

Modeling the behaviour of an oil spill in the marine environment

M.G. PSALTAKI, N.C. MARKATOS

School of Chemical Engineering
National Technical University of Athens
Iroon Polytechniou 9 Zographou Campus 15780
GREECE
n.markatos@ntua.gr

Abstract: Assessment of the risk of an oil spill in the marine environment is absolutely necessary as a great amount of petroleum is transported by cargo ships and pipelines through the marine environment. In 2004 the total amount of oil in the marine environment due to accidents was about 15.000 tons. The increase in offshore oil exploration, and the drilling and production activities enhance the potential for oil spills that damage marine ecosystems, given that oil toxicity creates major environmental problems. The mathematical modeling of oil spills is a very important tool for impact assessment studies, as oil toxicity creates major environmental problems. This paper describes briefly a deterministic model, developed to simulate the time-dependent behaviour of hypothetical oil spills near coastal regions. The model capabilities are demonstrated by applying it in two regions; near Carava, at the island of Lesbos, and near Eretria, in the Evvoikos bay, both being in the Aegean sea.

Keywords: Oil spill, computational fluid dynamics, turbulence, simulation, RNG (k-ε) turbulence model

1 Introduction

According to the International Union for Marine Pollution, during the last four months of 2004 five great accidents due to oil spills took place. The quantity of oil was over 9000 tons. The most important of them was due to a leakage from the ship "Al Samidon" at the Suez canal area (December 14, 2004), where the quantity of oil spilt was about 9000 tons.

The mathematical modeling of oil spills is a very important tool for impact assessment studies, as the effects of oil toxicity on the marine ecosystem create major environmental problems. Oil toxicity depends on the physical and chemical characteristics of the spilled oil, more toxic being the oils with a significant fraction of aromatics. The impact of oil toxicity on marine organisms depends on the organism itself and its age, on oil concentration, on the water salinity, its temperature and pH, and the presence of nutrients, pollutants (such as sulfides, phenols, detergents) and/or dispersants. Furthermore, the damage to the shore also depends on the contact duration of the slick with the coastline [1,2].

2 Problem Formulation

The spill is considered to be initially circular, formed under the action of gravity, inertia, viscous

and surface tension forces. The sequential balances, in time, among pairs of these forces allow for an estimate of the respective diameter, D , of the spill (Eqns. (1a,1b,1c) and of its thickness, provided that the spilled oil volume is known.

Gravity-Inertia forces:

$$D = 2k_1 \left(\frac{\rho_w - \rho}{\rho_w} g V t^2 \right)^{1/4} \quad (1a)$$

Gravity-Viscous forces:

$$D = 2k_2 \left(\frac{\rho_w - \rho}{\rho} g V^2 t^{3/2} \right)^{1.6} \quad (1b)$$

Surface tension-viscous forces:

$$D = 2k_3 \left(\frac{f_n^2 t^3}{\rho_w} v_w \right)^{1/4} \quad (1c)$$

Here ρ_w is the water density, ρ the oil density, V the oil volume, v_w the water kinematic viscosity, f_n is the oil-water surface tension and $k_1=1.14$, $k_2=1.45$, $k_3=1.6$ [2].

At subsequent times, the spill, while advected by the hydrodynamic field and subjected to various weathering processes, takes arbitrary shapes which are predicted by the present model. The model

utilizes an Eulerian two-phase flow approach [3,4,5]. The two phases are considered as “interpenetrating continua”, i.e. the two phases occupy the same space (although not necessarily at precisely the same time), their share of space being measured by their “volume fractions” r_i . It is, therefore, obvious that for two -phase flows:

$$r_1 + r_2 = 1 \quad (2)$$

A complete set of equations is formulated for each phase present, the phase equations being linked together through the processes of interphase momentum/heat and mass transfer.

The phase continuity equation has the following form:

$$\frac{\partial(\rho_i r_i)}{\partial t} + \text{div}(\rho_i r_i V_i - \Gamma_{ri} \text{grad}(r_i)) = \frac{dm}{dt} \quad (3)$$

Where r_i the volume fraction of each phase, m^3/m^3 , ρ_i the phase density, kg/m^3 , V_i the phase velocity, m/s , Γ_{ri} the phase diffusion coefficient, Ns/m^2 , dm/dt net mass transfer to phase i from phase j , $kg/(m^3s)$ (e.g. evaporation). The momentum equation for phase i is as follows:

$$\frac{\partial(\rho_i r_i u_{ik})}{\partial t} + \text{div}(\rho_i r_i V_i u_{ik}) = r_i(-K \text{grad} p + B_{ik}) + F_{ik} + I_{ik} \quad (4)$$

where p the pressure assumed here to be shared by the phases, B_{ik} body forces (e.g. gravity), F_{ik} turbulence forces to each phase from the tension forces within the phase, I_{ik} momentum transport due to phase interactions. In the total equation of phases $\sum I_{ik} = 0$

The energy equation is as follows:

$$\frac{\partial(r_i \rho_i h_i)}{\partial t} + \text{div}(r_i U_i \rho_i h_i - \Gamma_{hi} \text{div}(r_i h_i)) = S_{hi} \quad (5)$$

where $\Gamma_{hi} = \mu_i / Pr_i$, μ_i the dynamic viscosity and Pr_i Prandtl number of phase i , h_i the enthalpy of phase i per unit mass, and S_{hi} the source terms. All differential equations above can be cast in the following general form:

$$\frac{\partial}{\partial t}(r_i \rho_i \phi_i) + \text{div}(\rho_i r_i V_i \phi_i) = \text{div}(r_i \Gamma_{\phi_i} \text{grad}(\phi_i)) + S_{\phi_i} \quad (6)$$

where i takes the values 1 and 2 for the two phases (1 for the water and 2 for the oil phase); for particular phase i , the dependent variable ϕ_i denotes u , v , w , the three velocity components, or the

turbulence kinetic energy k , the turbulence dissipation rate ϵ ; $\phi_i = 1$ reproduces the continuity equation; \vec{U}_i is the hydrodynamic velocity vector; Γ_{ϕ_i} is an effective exchange coefficient [3] and S_{ϕ_i} is the appropriate source or sink term (i.e. for the momentum equations.: the terms representing interphase friction, gravitational acceleration, Coriolis force, surface tension and pressure gradient). The salinity equation has the following form:

$$\frac{DS}{dt} = \frac{\partial}{\partial X_j} \left(\frac{\nu_T}{\sigma_T} \frac{\partial S}{\partial X_j} \right) \quad (7)$$

where σ_T is a Prandtl/Schmidt number (= 2.5)

ν_T turbulence viscosity. Also, the equation for the density is as follows:

$$\rho = \rho_0 (1 + \alpha S) \quad (8)$$

where $\rho_0 = 1000 \text{ kg/m}^3$, α a coefficient (= 8×10^{-4}).

The present model employs a version of the RNG (k- ϵ) turbulence model [6], modified properly to incorporate the aspects associated with the presence of waves, wave breaking, natural dispersion of oil mass, etc. The finite volume method was implemented for the numerical solution of the above system [3,4].

The model is implemented in the CFD code PHOENICS -V.3.1, V.3.4 which utilizes the SIMPLEST algorithm to solve the Navier-Stokes equations for transient, two phase, 3-D turbulent flow [4]. The model also employs some simple expressions for describing the slick advection by the wind and wave-induced currents, the presence of waves and the impact of breaking waves on the dispersion of oil mass in the water column. The surface wind- and wave-induced currents, U_{sa} and U_{sw} , that advect the oil slick along with other permanent currents are given by the following simple expressions [2,7]:

$$\begin{aligned} U_{sa} &= 0.01 \exp(0.03 + 0.14 U_a) \\ U_{sw} &= 0.015 U_a \end{aligned} \quad (9a,b)$$

where U_a is the wind speed measured at some elevation above the mean sea level (usually 10 m). Tidal Currents are also included in the advection scheme of oil slicks. For the application presented below Evvoikos bay is influenced [8] by M_2 , S_2 , K_1 , O_1 tides (Table 1.)

For tides simulation the widths of the main diurnal (O_1, K_1) and the widths of the semi-diurnal (S_2, M_2) were considered. If $(O_1 + K_1) / (S_2 + M_2) \geq 3.0$ we have the diurnal type, if ≤ 0.25 we have the semi-

diurnal type. If it is greater than 0.25 and smaller than 3.0 we have the mixed type.

M ₂	M ₂	S ₂	S ₂	K ₁	K ₁	O ₁	O ₁
cm	deg	cm	deg	cm	deg	cm	deg
19.0	92	13.2	119	2.9	356	1.4	328
19.1	92	13.3	119	2.9	356	1.4	328
19.2	92	13.4	119	2.9	356	1.4	328

Table 1. M₂, S₂, K₁, O₁ tides

The evaporation rate E is estimated by a simple relation of the form:

$$E = kU_a P, \quad (10)$$

where P the oil vapour pressure and k a relevant coefficient [2].

The rate of the natural dispersion of the oil, that is the rate Q at which oil entrains in the water column, is estimated according to an expression proposed in [9,10].

$$Q = c_{oil} V_{oil} f_{bw} D_e^{0.57} \quad (11)$$

where c_{oil} represents a factor that can be experimentally calculated, V_{oil} is estimated as:

$$V_{oil} \propto \int_{d_{min}}^{d_{max}} N(\delta) \delta^3 d\delta, N(\delta) = N_0 (d/d_0)^{-2.3} \quad (12)$$

where D_e is the wave energy dissipation due to breaking, per unit time and unit area. According to [9] D_e is estimated as:

$$D_e = 0.0034 \rho g H_{rms}^2, \quad H_{rms} = H_s / \sqrt{2}, \quad H_s = 4 \sqrt{m_0} \quad (13a,b, c)$$

where m_0 is the sea surface variance ($= \overline{\eta^2}$) where η is the water surface displacement from the mean water level. The wave energy is given as $\rho_w g \overline{\eta^2}$.

Photo-oxidation is estimated according to an expression proposed in [11]. The oil-volume change due to photo-oxidation is given by:

$$\frac{dV}{dt} = -k_p \xi V \quad (14)$$

where $\xi = \exp(T - 20) \ln(k_t) IOS / (IOD_{max} RD)$, T is the temperature of the oil, IOS is the total photosynthetically-activated radiation, IOD_{max} the maximum photosynthetically-activated radiation, and RD the relevant daily light constant $k_t = 1.05$ and k_p is a coefficient.

Emulsification is estimated by an expression proposed in [12], namely:

$$\frac{dY}{dt} = kU^2 \left(\frac{Y}{Y_f} \right) \quad (15)$$

where Y is the water volume entrainment to the oil spill and Y_f is the maximum amount of water in the emulsion; $k = 1.6 \times 10^{-6}$. As an interim approach, ADIOS2[11] uses a simple model which relates sedimentation rate to oil stickiness, oil droplet concentration, sediment concentration, and dissipation energy rate for surface water:

$$Q_{sed} = k_a \sqrt{\frac{D_e f_{bw} C_0 C_{sed}}{H_{rms} \rho_w v_w}} \quad (16)$$

where C_0 is the entrained oil volume concentration and C_{sed} is the suspended sediment volume concentration. k_a is a sticking parameter that depends on the type and size of the sediment particles.

Dissolution is estimated by the following expression [13]:

$$M_d = K_d A t X S \quad (17)$$

where M_d is the dissolved amount of oil (moles), K_d a coefficient ($= 3.0 \times 10^{-6}$), X the mole fraction, A oil surface (m^2), S solubility.

Biodegradation is estimated as:

$BE(\%) = 100 - (Asx100/Aac)$, where $BE(\%)$ is the effective biodegradation, As the total peak area per sample and Aac the total peak area of the relevant abiotic control [14]

3 Problem solution

The model capabilities are demonstrated by applying it in two regions of different topography and bathymetry, in the framework of impact assessment studies. These two regions are near Carava (Figure 1), at the island of Lesvos, and near Eretria (Figure 2), in the Evvoikos bay, both being in the Aegean sea. The first region has an extent of $12 \times 9.5 \text{ km}^2$ and a maximum depth of 55m, whereas the second occupies an area of $10 \times 18 \text{ km}^2$ and has a maximum depth of 25 m. The model predicts the position of the centre of mass and the shape of the oil spill in time, as it spreads under the action of hydrodynamic dispersion and turbulence diffusion, both at the sea surface and throughout the water column, while it is being advected by wind and wave-induced or other currents. The effects of evaporation, natural dispersion, dissolution, emulsification, sedimentation, photo-oxidation and biodegradation on the spilled oil are also considered in this work. Furthermore, the model handles the enhanced turbulence diffusion, caused

by surface wave breaking, and the impact of breaking waves on the dispersion of oil in the water column. The spill is considered to be initially circular, formed under the action of gravity, inertia, viscous and surface tension forces. A time step of 800s proved to be adequate for time-step independent solutions, while using 100 iterations per time step. The runs were performed on a Silicon Graphics Origin 200 (4 CPU R 10000). A typical run using a 120x95x16 grid (that leads to grid independent solutions) for 20 time steps and 23.200 secs real time, requires 12 hrs on the above machine using UNIX and 5 hrs using LINUX on a Pentium IV, 2.4 GHz, 512 MB. The hydrodynamic field was predicted considering a NW wind of 10 m/s and assuming a logarithmic wind profile.

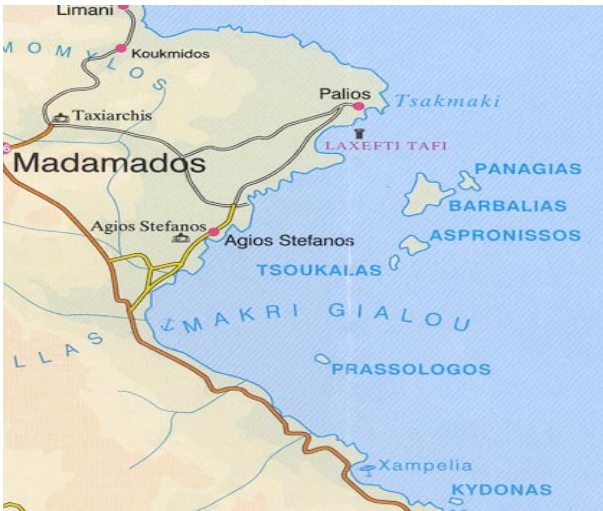


Figure 1. The region of Carava area



Figure 2. The region of Evvoikos bay

The above fields were simulated first under steady-state and single phase flow conditions, using the RNG (k-ε) turbulence model for the water phase only. Then, the fate of hypothetical oil spills was simulated, under transient, two-phase flow conditions. Figures 3,4 present the hydrodynamic field of Carava area and Eretria , respectively.

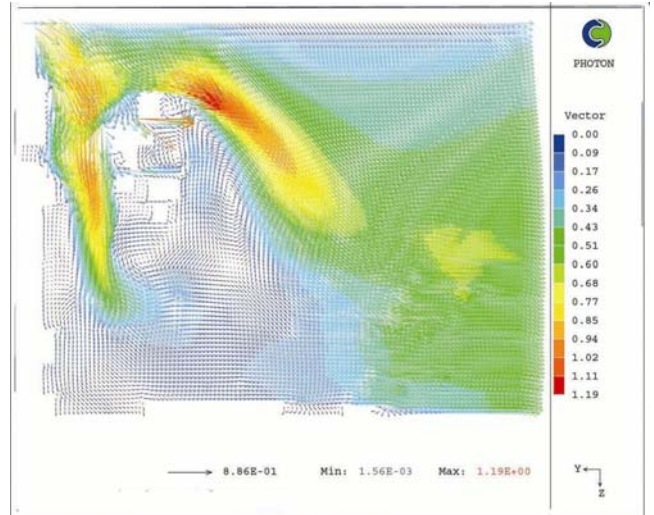


Figure 3. The hydrodynamic field at the surface

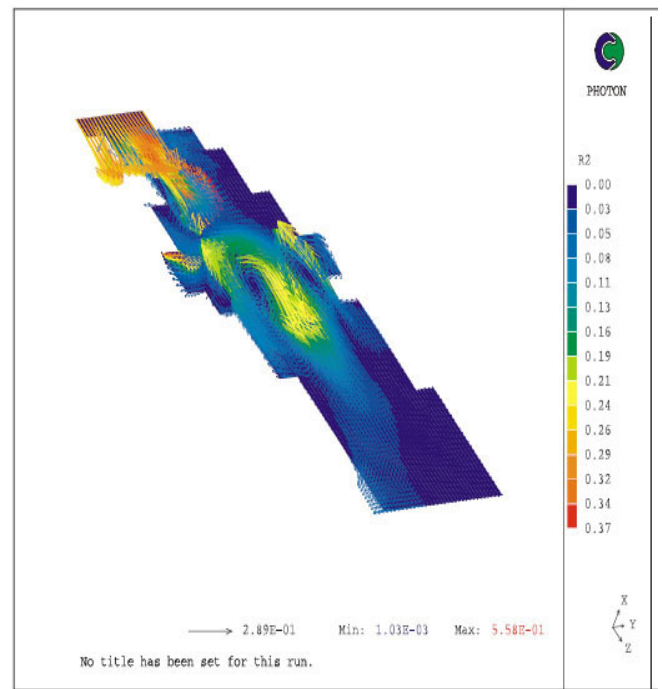


Figure 4. The hydrodynamic field at the surface

Figure 5 presents an oil spill of 800kg/m³ at a distance of 500μ. from the coast of Lesbos Island at the upper western part of the study field

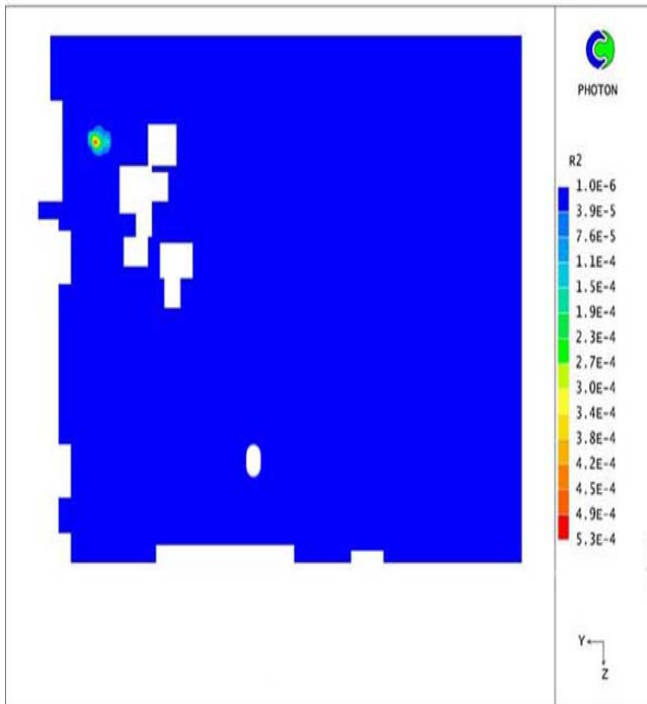


Figure 5. The spill at the surface 10secs after the accident

Figures 6,7 present the fate of the spill at the surface and at a depth of 25m, 6.5 hours after the accident.

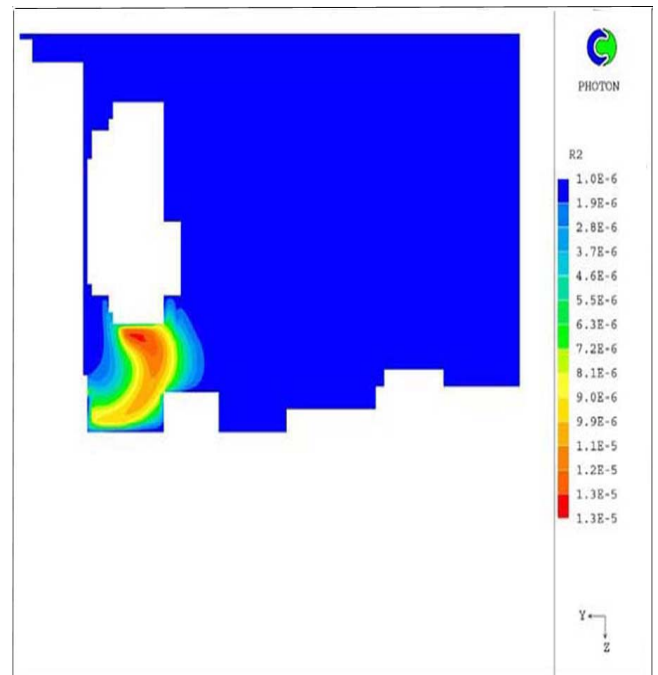


Figure 7. The spill at a depth of 25m. 6.5 hours after the accident

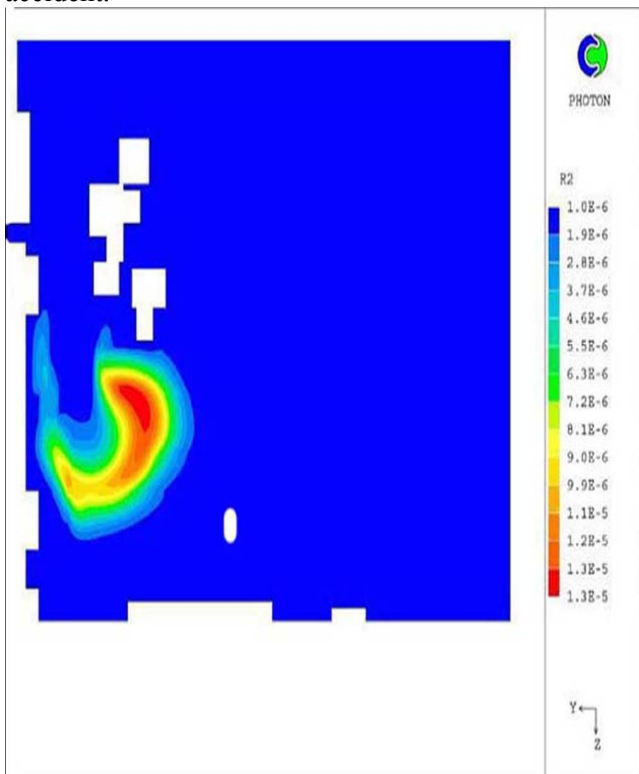


Figure 6. The spill at the surface 6.5 hours after the accident

Figure 8 presents the percentage of the water uptake with time, while figure 9 presents the evaporation percentage versus time.

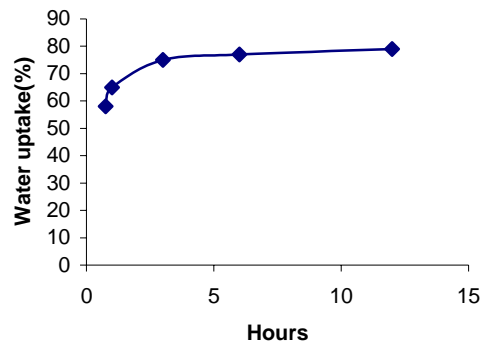


Figure 8. Water uptake (%) versus time

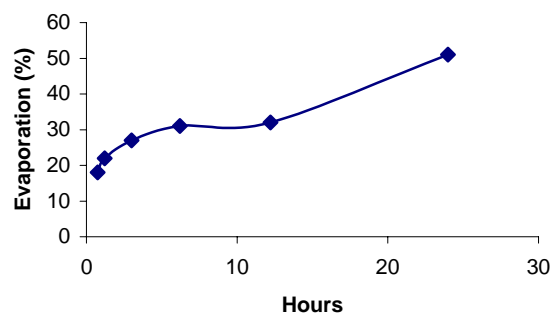


Figure 9. Evaporation (%) versus time

All the simulation cases were conducted using salt water and meteorological /oceanographical data for a given period of time (May-June 2004). Figure 10 presents the fate of an oil spill, a few minutes after a spill of 830 m³ with density of 830kg/m³ had occurred at a distance of 200 m from the upper western coast of Prasologos, a small island and a region of rather shallow waters, considering a NE wind of 10m/s.

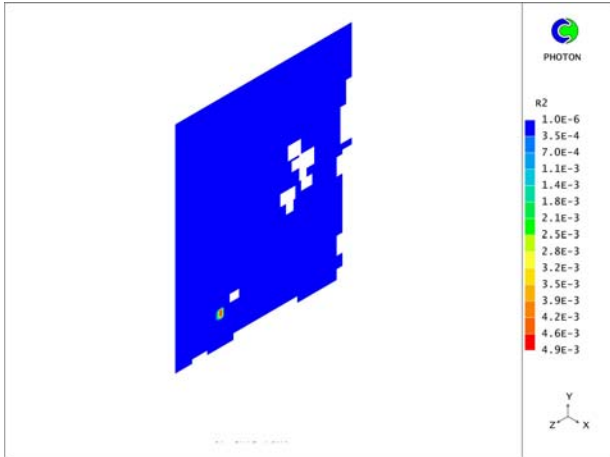


Figure 10. The spill 10s after the accident

Figure 11 presents the fate of the above spill at the surface 6 hrs after the accident.

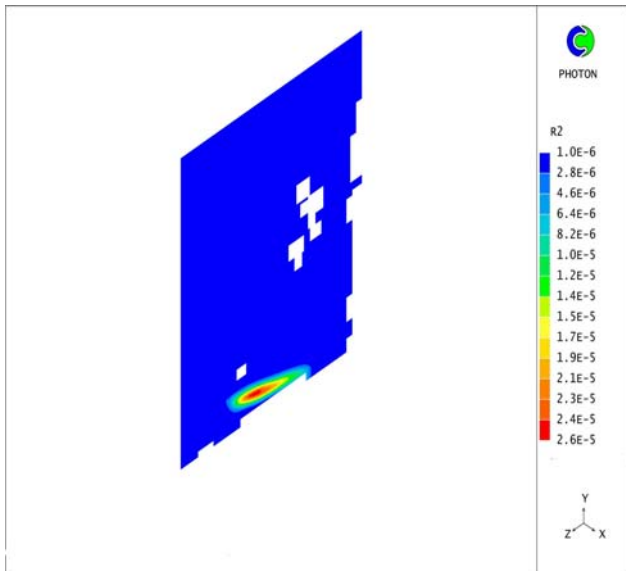


Figure 11. The spill at the surface 6 hrs after the accident

Figure 12 presents the spill balance 3 days after the accident.

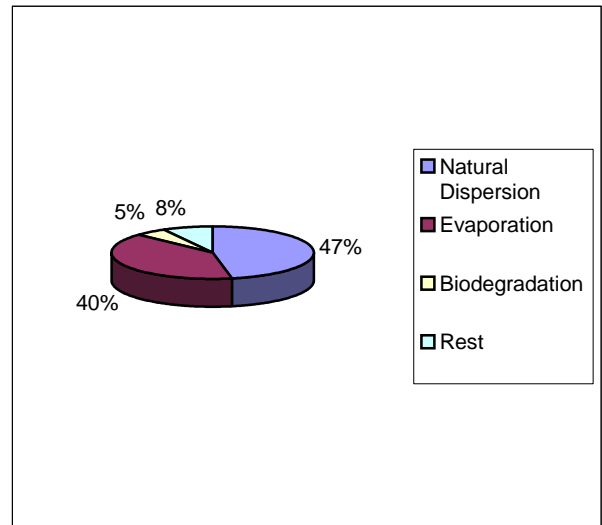


Figure 12. The spill balance 3 days after the accident

Figure 13 presents the fate of the spill 10s after a hypothetical accident 500m southwestern of Eretria, a region of Evvoikos bay, considering a NW wind of 10m/s and an oil density of 860kg/m³. Figure 14 presents the fate of the above spill 12 hrs after the accident.

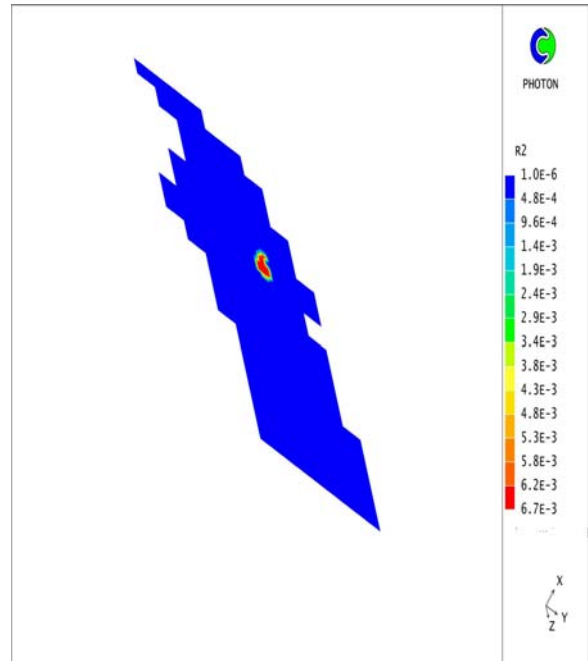


Figure 13. The spill 10s after the accident

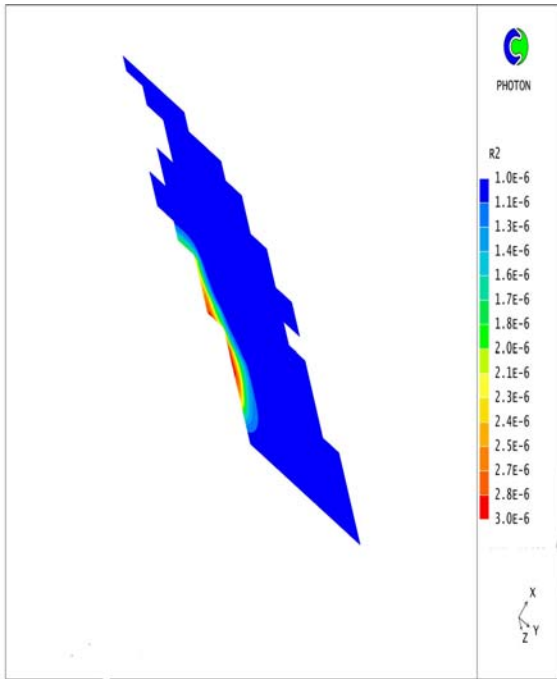


Figure 14. The spill at the surface 12 hrs after the accident

Figure 15 presents the fate of the above spill at a depth of 15m. 12 hours after the accident

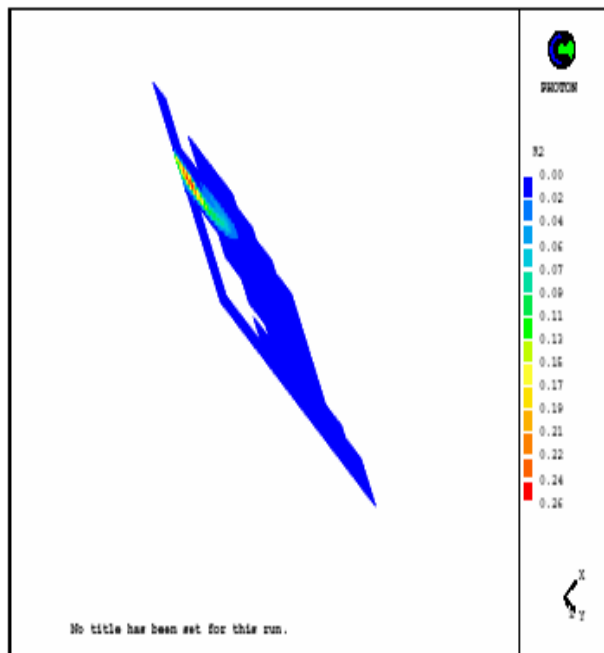


Figure 15. The spill at a depth of 15 m. 12 hours after the accident

Figure 16 presents the fate of the spill 10s after a hypothetical accident 300m western of Eretria, a

region of Evvoikos bay, considering a NE wind of 10m/s and an oil density of 880kg/m³. Figure 17 presents the emulsion 16 hrs after the accident.

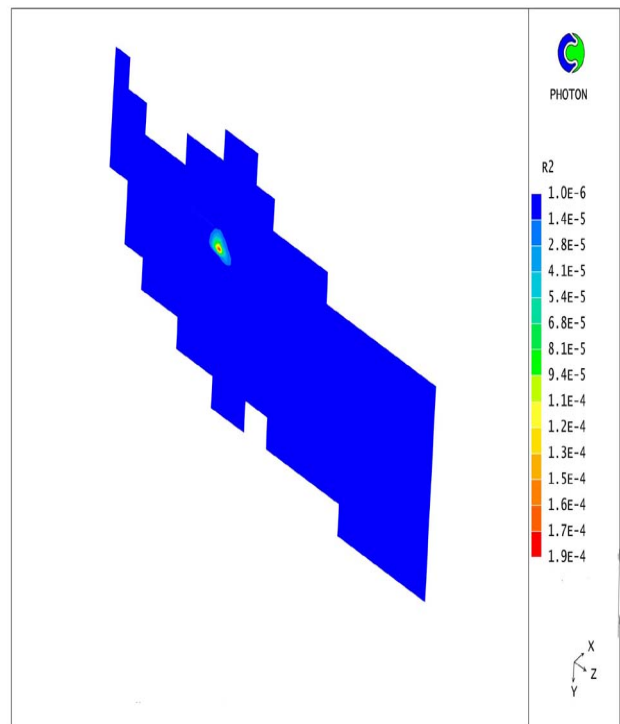


Figure 16. The spill 10s after the accident

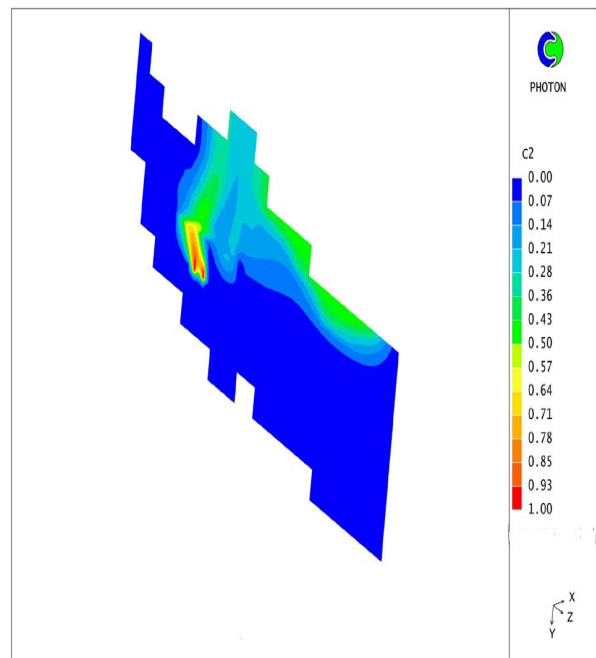


Figure 17. The emulsion at the surface after 16hrs

A 1D version of the present model was used to simulate the oil concentration profile in the water

column under the oilspill at the surface, taking into account the effect of wave breaking, and considering the following:

Wind velocity: 17.5m/s,; Wind Height: 1.60m, Wave period=4.8s, coefficient of vertical diffusion [10] $\epsilon_z=0.015$, Water depth 4.7m. The vertical oil mass transport is as follows::

$$T(z)=\epsilon_z\theta c/\theta z + W_C, \quad (18)$$

where c is oil concentration and the boundary conditions are:

$$T_b=0 \quad (19)$$

$$T_s=W_C \quad (20)$$

Oil droplets were also simulated by the model:

Oil density :900 kgr/m³

The mass of the droplets per time step is as follows:

$$Q_r(d_0)=C(0)D_{ba}^{0.57}S_{cov}F_{wc}d_0^{0.7}\Delta d \quad (21)$$

where : $Q_r(d_0)$ the mass of the oil droplets per unit area and unit time, $C(0)$ empirical diffusion coefficient , D_{ba} energy of wave breaking per unit area and breaking case, F_{wc} percentage of sea surface attacked by the wave breaking per unit time, d_0 droplets diameter, S_{cov} percentage of sea surface covered by oil. For the present simulation we considered $d_0=400-800\mu m$. Figure 18 presents the concentration of oil droplets versus height in the water column.

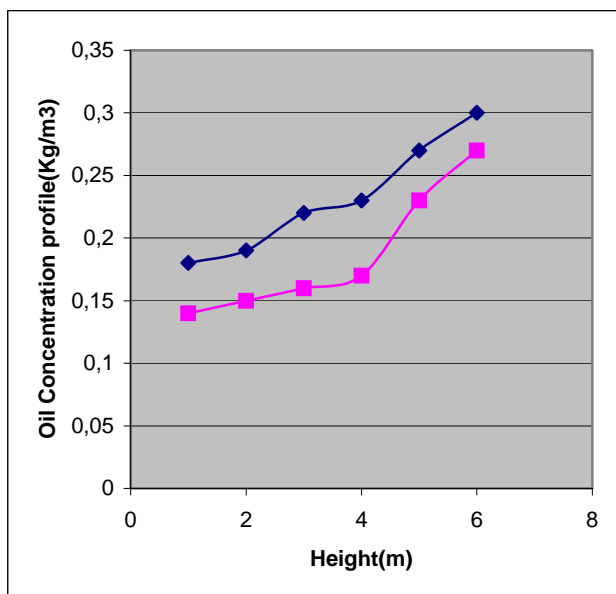


Figure 18. Oil concentration profile in the water column

The blue and the red lines correspond to the model results without and with oil droplets, respectively. The present model was also used, to simulate the natural dispersion of the oil in an area of 100mx50m considering a depth of 50m and a wind of 8m/s. Figure 19 presents the oil volume fraction which was naturally dispersed in the water column after 17 hours

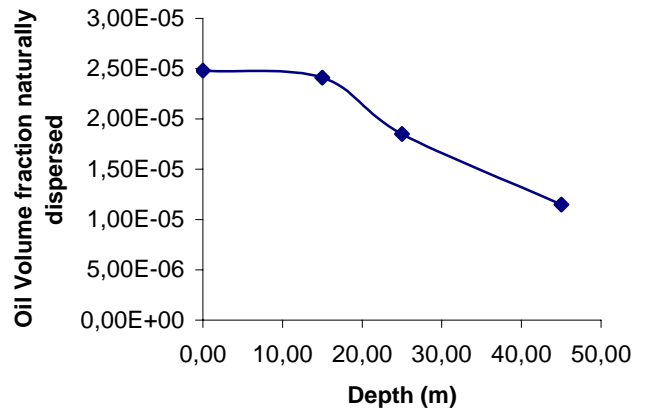


Figure 19. Oil volume fraction naturally dispersed

4 Conclusions

The model developed and used in this work incorporates most of the physical processes, that are considered necessary for the particular application, given the conditions of each simulation (depth, oil density, etc). Yet, it has a general structure that can accommodate any other processes deemed necessary.

Furthermore, the model covers the general circulation, the wave field and the processes that govern the fate of an oil spill in a marine environment, using a single computer code. The results of the simulations near coastal regions indicate that oil turbulence diffusion and dispersion are larger closer to the coasts than in deeper waters, and decay with depth away from the surrounding islands. These results are in accordance with observations, as turbulence diffusion and dispersion follow a similar trend.

The present model can respond to the demand for action following an accident. In that case, it is necessary to have input data for only two parameters: the area and the initial quantity of the oil at the sea surface.

Then, using the meteorological and oceanographical conditions of the open sea for a specific area we can predict the fate and the final place of the oilspill. Furthermore, if the ecosystems of the area

are known, it is feasible to estimate the ecological and environmental risk .

It may then be concluded that the prediction of the time dependent behaviour of oil spills in complicated 3D environments is feasible and can be accomplished within practical computer resources.

Referenecees

- [1]Findikakis A.N., A.W.K. Law & Y.Papadimitrakis (1998), "Assessment of the risk of shore contamination by offshore oil spills model formulation" Proc. of 1st Int. Conf. *Oil and Hydrocarbon Spills Modelling Analysis and Control (Oil Spill '98)*. Edited by. Garcia - Martinez, C.A. Brebbia, pp 209-220.
- [2]Stolzenbach K.D., O.S Madsen,. E.E..Adams, A.M. Pollack & C.K.Cooper (1977) " A Review and Evaluation of basic techniques for predicting the behavior of surface oil slicks", R.M.Parsons, Laboratory for Water Massachusetts Institute of Technology, Cambridge Massachusetts. Resources and Hydrodynamics, Dept. Of Civil Engineering, *M.I.T Sea Grant Program*
- [3]Spalding D.B. (1981), "A general purpose computer program for multi-dimensional one-and two –phase flow". *Maths and Computers in Simulation*, North Holland Press, Vol. 13 pp.267-276.
- [4]Markatos N.C. (1993), "Mathematical modelling of single-and two-phase flow problems in the process industries", *Revue de l'Institut Francais du Petrole* 48 (6) 631-661.
- [5]Markatos N.C. (1986.),"Modelling of two –phase transient flow and combustion of granular propellants", *Int. J.Multiphase Flow*, Vol.12, (6), pp 913-933,
- [6]Yakhot V.and S.Orszag, S.Thangam, T.B Gatski and. C.G.Speziale (1992) "Development of turbulence models for shear flows by a double expansion technique",*Physical Fluids A*,Vol. 4,No 7
- [7]Sobey R.J & C.H Barker.(1997) "Wave-driven transport of Surface Oil",*Journal of Coastal Research*, 13(2),490-496.
- [8]Tsimplis M.N (1997) "Tides and Sea-level Variability at the Strait of Euripus", *Estuarine, Coastal and Shelf Science*, Volume 44,Issue 1, , pp.91-101
- [9]Papadimitrakis Y., "Oil Natural Dispersion in the water column due to wave breaking", Proc. Of the 2nd Panhellenic Conference "*Management and amelioration of coastal zones*" School of Civil Eng., NTUA, 2002
- [10]G.A.L Delvigne & C.E. Sweeney (1988) "Natural Dispersion of Oil", *Oil and Chemical Pollution* 4pp.281-310.
- [11]Lehr W,. R. Jones, M. Evans, D. Simecek- Beatty & R. Overstreet (2001) "ADIOS, ADIOS2, Revisions of the ADIOS oil spill model", *National Oceanic & Atmospheric Environment (NOAA)-HAZMAT*, 7600, Sand Point Way NE, Seattle,WA 98115,USA
- [12]Lintrup M. J & A. K. VintherFalk, Bengtssen G. & N. Torneman (2000) "Oil Spill modelling in ORESUD-the influence of seasonal variation of photo-oxidation on the distribution of a spilled oil slick", *DHI-Water & Environment*, Denmark, Dept. of Ecology, Lund University, Sweden.
- [13]Xiaobo Chao, N.Jothi Shankar, Cheong Hin Fat (2001) "Two -and three-dimensional oil spill model for coastal waters", "*Ocean Engineering*"28 pp.1557-1573
- [14]J.P.Del'Arco,F.P.de Franca(1999) "Biodegradation of crude oil in sandy sediment",*International Biodeterioration& Biodegradation*,Volume 44,Issues 2-3 pp.87-92