The thickness of slick is sum of spillets

$$h(x,y) = \sum_{i=1}^{N_p} h_i(x,y).$$
 (8)

In Lagrangian coordinates, the position of centre mass of spillet at time $t^{n+1} = t^n + \Delta t$ is given by

$$\vec{x}^{n+1} = \vec{x}^n + \Delta t \vec{u}_o^n \,, \tag{9}$$

where \vec{u}_o^n is spillet velocity. It is determined from (1) as

$$\vec{u}_{o}^{n} = \vec{u}_{w}^{(s)n} + \left(\frac{h\rho_{o}\sqrt{L}}{C_{w}\rho_{w}\sqrt{v_{w}}}\right)^{2/3} \vec{F}^{n} (h,\chi_{1},W) / \left|\vec{F}^{n} (h,\chi_{1},W)\right|^{1/3}, \tag{10}$$

with omitted inertial terms that are not important in spreading process, except very early stage. Following [5] the gravitational forcing in (3) can be efficiently calculated using relations

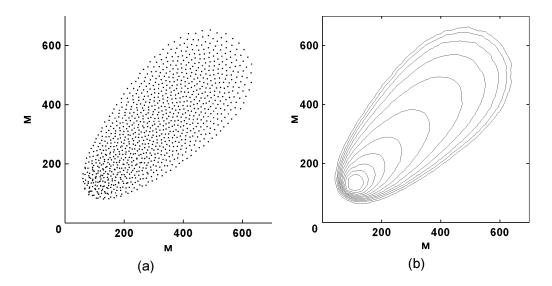


Figure 1. Spreading of oil slick for continuous spill: Scatterplot for spillets (a) and corresponding contour plot (b) at t = 1300 s.

$$\frac{\partial h}{\partial x} = -\sum_{i=1}^{N_p} \frac{(x - x_i)}{\lambda_x^2} h_i(x, y), \quad \frac{\partial h}{\partial y} = -\sum_{i=1}^{N_p} \frac{(y - y_i)}{\lambda_y^2} h_i(x, y). \tag{11}$$

The described approach allows take into account interactions of spillets in ensemble. Similar methods were developed in plasma physics for description of collisionless systems by "particle-particle" methods [10]. For practical calculations the relation $\lambda_x = \lambda_y = \sqrt{S/N_p}$ was used, where S is the slick area. To take into account interactions of all particles in general case one have to make the number of calculation of the $\left(N_p\right)^2$ order. To save calculation time we use effective radius of interaction D = 3w, the distance where interaction forces can be neglected. The problem of particle sorting by the coordinates to calculate the distance only for a some subset $N_{\scriptscriptstyle n}$ of general number of particles $N_{\scriptscriptstyle p}$ is appeared. Following [10] we used chain grid for this purpose. It is mesh with dimensions $M_x \times M_y$, which covers the calculation area with the cell size equal D. The non-zero contribution in the force acting the particle will have only those particles, which located in the same grid cell or in the nine adjacent cells. To determine what particles are in adjacent cells one needs to carry out the presorting of the particles. To keep calculation time down we use the algorithm [15] to sort the coordinate addresses instead the coordinates. It is rational to take the lateral (minimal) length of slick as the estimate of linear length scale L using relation $L_{\min} = S/(\pi L_{\max})$. The root-mean-square distance between the particles is taken as $L_{
m max}$. It is easy to show that $L_{
m max}$ is the estimation for the maximum length scale for the elliptic slick with the uniform particles distribution.

In Figure 1 the example of spreading of oil slick for continuous spill in the field of water velocity $\vec{u}_w = (0.3; 0.3)$ m/s. Spill rate was 0.28 m³/s. Figure shows that at moderate water velocity the different mechanism of slick spreading (advection, viscous-gravitational, surface tension) can be equally important. With large time and spatial scale the horizontal turbulent diffusion will be essential factor.

The water velocity $\overset{\neg(s)}{u_w}$ can be decomposed on deterministic advective component $\overset{\neg(s)}{u_{adv}}$ and random component $\overset{\neg(s)}{u_{diff}}$, which caused by horizontal turbulent diffusion

$$\frac{du}{du} = \frac{du}{du} + \frac{du}{du} = \frac{du}{dt} + \frac{du}{dt} = 0.$$
(12)

The advective velocity is found from the solution of hydrodynamic model equations or set from observations. Random component is simulated by random walk method

$$\vec{u}_{diff}^{(s)} = P_d^{(u)} \sqrt{6K_H / \Delta t} , \qquad (13)$$

where $P_d^{(u)}$ is the uniformly distributed in $[-1;1] \times [-1;1]$ random vector; K_H is the isotropic turbulent coefficient. The experimental relation [11]

$$K_H = 1.17 \cdot 10^{-6} t_k^{1.34} \tag{14}$$

where t_k is the age of spillet. Maximum value of K_H should be equal to sub-grid diffusion coefficient in the hydrodynamic model.

Oil-in-water phase.

In stormy conditions breaking wind waves cause oil droplets entrainment into the water column. Therefore, in shallow waters the great amount of oil can be deposited on the bottom. Dispersion processes are governed by mechanical factors such as breaking waves and turbulent mixing in the near surface layer. They depend on the physical-chemical oil properties: density, viscosity, surface tension. The oil droplet concentration in water is described by equation

$$\frac{\partial C_d}{\partial t} + \vec{\nabla}(C_d \vec{u}) = Q_d^{(dis)} + Q_d^{(sed)}, \tag{15}$$

where C_d - volume concentration of oil droplets with diameter d, $\vec{u} = (u_w, v_w, w')$, $w' = w_w + w_d$, w_d is the velocity of oil droplet due to buoyancy force. The mass flux caused by breakup the surface slick by breaking waves $Q_d^{(dis)}$ is assumed to be uniformly distributed over the wave mixing depth $Z_s \approx 1.5H_s$, where H_s is the significant wave height [13]. The flux of droplets of diameter d is estimated according [12]

$$Q_d^{dis} = \frac{C(o)}{\rho_o Z_s} F_{wc} D_{ba}^{0.57} d^{0.7} , {16}$$

where C(o) - is the empirical constant, dependent on the oil properties; D_{ba} - dissipated breaking wave energy per unit surface area

$$D_{ba} \approx 0.0034 \rho_w g H_{rms}^2$$
, (17)

where H_{rms} is r.m.s. value of the wave height, $H_{rms} \approx 0.7 H_s$; F_{wc} is fraction of sea surface hit by breaking waves ('white caps') per unit time

$$F_{wc} = c_b (W - W_i) / T_w \,, \tag{18}$$

where W_i initiation of breaking wind speed ($\approx 5\,\mathrm{m/s}$); T_w - wave period, c_b is constant ($\approx 0.032\,\mathrm{s/m}$). The total oil droplet flux and total oil concentration are calculated as

$$Q^{(dis)} = \int_{d_{min}}^{d_{max}} Q_d^{(dis)} Z_s \delta d, \quad C = \int_{d_{min}}^{d_{max}} C_d \delta d$$
(19)

 d_{\min} , d_{\max} - are the minimum and maximum oil droplet diameters respectively. According to experiments [12], $d_{\min} \approx 5 \mu m$. For d_{\max} we use relation [13]

$$d_{\text{max}} = 0.363(\sigma/\rho_w)^{3/5} \varepsilon^{-2/5}, \tag{20}$$

where ε is the dissipation rate of turbulence energy. The

$$Q^{(res)} = \int_{d_{min}}^{d_{max}} u_d C_d(0) \delta d$$
 (21)

where $C_d(0)$ is surface volume concentration of particles with size d. The 3D equation (15) is integrated using Lagrangian approach. The water velocities u_w , v_w , w_w are decomposed on deterministic advective components and random components, which caused by vertical and horizontal turbulent diffusion. Random components are simulated by random walk method. The coefficient of vertical diffusion is calculated in the hydrodynamics model whereas horizontal diffusion is similar (13).

Oil-on-sediment phase

The scavenging of dispersed oil from water by adhesion to the sediment and particulate matter (SPM) is parameterized with use model [15]. The sedimentation rate is

$$Q_d^{(sed)} = -1.3\alpha [\varepsilon/\nu_w]^{1/2} C_d S, \tag{22}$$

where α is a sticking coefficient, S is volume suspended sediment concentration.

Oil-on-bottom phase

The flux of oil in the bottom include flux by scavenging of oil by SPM (22) and direct sticking to the bottom, that is parameterized by empirical relations.

Oil-on-shore phase.

Following [9] we represent the shoreline as the sequence of straight line segments with shore type attributes: exposed headlands, sand beaches and sheltered marshes. Each particle moves until it 'crosses' one of the shoreline segments. After particle has been beached it may remain on the shore or refloat after a specified time depending on the shoreline type. The refloating algorithm is based on the specified half time of the oil to determine the time of

particle remaining at the shore [16]. The number of particles at time $t+\Delta t$ denoted as $s(t+\Delta t)$ can be estimated as

$$s(t + \Delta t) = s(t) \left(\frac{1}{2}\right)^{\Delta t/\tau},\tag{23}$$

where τ is the half life, i.e. at the time τ half of particles refloating. So, the number of particles which have to be refloat during one time step can be calculated as

$$s(t) - s(t + \Delta t) = s(t) \left(1 - \left(\frac{1}{2} \right)^{\Delta t/\tau} \right). \tag{24}$$

To select which particle has to refloat we allow them to refloat in the same order in which they arrived. For different types of shore we used the next values for oil half time. For exposed headland, sand beach and sheltered marsh $\tau = 1$ hour; 1 day; 1 year, respectively.

3. The weather and sea state models

The weather forecast model.

The limited area model MM5 V.3 is a core of the weather forecasting system that was developed by IMMSP and UCEWP with support Ukrainian Hydrometeorological Service to produce the operational forecasts for the Ukraine. The Fifth-Generation NCAR / Penn State Mesoscale Model MM5 [17] is nonhydrostatic model that contains capabilities of multiple nesting, four-dimensional assimilation and set of parameterizations of the microphysical fields and planetary boundary layer. The forecasting system includes preprocessor, MM5 model and postprocessor. Preprocessor retrieves every 12 hr GRIB bulletins from DWD with analyses and global model forecasts which contain horizontal winds, temperature, geopotential and moisture on 11 levels. These fields are necessary to provide initial and boundary conditions on the coarse grid. The coarse grid 37x37 with 81 km mesh cover large area in the Eastern Europe. The lateral conditions are updated every 12 hr. The nested grid 73x73 with 27 km allows refine forecast on the Ukraine territory and the Black Sea. The model uses 31 sigma levels in vertical. A planetary boundary layer was parameterized using scheme NCEP MRF model. The roughness height over sea was parameterized by modified Charnock relation. The forecasts at 48 hr are run once a day at 6 UTC. The procedure of initialization includes assimilation of data retrieved from meteorological stations bulletins and soundings on coarse grid area in -24-0 hr of model time. The Black Sea surface temperature for the forecast period is taken from DWD analysis. The available data from meteorological bulletins are assimilated in the 0-6 hr of model time. Postprocessor produces forecasts for specific locations, 2D field of meteorological parameters for other models and visualizes results at the web page http://www.meteoprog.com.ua.

The wave model.

The wave model WAVEWATCH III V. 1.18 (WW3) is a third generation wave model developed at NOAA/NCEP [18]. The governing equations include refraction and straining of the wave field due to temporal and spatial variations of the mean water depth and the mean current and wave growth and decay due to the actions of wind, nonlinear resonant interactions, dissipation ('whitecapping') and bottom friction. The prognostic parameters are

gridded fields of 16 mean wave parameters such as the significant wave height and directions and significant wave period. WW3 is forced by MM5 10 m height winds. The surface currents are supplied by circulation model. The wind and currents time step is 3 hr. The model uses the forecasts wave spectra as the initial conditions for the next run. The finest spatial resolution is 6', number of nodes is 160×60 , number of spectral components is 25 and directions is 24. Timestep is 300 s.

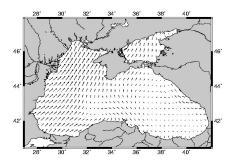


Figure 2 Wind field at 10 m predicted by MM5 at 10.00 UTC 25 September 2002

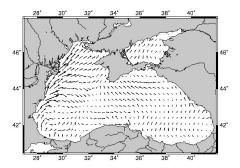


Figure 3 Surface currents predicted by circulation model at 10.00 UTC 25 September 2002

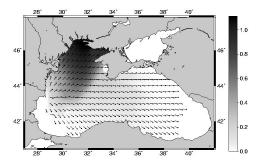


Figure 4 Wave direction and height predicted WW3 at 10.00 UTC 25 September 2002



Figure 5. 3D representation by interactive visualisation tool of the oil spill at the North-western shelf of the Black Sea. The surface slick, oil-in-water and oil-on-bottom concentrations are shown by black, light grey and dark grey, respectively.

The circulation model

The hydrodynamics code THREETOX based on the three-dimensional, time-dependent, free surface, primitive equation model [19]. The prognostic variables of the hydrodynamics code are the three components of the velocity, temperature, salinity and surface elevation. The σ -coordinate system, mode splitting and two-equation model of turbulence are important features of model. The model of turbulence provides necessary values of vertical diffusion coefficient and dissipation. Model also describes wave breaking effects on the surface layer [13]. Suspended sediment transport is an option of model [20]. The surface wind stress and heat fluxes are provided by MM5 with time step 3 hr. The resolution is 10x10 km, number of nodes is 137×68 and number of σ - layers is 21. Internal mode time step is 1000 s

4. Modelling system design

The OILTOX model includes computational engine, oil database and Graphical User Interface. The database of the model includes information about a hundred types of oil transported in the Black Sea and their main physical-chemical properties. Together with the standard 2D visualization tools, the oil spill evolution was tracked by an interactive 3D tool based on OpenGL technology. The forecasting system was designed to operate at on a Linux-based PC network. OILTOX can be used in different configurations:

- 1. Stand-alone version with environment parameters specified by user, including climate database;
- 2. Version, linked with circulation model with meteorological parameters specified by user;
- 3. Full scale version linked with weather, wave and circulation models.

5 Applications

The modelling system was adapted to the Black Sea basin. The results of simulations of surface wind, waves and currents in the Black Sea as obtained by the coupled model system are shown in Figures 1-3. The hypothetical scenario of an oil spill of 75 000 tons of crude oil on the north-western shelf of the Black Sea on 25 September 2002 at a distance of around 50 km from the Odessa oil terminal was considered. The oil slick drifted by wind and surface

current to a shallow area. The oil from slick was entrained by breaking waves with rate that depends on calculated by WW3 wave parameters. The oil droplets were transported by currents, dispersed by turbulence, interacted with suspended and bottom sediments and gradually resurfaced by buoyancy forces, forming thin film ("sheen") behind the thick slick area. The resulting 3D distribution of oil concentration in three phases (surface, water and bottom) is shown in Figure 5.

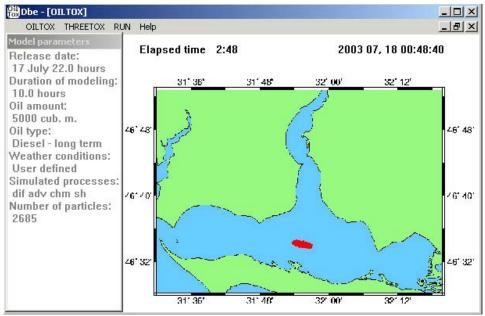


Figure 5. 2D representation of the oil spill in the Dnipro-Boog Estuary on the OILTOX interface.

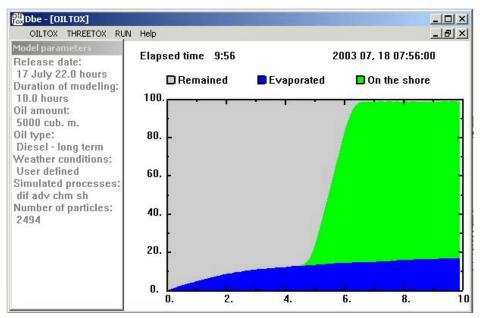


Figure 6. Oil spill mass budget on the OILTOX interface.

Another example is the Dnipro-Boog Estuary that is the largest in the Black Sea basin. Two large cities (Mykolayiv and Kherson) with ports and refineries are located in the estuary and it is on the way to the Dnipro basin system. From 2004 the version of the system which contains the circulation model and OILTOX complemented by a database and GUI will be in use by State Departments on the Environment and Natural Resources in the Kherson and Mykolayiv. Figure 5 shows GUI representation of the simulated spill in the Dnipro-Boog Estuary after a hypothetical spill of 5000 tons of diesel fuel. The atmospheric forcing (observed wind, air temperature, humidity and cloudiness), river discharge and level in estuary mouth were available every 3 hours. The plot with spill budget is given in Figure 6.

5. Future development and conclusions

This paper presents the development of a 3D oil spill model OILTOX based on an extended Lagrangian concept that includes five interactive phases of an oil spill. New spreading algorithm allows simulate most processes governs evolution of surface slick. It can be used to simulate slick retention by booms and barriers. The model is coupled with a weather forecast model and wave and circulation models. The whole system was adapted to the Black Sea and the first test results showed potential for a multipurpose modelling system. Future development include: (a) extension of oil spill model capabilities to support use chemical dispersants and cleanup operations; (b) full coupling of weather, wave and circulation models with detailed modelling of wave breaking and Stokes drift effects on vertical and horizontal dispersion of oil.

Acknowledgements

Current development of the system is funded within the INTAS project No 01- 0330 and the US AID project "Water quality program assessment and abatement Dnipro Estuary, Phase 2".

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