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Three Dimensional Numerical Modeling of Oil Spill Behavior in Marine Environment

Aghajanloo, K.* and Pirooz, M.D.

School of Civil Engineering, College of Engineering, University of Tehran, Tehran, Iran

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ABSTRACT: In this research a three dimensional model is explained which simulate the oil spill behavior in seas. This model is the developed version of previous two-dimensional study of Aghajanloo *et al.,* 2013. Because of three-dimensional nature of the oil dispersion/movement in water, this is a more realistic model of oil spill transport and fate in marine environment. The model is based on Eulerian approach and the governing equations have been discretized by finite volume method. The main model is a combination of several major sub-models that predict the oil slick transport on the sea surface, oil losses due to natural weathering processes and oil dispersion in water column. The oil pollution distribution in water column have been modeled in a sigma-coordinate system and the effects of current, wave and wind forces and turbulent diffusion have been included. Also a hydrodynamic model is provided to simulate the tidal current which is based on two dimensional depth averaged equations of shallow water. A test case including analytical solution is chosen to ensure the model capability in oil spill simulation. The oil spill accident in the Persian Gulf has been simulated by the model.

Key words: Three Dimensional, Oil Spill Numerical Model, Vertical Dispersion, Sigma Coordinate

INTRODUCTION

Due to the 3D nature of the oil dispersion in water, the 3D modeling of oil concentration is important while the most oil spill models are based on the prediction of oil slick path on the water surface. In past years, many mathematical models were presented to simulate the oil spill behavior in marine environment (Al-Rabeh *et al.*, 2000; Chao *et al.*, 2003; Papadimitrakis *et al.*, 2006; Perianez, 2005, 2007; Perianez and Pascual-Granged, 2008; Shen and Yapa, 1988; Wang *et al.*, 2008, 2005; Yapa *et al.*, 1994). Most of these models were only capable of two-dimensional modelling of oil spreading, prediction of oil slick movement on the sea surface and estimation of the oil fate; and vertical dispersion of oil in water column was estimated based on empirical equations. In recent years, the marine environment researchers have paid more attention to fully 3D simulation of the oil distribution in the water and attempted to develop numerical models. Boufadel et al. (2006) simulated the movement of oil droplets in the non-breaking wave. In their Lagrangian model, the effects of wave forces and droplets buoyancy on dispersion were considered and they improved the Eulerian advection-diffusion equation to apply in their Lagrangian model to calculate the oil concentration in the water in 3D space. Boufadel et al. (2007) promoted their previous studies on regular wave occurrence. They expressed that the waves at sea play an important role in the transport and fate of oil particles. Perianez and Pascual-Granged (2008) proposed a Lagrangian model for 3D dispersion of chemical pollution and oil spills in marine environments, in the case of the Strait of Gibraltar. In their studies, the effects of wind and current velocities and turbulence diffusion in the oil droplets transfer have seen. Wang et al. (2008) proposed a 3D Lagrangian model, based on the particle approach, for the oil concentration in the sea in which the oil droplets buoyancy speed was calculated as a combination of wind, current and wave speed. The effective coefficient of current and wind speed was 0.03 and 1.10 respectively and the wave velocity was computed by Stokes wave law. Wang and Shen (2010) developed the previous work using an ocean wave model. Their model was tested by an idealized test case, a cylindrical flat lake and the results showed a successful numerical modeling. In their transport-fate module the oil dispersion was solved using a particle-

*Corresponding author E-mail:aghajanloo@ut.ac.ir

tracking method. Horizontal diffusion was simulated using random walk techniques in a Monte Carlo framework, whereas the vertical diffusion process was solved on the basis of the Langeven equation. Papadimitrakis et al. (2011) used a 3D hybrid turbulence model, simulating the transport and fate of oil spills in various waters, to evaluate the influence of natural dispersion on the spreading of water-in-oil emulsions formed in the water column. The model combined the Navier-Stokes equations for two-phase flows, the RNG k-å submodel, and parameterized expressions of the basic processes affecting the fate of oil spills. Their model also considered the presence of waves, the wind- and wave- induced surface drifts, and the influence of surface wave breaking on the oil spills.

In this paper, an Eulerian approach has been applied to simulate the transport and fate of the oil slick, which is adjusted by hydrodynamic model.

MATERIAL & METHODS

In this research, to simulate oil spill behavior in marine environment, a 3D numerical model has been developed. Coding of the model has been done in Visual Fortran language. The model is based on Eulerian approach and all of the mathematical equations have been solved by Finite Volume Scheme. In each time step, a set of several sub-models work together to calculate the different parameters of oil dispersion/ movement procedure in polluted area. The marine situation and surface current velocity are computed by the hydrodynamic sub-model. 2D governing equations of shallow water have been discretized on the structured staggered grid system and the ADI technique has been used to solve the resulted algebraic expressions. The oil slick movement on the sea surface has been modeled by an advection-diffusion equation. Also, oil mass losses from the slick due to natural weathering processes and the changes of remained oil have been estimated by the oil weathering sub-model. The verification of each sub-model was done and cited in literature (Aghajanloo and Pirooz, 2011; Aghajanloo *et al.,* 2011, 2013).

The fraction of oil entering into water column can pollute the underlying water. This process could be important when dispersant were used for cleanup operation. Oil mixing near the surface by breaking wave forms a mixing layer beneath the slick in that the oil concentration is uniform. Bellow this layer the oil distribution is governed by advection due to tidal current, wind and wave actions in horizontal direction, buoyancy speed in vertical direction and turbulent diffusion due to horizontal and vertical diffusion. Fig. 1 shows a schematic layout of the computational layers in the water column (h_w is the water depth). Therefore to compute the oil concentration below the water surface in polluted area, the 3D oil distribution model has been provided based on 3D advection-diffusion equation has been provided.

In this model, the computational domain is divided into several layers and the governing equations are solved in these layers. Because of the water depth variations due to variations in marine bottom elevation and water surface fluctuations, the sigma coordinate is chosen to the vertical domain discretization. In fact, in each point of horizontal grid, the water column is divided into a certain number of layers and the vertical computational lines are formed. The solution procedure of the 3D oil distribution model is similar to the

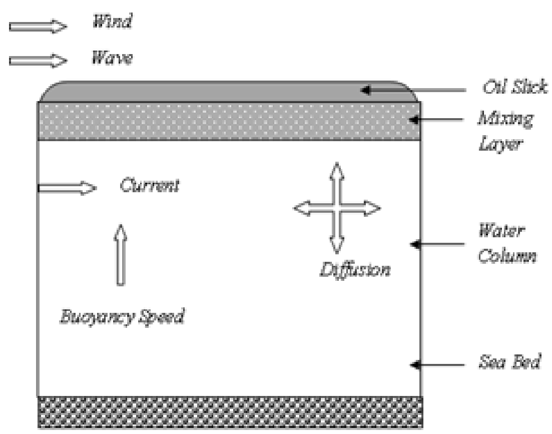

Fig. 1. The Schematic layout of the computational layers for the 3D oil distribution model

$$\frac{\partial \xi}{\partial t}+\frac{\partial (u_i h)}{\partial x_i}+\frac{\partial (u_j h)}{\partial x_j}=\frac{\partial z}{\partial t} \qquad (1)$$

$$\frac{\partial (u_i h)}{\partial t}+\frac{\partial}{\partial x_i}\left(u_i^{\,2} h\right)+\frac{\partial}{\partial x_j}\left(u_i u_j h\right)=-gh\frac{\partial \xi}{\partial x_i}-\frac{\tau_{bi}}{\rho_w}+\frac{\tau_{si}}{\rho_w}\pm f_{ci}+\frac{\partial}{\partial x_i}\left(\upsilon_t \frac{\partial (u_i h)}{\partial x_i}\right)+\frac{\partial}{\partial x_j}\left(\upsilon_t \frac{\partial (u_i h)}{\partial x_j}\right) \qquad (2)$$

$$\frac{\partial h_s}{\partial t}+\frac{\partial}{\partial x_i}\left(h_s v_j\right)-\frac{\partial}{\partial x_i}\left(D_s \frac{\partial h_s}{\partial x_i}\right)=\pm Q_s \qquad (3)$$

procedure of the transport terms in other sub-models, of course, with slight changes due to the application of sigma coordinate system to calculate overflowing and flux.

where, ξ, h and z are water surface elevation, flow depth and bed elevation, respectively ($\xi = h+z$); i and j are coordinate directions; u is surface current velocity; g is gravitational acceleration, $_t$ is eddy viscosity coefficient; f_c is Coriolis forces due to earth rotation; τ_b and τ_s are bed friction and wind stresses terms and ρ_w is water density.

The oil slick transport in the aquatic environment could be expressed by the following equation.
Where, h_s is the oil slick thickness; Q_s is source/sink term and D_s is the slick spreading function ($D_s = g\,h_s\,((\rho_w/\rho_o-1)/(f\rho_w))$); ρ_o is oil density; f is oil-water interface friction. The oil drifting velocity component v_j ($v_j = u_j + \tau_j/f$) is computed using the shear stresses $\tau_j = 0.03U_j$ due to the wind velocity U_j in x and y directions (Tkalich et al, 2003; Tkalich, 2006). The selected techniques to solve the equations of this model are similar to hydrodynamic model.

The most effective processes of oil weathering in the first days of spillage are evaporation, vertical dispersion, water-in-oil emulsification and dissolution that are mentioned in most oil spills models (Wang *et al.*, 2008; Tkalich, 2006; Nagheeby and Kolahdoozan, 2010). In this study the oil mass losses due to these natural processes are predicted by following:
To estimate the evaporation rate (F_E), the analytical equation of Stiver and Mackay (1984) is used as follows:

$$F_E = \left[\frac{T_E}{BT_G}\right] \times \ln\left[1 + B\left(\frac{T_G}{T_E}\right)\left(\frac{K_E \cdot A_S \cdot t}{V_0}\right)\exp\left(A - \frac{BT_B}{T_E}\right)\right] \quad (4)$$

Where, K_E is mass transfer coefficient, A_s is spilled oil area; V_0 is initial volume of spilled oil, t is time; T_E is environmental temperature (K); T_B is initial boiling point (°K); T_G is the gradient line of T_B and T_E; A and B are constants derived from distillation data.

Tkalich and Chan (2002) proposed the rate of oil input mass into the water column as a function of the rate of droplets separation from the oil and entry into the water column (λ_{ow}) which is heavily dependent on the breaking wave energy and the rate of oil droplets returning to the water surface (λ_{wo}). Their equation is presented as $dM_e/dt = K(\Lambda M_s - M_e)$, where, M_s and M_e are the mass of oil in the slick and the mixing layer, respectively. The dimensionless "Mixing Factor" is defined as $\Lambda = \lambda_{ow}/(B_1\lambda_{wo})$.

$$\lambda_{ow} = \frac{k_b \gamma \omega H}{16\alpha L_{ow}} \quad (5)$$

$$\lambda_{wo} = \frac{w_b(d_m)}{L_{wo}} \quad (6)$$

where, B_1 is the fraction of resurfacing oil, $k_b = 0.3 \sim 0.5$ is the fraction of the energy from the breaking wave that is used for separating the oil droplets from the slick and their entry into the water (Lamarre and Melville, 1991); L_{ow} is the vertical length scale parameter that depends on the kind of breaking wave; $w_b(d_m)$ is the average droplets buoyancy calculating for a droplet with the diameter of $d_m = 0.5d_{ax}$ (Spaulding *et al.*, 1992).
The change in water content is expressed by equation of Mackay et al. (1980) as:

$$\frac{dF_{wc}}{dt} = K_{wc}\left(U_{wind} + 1\right)^2\left(\frac{1-F_{wc}}{OC}\right) \quad (7)$$

Where, F_{wc} is the water content, K_{wc} is the emulsification coefficient that is equal to 2×10^{-6} for light oil and 4.5×10^{-6} for heavy oil, OC is equal to 0.7 for light oil and 1.15 for heavy oil (Rasmusen,1985; Reed *et al.*, 1988).
The proposed equation of Riazi and Edalat (1996) for the rate of dissolution (F_{dis}) is:

$$F_{dis} = 1 - \exp\left(-\left(\frac{K^{dis}}{y}\right)\cdot\left(\frac{C_s}{\rho_m}\right)\cdot t\right) \quad (8)$$

Where, K^{dis} is the mass transfer coefficient; υ is the kinematic viscosity of seawater; D_v is the diffusion coefficient of oil in water and L is the square root of surface area A.
The following equations are applied to predict the oil properties changes due to the weathering processes, specially evaporation and emulsion, in each time step (Mooney 1951; Mackay *et al.*, 1980; Perry 1992):

$$\mu = \mu_{ref}\exp\left(C_{E1}F_E + \frac{C_{wc1}F_{wc}}{(1 - C_{wc2}F_{wc})}\right) \quad (9)$$

$$\rho_o = F_{wc}\rho_w + (1 - F_{wc})(\rho_{ref} + C_{E2}F_E) \quad (10)$$

Where, μ_{ref} and ρ_{ref} is the viscosity and density of fresh oil at reference temperature T_{ref}. The constants C_{E1},

C_{wc1} and C_{wc2} are assigned values by the user based on the general oil type and C_{E2} is an experimental coefficient obtained in laboratory for each oil.

To model the oil pollution distribution in 3D space, the common approach is the basic advection-diffusion equation. This method can be used for all types of scalar quantities spreading in water (Fischer et.al, 1979; Guymer, 1998; Wallis and Manson, 2004; Socolofsky and Jirka, 2005):

where, $C(x,y,z,t)$ is the oil concentration, (u,v,w) are the current velocity components in the x, y and z directions, w_s is the oil droplets buoyancy speed in water, S is the concentration source term and D_h and D_z are the diffusion coefficients in the horizontal and vertical directions. In the present model, the velocity component in the vertical direction is neglected and thus the effective velocity in the vertical direction is only the oil droplets buoyancy speed. Tkalich et al. (2003) and Boufadel et al. (2007) confirmed validity of this equation by using it in the simulation of oil pollution dispersion in water.

In the present model, the effective velocities in the horizontal movement of oil in computational layers are the results of the wind speed (u_w), the current velocity (u_c) and the current due to waves (u_{wave}) which are calculated by the following equation, $u=\alpha_c u_c+\alpha_w u_w+u_{wave}$, where α_c and α_w are the efficacy coefficients of the wind and current velocities in the oil transport in horizontal directions that have the values of 0.03 and 1.10, respectively.

Because of mixing layer formation beneath the oil slick, the vertical boundary condition for the equation (11) is $C(h_w\text{-}Z_{ML}) = C_{ML}$, C_{ML} is the computed concentration of mixing layer. In the present model, it is assumed that the oil droplets don not stick themselves to the suspended sediments in the water column and as a result are not deposited in the sediments of the sea bed. Thus, in the sea bottom, the other vertical boundary condition for the equation (11) is $C(Z_{v0}) = 0.0$.

Tkalich & Chan (2002) showed that a mixing layer of oil and water is formed beneath the oil slick, where the oil concentration is uniform. Also, they suggested that the oil concentration below this layer followed the turbulence advection and diffusion formula. According to studies conducted by Li and Garrett (1998), the thickness of mixing layer is a function of wave height, as $Z_m=\alpha H_s$, where α=1.2~1.6 is a dimensionless scaling factor depending on the sea state. Following the laboratory studies conducted by Delvign and Sweeny (1988), it was suggested that α=1.5±0.35 was suggested. Kantha and Clayson (2004) presented a relationship as Z_m=1.6 H_s.

The buoyancy speed of the oil droplets is a function of their diameter, d_i, seawater viscosity, υ, seawater and oil density. The buoyancy speed of the oil droplets can be obtained using the following equation (Proctor, 1994; Korotenko *et al.*, 2004):

where d_c is the critical diameter of oil droplets calculated by the following formula (Lou *et al.*, 2001):

The buoyancy speed formula has been reached by using Stock law for small oil droplets $d_i < d_c$ and Reynolds law for larger oil droplets $d_i \geq d_c$.
Stokes proposed that forward velocity u_{wave} to transport the mass with free surface wave motion based on single Stoke wave, was calculated as:

where u_{wave} is the net wave current velocity at depth-z below the water surface, is the wave frequency (2π/wave period), k is the wave number (2π/wave length), H_s is the significant wave height and h is the water depth.

$$\frac{\partial C}{\partial t}+\frac{\partial (uC)}{\partial x}+\frac{\partial (vC)}{\partial y}+\frac{\partial ((-w_b)C)}{\partial z}=\frac{\partial}{\partial x}\left(D_h\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_h\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\pm S \tag{11}$$

$$w_b=\begin{cases}\dfrac{gd_i^2(1-\rho_o/\rho_w)}{18\upsilon} & d_i<d_c\\ \sqrt{\dfrac{8}{3}gd_i^2(1-\rho_o/\rho_w)} & d_i\geq d_c\end{cases} \tag{12}$$

$$d_c=\frac{9.52\upsilon^{2/3}}{g^{1/3}(1-\rho_o/\rho_w)} \tag{13}$$

$$u_{wave}=\frac{K\omega H_s^2}{8\sinh^2(Kh)}\cosh(2Kz_0) \tag{14}$$

Determining the diffusion coefficients of oil droplets in the water column, whether in horizontal or vertical direction, have some complexities and considering with previous researches. Johansen (1982) proposed that the vertical diffusion coefficients can be computed by $D_z=0.028(H_s^2/T)e^{-2Kz}$ in z level. Thrope (1984) presented the $D_z = 0.0015U_{wind}$ equation in which the vertical diffusion coefficient is constant and only associated with the measured wind speed 10*m* above the water surface. This equation was used by Reed et al. (1999) for modeling the oil vertical dispersion in the water column. Dick and Schonfeld (1996) stated that the horizontal diffusion coefficient was a function of the grid dimension and its value was determined by $D_h=0.2055\times10^{-3}\Delta x^{1.1}$. This equation was used by Perianez and Pascual-Granged (2008). Elliot et al. (2001); Schonfeld (1995); Dick and Schonfeld (1996) and Elliot (1999) used the vertical diffusion coefficient of 0.001 m^2/s in their studies. Gemmrich and Farmer (1999) proposed the $D_z=2.6\times10^{-5}(U_{wind}^3/g)$ equation for the vertical diffusion coefficient for the turbulence caused by winds which had a constant value at various water depths and was not a function of depth.

To distribute the current velocities, obtained by 2D depth-averaged hydrodynamic model, in different layers of the water column, the logarithmic equation of Van Rijn et al. (1990) has been used which is as follows:

$$u_z = \frac{u}{\left[\frac{z_0}{h} - 1 + \ln\left(\frac{h}{z_0}\right)\right]} \ln\left(\frac{z}{z_0}\right) \qquad (15)$$

where, u_z is the velocity in depth-z, u is the depth-averaged velocity, h is water depth and z_0 is the zero level and normally follows the $z_0/h<<1$.

Moreover, the wind induced current has a velocity equal to 3% of the wind speed at 10*m* above the sea surface. This current velocity would decrease logarithmically and will be zero at the z_1 level. This level is assumed to be equal to 20*m* (Elliott, 1986). The wind induced velocity distribution in the underlying water can be expressed as follows (Pugh, 1987):

$$u_z = \begin{cases} u_0 - \frac{u^*}{\kappa}\ln\left(\frac{z}{z'}\right) & if \quad z < z_1 \\ 0 & if \quad z \geq z_1 \end{cases} \qquad (16)$$

In which the u_0 is the wind induced current velocity, $\kappa = 0.4$ is the Van Karman constant and the z' is the sea surface roughness length which is proposed to have a value about 0.5~1.5 *mm* (Pugh, 1987) and the u^* is the friction velocity which can be calculated by $u^*=0.0012U_{wind}$.

RESULTS & DISCUSSION

The governing equations, the solution techniques and all parameters of 3D numerical model have been described in previous sections. In this section the results of model implementation for a test case study and a hypothetical oil spill in Persian Gulf is considered. To ensure the validity of the 3D advection-diffusion numerical model, a case study with analytical solution has been chosen in that the complete mixing layer formation due to breaking waves has been neglected. Sankaranarayanan et al. (1998) proposed the following equations to compute the real concentration of $C(x,y,z)$ at t time for a pointed pollution source in the (x_c,y_c,z_c) positions in an unlimited field:

$$C(x,y,z,t) = C_x(x,t,u)C_y(y,t,v)C_z(z,t,w) \qquad (17)$$

Where,

$$C_x(x,t,u) = \frac{1}{\sqrt{4\pi K_x t}} \exp\left[-\frac{(x - x_c - ut)}{4D_x t}\right] \qquad (18)$$

$$C_y(y,t,v) = \frac{1}{\sqrt{4\pi K_y t}} \exp\left[-\frac{(y - y_c - vt)}{4D_y t}\right] \qquad (19)$$

$$C_z(z,t,w) = \frac{1}{\sqrt{4\pi K_z t}} \exp\left[-\frac{(z - z_c - wt)}{4D_z t}\right] \qquad (20)$$

In order to compare the results of numerical simulations with analytical solution, some assumptions have been adopted as follows:
(a) The existence of mixing layer in upper layer has been neglected (b) The current velocity in the vertical direction, w, has been replaced by $(-w_b)$, to include the buoyancy velocity. (c) The combination of the wind speed, the tidal current velocities and the current speed due to waves has been used for the velocities in horizontal directions. (d) The vertical diffusion coefficients throughout the water column have been assumed constant.

The case study properties are as follows. A computational domain with 100,000×100,00 m^2 dimensions has been covered by a regular grid with the dimensions of $\Delta x = \Delta y = 5000$ *m*. The horizontal diffusion coefficients and the vertical diffusion coefficients are $D_x = D_y = 2000$ m^2/s and $D_y = 0.01$ m^2/s respectively. Also, the wind speed was 1.0 *m/s* and the time step was 50 *s*. The water column has been divided into 10 layers with the thickness of $\Delta z = 6.5$ *m*. In Figs (2) and (3), the comparisons between the results of numerical model and analytical solution are shown. These Figs are represented as 2D and 3D layouts of the concentration on the layers to a depth of 26 *m* and 52 *m*. Considering the results of the study, it can be

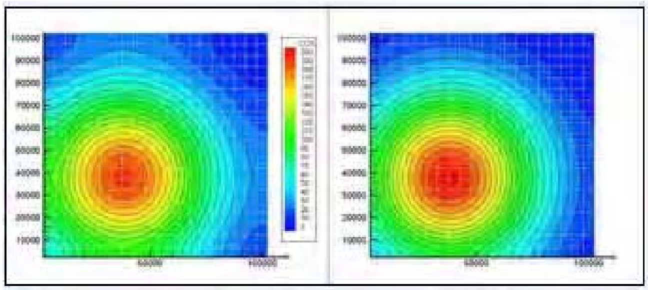

Fig. 2. 2D view of pollution concentration on the layer to a depth of 26 *m*; (a) numerical modeling; (b) analytical solution

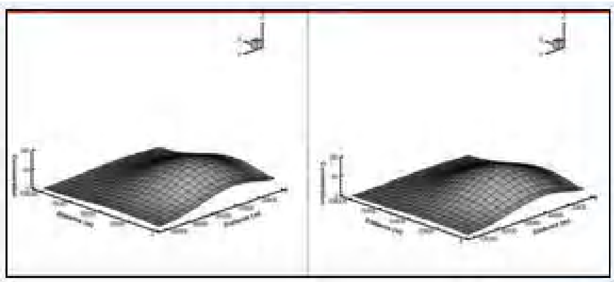

Fig. 3. 3D view of pollution concentration on the layer to a depth of 52 *m*; (a) numerical modeling; (b) analytical solution

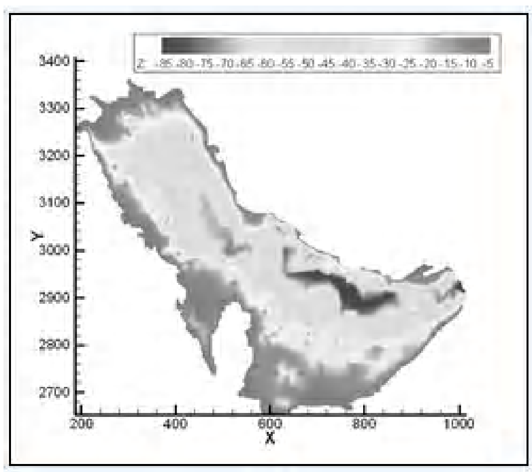

Fig. 4. The Bathymetry of study area

seen that the model is highly capable to simulate the pollutant concentration dispersion in a 3D domain.

A hypothetical instant incident in the Persian Gulf is considered to indicate its capability be used in a real marine environment (Aghajanloo *et al.*, 2013). The model covers the area by a structured rectangular mesh with grid size of ($\Delta x = \Delta y = 2\ km$), including 58417 nodes and 57401 elements. Because of varied range of bed elevation in the Persian Gulf, a high accuracy 3D bathymetry map has been provided (Fig. 4). Table 1 presents the other modelling conditions of this real case.

The current velocities and the Gulf situations have been taken from output of hydrodynamic sub-model (Aghajanloo and Pirooz, 2011). The tidal current in the Gulf is made by imposing tidal fluctuation to the main open boundary at Hengam Island, Hormuz Strait (26°39'N 55°53'E). Required data for water surface fluctuations in certain period of time are available and plotted in Fig. 5 from 2010/01/01 to 2010/10/21. The comparison between predicted results and measured data in Assaluyeh Port, in the northern coastline of the Gulf (27°30'N 52°36'E), is presented in Fig. 6 that shows a good agreement between them.

To simulate an oil spill event, a hypothetical spill of crude oil in a position close to Assaluyeh Port is considered (Aghajanloo *et al.*, 2013). It is assumed that the oil spill is occurred four days after starting the hydrodynamic model. During the next 4 days, the amount of 280 tons of Ahwaz crude oil is released continuously. The chemical and physical properties of Ahwaz crude oil are presented in Table 2.

The environment temperature, wind speed and wind direction are assumed as, 15°C, 5*m/s* and 315°, respectively. Fig.7 shows the slick thickness on the sea surface and its path during the time. The Fig. shows that the wind direction is an effective parameter on slick diversion to the coastline and the sensitive area, as well as tidal currents.

To simulate the 3D distribution of oil, the water body is divided to 10 layers and Figs (8) and (9) presents the oil concentration in different layers. Unfortunately, there is no observed and measured vertical distribution of oil slick for comparison. Nevertheless, the results show the model ability to predict the 3D distribution of spilled oil in marine environment. The improvement of the reliability of environmental information such as wind conditions may be resulted in better results of the numerical model.

Table 1. The modelling conditions of real application, Persian Gulf

Grid size (*m*) (Δx=Δy)	**2000**	**Environment Temperature (°*K*)**	**288**
Simulation time (*day*)	11	Wind Speed (*m/s*)	5
Time step (*sec*)	50	Wind Direction	315°
Released Time (*day*)	4		

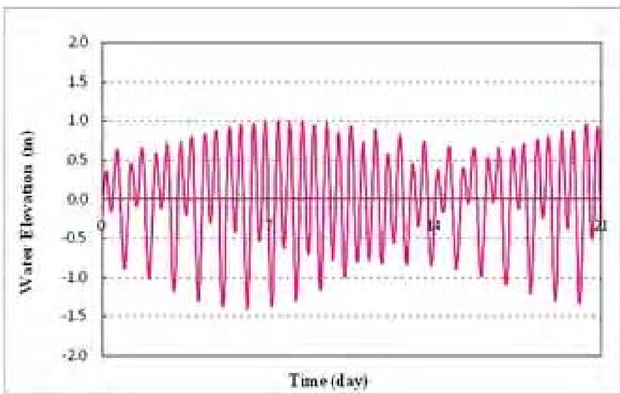

Fig. 5. Measured tidal fluctuation at Hengam Island, Hormuz Strait

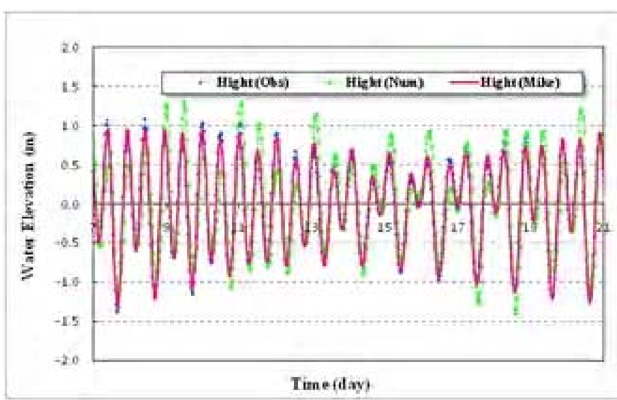

Fig. 6. The water surface elevations comparison at Assaluyeh Port

Table 2. The chemical and physical properties of Kuwait crude oil (ITOPF, 2002)

Specific Gravity	**0.87**	**Pour Point (°*C*)**	**-21**
API	31.31	Viscosity @ 40 °*C* (*cP*)	3.03
Molecular weight (*g/mol*)	210	Solubility @ 25 °C (g/m^3)	2.5
Paraffin Content (%)	63	Aromatic Content (%)	24
Naphthalene Content (%)	20	Sulfur Content (%)	2.4

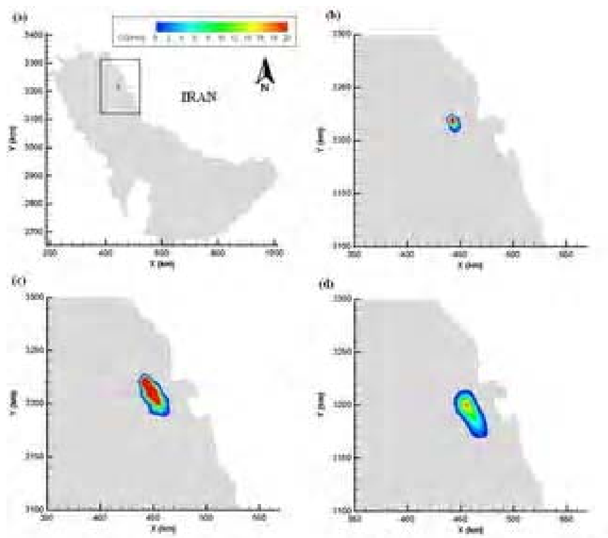

Fig. 7. Distribution of oil simulated in the surface layer (a) initial condition; (b) 12 hours; (c) 3 days; (d) 5 days after spillage

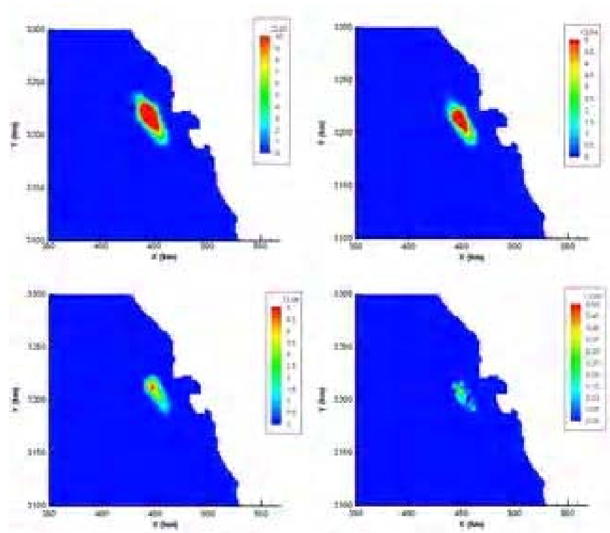

Fig. 8. Oil concentration on different sub-layers in 4days after spillage; (a) 2nd layer; (b) 4th layer; (c) 6th layer; (d) 8th layer

Unfortunately, no observed data for verification of the 3D oil concentration model is the major problem of these numerical models (Wang *et al.*, 2008; Tkalich, 2006; Tkalich *et al.*, 2003). Nevertheless, the results show that it is possible to predict the distribution of the spilled oil slick in the water body using this model. With improvement of reliability of external information, better-simulated results may be achieved.

CONCLUSION

In this work, a 3D mathematical oil spill model has been developed to simulate the oil behavior in the marine environment. This model is based on Eulerian approach and includes several major sub-models including, the hydrodynamic model to simulate the tidal currents; the oil slick movement model to simulate its transport on the sea surface, the oil weathering model to predict the rates of oil losses due to natural processes and the changes of oil properties, the 3D σ-coordinate oil concentration model to simulate the oil dispersion under the sea surface. The detailed characteristics of sub-models were presented in recent works of the authors (Aghajanloo and Pirooz, 2011; Aghajanloo *et al.*, 2011; 2013). The high order solution techniques have been increased the accuracy of predicted parameters. The model verification has been carried out using a computational test case including an analytical solution and the results show the model capability in selected case study. Therefore, the model

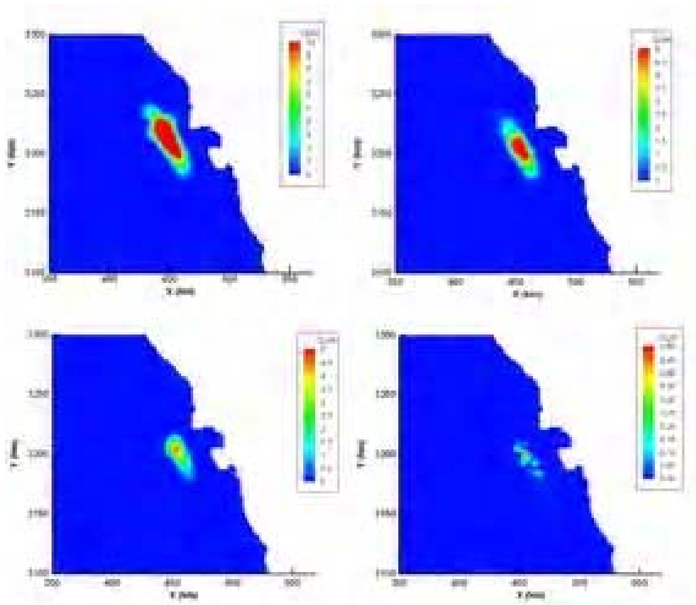

Fig. 9. Oil concentration on different sub-layers in 5days after spillage; (a) 2nd layer; (b) 4th layer; (c) 6th layer; (d) 8th layer

is run for a real marine environment, Persian Gulf and a hypothetical instant is chosen to indicate the model capability in prediction of oil spill behavior in real field. The validation of the model results for spreading and weathering processes was not carried out as there were no observational data to verify. In general, the simulated results show that the model is capable to investigate the oil spill behavior in marine environment.

REFERENCES

Aghajanloo, K., Pirooz, M. D. and Namin, M. M. (2013). Numerical Simulation of Oil Spill Behavior in the Persian Gulf, The Simulation of the Oil Weathering Processes in Marine Environment. Int. J. Environ. Res., **7 (1)**, 81-96.

Aghajanloo, K. and Pirooz, M. D. (2011). The Simulation of the Oil Weathering Processes in Marine Environment. Proceeding of the 4th International Conference on Environmental and Computer Science, ICECS 2011. Singapore.

Aghajanloo, K., Pirooz, M. D. and Namin, M. M. (2011) Numerical Simulation of Tidal Currents in Persian Gulf. Proceeding of International Conference on Civil, Environmental and Chemical Engineering, ICCECE 2011. Bali.

Al-Rabeh, A. H., Lardner, R. W. and Gunay, N., (2000). Gulfspill version 2. 0: a software package for oil spills in the Arabian. Gulf. Environ. Modell. Softw., **15**, 425–442.

Boufadel, M. C., Bechtel, R. D. and Weaver, J. (2006). The Movement of Oil under Non-Breaking Waves, Marine Pollution Bulletine, **52**, 1056-1065.

Boufadel, M. C., Suidan, M. T. and Venosa, A. D. (2007) Tracer Studies in a Laboratory Beach Subjected to Waves, Journal of Environmental Engineering, **133 (7)**, 722.

Chao, X. B., Shankar, N. J. and Wang, S., (2003). Development and Application of Oil Spill Model for Singapore Coastal Waters. J. Hydraul. Eng., **129**, 495–503.

Delvigne, G. A. L. and Sweeney, C. E. (1988). Natural dispersion of oil. Oil and Chemical Pollution, **4,** 281-310.

Dick, S., and Schönfeld, W. (1996). Water Transport and Mixing Times in the North Frisian Wadden Sea – Results of Numerical Investigations, Deutsche Hydrographische Zeitschrift, **48**, 27–48.

Elliott, A. J. (1986). Shear Diffusion and the Spread of Oil in the Surface Layers of the North Sea. German Journal of Hydrography., **39**, 113–137.

Elliott, A. J. (1999). Simulations of Atmospheric Dispersion Following a Spillage of Petroleum at Sea. Spill Science and Technology Bulletin., **5**, 39–50.

Elliott, A.J., Wilkins, B.T. and Mansfield, P., (2001). On the Disposal of Contaminated Milk in Coastal Waters. Marine Pollution Bulletin. **42,** 927–934.

Fischer, H. B., List, E. J., Koh, R., Imberger, J. and Brook, N. H. (1979), Mixing in Inlandand Coastal Waters, Academic Pree.

Gemmrich, J. R. and Farmer, D. M. (1999). Near-Surface Turbulence and Thermal Structure in a Wind-Driven Sea. Journal of Physical Oceanography, **29**, 480–499.

Guymer, I. (1998). Longitudinal Dispersion in Sinuous Channel with Changes in Shapes. Journal of Hydraulic Engineering, ASCE, **124 (1)**, 33–40.

Johansen, Ø., (1982). Dispersion of Oil from Drifting Slicks. Spill Technology Newsletter, 134–149.

Kantha, L.H. and Clayson, C. A. (1994). An Improved Mixed Layer Model for Geophysical Applications. J. Geo. Res., **99**, 25235–25266.

Korotenko, K. A., Mamedov, R. M., Kontar, A. E. and Korotenko, L. (2004). Particle-Tracking Method in the Approach for Prediction of Oil Slick Transport in the Sea: Modelling Oil Pollution Resulting from River Input. J. Marine Sys., **48**, 159–170.

Lamarre, E. and Melville, W. K. (1991). Air Entrainment and Dissipation in Breaking Waves. Nature, **351**, 469–472.

Li, M. and Garrett, C. (1998). The relationship between oil droplet size and upper ocean turbulence, Marine Pollution Bulletin, **36 (12)**, 961-970.

Lou, A. G., Wu, D. X., Wang, X. C. and Xi, P. G. (2001). Establishment of a 3D Model for Oil Spill Prediction. Journal of Ocean University of Qingdao, **31 (4)**, 473–479.

Mackay, D., Mascarenhas, I. B. and Paterson, S. (1980). Oil Spill Processes and Models. Environment Canada Report. EE–8.

Mooney, M. (1951). The viscosity of concentrated solutions of spherical particles. J. Colloid Sci., **6**, 162–167.

Nagheeby, M. and Kolahdoozan, M. (2010). Numerical modeling of two-phase fluid flow and oil slick transport in estuarine water. Int. J. Environ. Sci. Tech., **7 (4)**, 771-784.

Namin, M. M. (2004). A Fully Three-Dimensional Non-Hydrostatic Free Surface Flow Model for Hydro-Environmental Predictions. Phd Thesis. Cardiff University.

Papadimitrakis, J., Psaltaki, M., Christolis, M. and Markatos, N. C. (2006). Simulating the Fate of an Oil Spill Near Coastal Zones: The Case of a Spill (from a Power Plant) at the Greek Island of Lesvos. Environ. Modell. Softw., **21**, 170–177.

Papadimitrakis, I., Psaltaki , M. and Markatos, N. (2011). 3-D oil spill modelling. Natural dispersion and the spreading of oil-water emulsions in the water column, Global NEST Journal, **13 (4)**, 325-338.

Perianez, R., (2005). Gispart: a Numerical Model to Simulate the Dispersion of Contaminants in the Strait of Gibraltar. Environ. Modell. Softw., **20**, 797–802.

Perianez, R. (2007). Chemical and oil spill rapid response modelling in the Strait of Gibraltar–Alboran Sea. Ecol. Model., **207**, 210–222.

Perianez, R. and Pascual-Granged A. (2008). Modelling surface radioactive, chemical and oil spills in the Strait of Gibraltar, Computers & Geosciences, **34**, 163–180.

Perry, C. (1992). Manual del Ingeniero Químico. México: McGraw-Hill.

Pugh, D.T. (1987). Tides, Surges and Mean Sea Level. Wiley, Chichester, UK.

Proctor, R., Elliott, A. J. and Flather, R. A. (1994). Forecast and hindcast simulations of the braer oil spill. Marine Pollution Bulletin, **28**, 219–229.

Rasmusen, D. (1985). Oil spill modeling-a tool for cleanup operations. Proceedings of the 1985 Oil Spill Conference. Washington: American Petroleum Institute, 243-249.

Reed, M., Johansen, O., Brandvik, P., Daling, P., Lewis, A., Fiocco, R., Mackay, D. and Prentki, R.R. (1999). Oil spill modelling towards the close of 20th century: overview of the state of the art. Spill Sci. Technol., **5 (1)**, 3-16.

Reed, M., Kana, T. and Gundlach, E. (1988). Testing and Verification of a Spill Surf Zone Mass Transport Model. Alaska. OCS Region. Minerals Management Service.

Riazi, M.R. and Edalat, M. (1996). Prediction of the rate of oil removal from seawater by evaporation and dissolution. J. Petrol Sci. Eng., **16**, 291-300.

Sankaranarayanan, S., Shankar, N. J. and Cheong, H. F. (1998). Three dimensional finite difference model for transport of conservative pollution, Ocean Engineering, **25**, 425–442.

Schönfeld, W. (1995). Numerical Simulation of the Dispersion of Artificial Radionuclides in the English Channel and the North Sea. J. Mar. Sys., **6**, 529-544.

Shen, H.T. andYapa, P. D. (1988). Oil Slick Transport in Rivers. J. Hydraul. Eng. **114,** 529–543.

Socolofsky, S. A. and Jirka, G. H. (2005). Special topics in mixing and transport processes in the environment. engineering – Lectures. 5th Edition. Coastal and Ocean Engineering Division. Texas A&M University, 184.

Spaulding, M. L., Howlett, E. anderson, E. and Jayko, K. (1992). OILMAP: a global approach to spill modelling. Proceedings of the 15th Arctic and Marine Oil Spill Program Technical Seminar. Environment Canada, 15–21.

Stiver, W. and Mackay, D. (1984). Evaporation rate of spills of hydrocarbons and petroleum mixtures. Environ. Sci. Technol., **18**, 834-840.

Tkalich, P. (2006). A CFD solution of oil spill problems, Environ. Modell. Softw., **21**, 271–282.

Tkalich, P., Huda, K. and Hoong-Gin, K. Y. (2003). A multiphase oil spill model. J. Hydro. Res., **1 (2)**, 115-125.

Tkalich, P. and Chan, E. S. (2002). Vertical mixing of oil droplets by breaking waves, Marine Pollution Bulletin, **44**, 1219–1229.

Thorpe, S. A. (1984). On the determination of K_v in the near surface ocean from acoustic measurements of bubbles. J. Phys. Oceanogr., **14**, 855 – 863.

Van Rijn, L. C. (1986). Mathematical Modeling Suspended Sediment in Nonuniform Flows, J. Hyd. Eng., **112 (6)**, 433-455.

Wallis, S. and Manson, J. (2004). Methods for predicting dispersion coefficients in rivers. Proceedings of the Institution of Civil Engineers. Water Management, **157**, 131-141.

Wang, S. D., Shen, Y. M. and Zheng, Y. H. (2005). Two-dimensional numerical simulation for transport and fate of oil spills in seas. Ocean Eng., **32**, 1556–1571.

Wang, S. D., Shen, Y. M., Guob, Y. K. and Tanga, J. (2008). Three-dimensional numerical simulation for transport of oil spills in seas. Ocean Eng., **35**, 503–510.

Wang, S. D. and Shen, Y. M. (2010). Modeling oil spills transportation in seas based on unstructured grid, finite volume, wave ocean model, Ocean Modeling, **35 (4)**, 332–344.

Yapa, P. D., Shen, H. T. and Angammana, K. S. (1994). Modeling oil-spills in a river lake system. J. Mar. Syst., **4**, 453–471.