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Biodegradation: Study of Modelling and Simulative of Oil Spill in Marine

Engineering

KEYWORDS : Oil transformation, Evaporation, Emulsification, Ordinary differential equation and Polymath

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ABSTRACT

Complex biochemical processes of oil transformation in the marine environment start developing from the first hour of oil's relationship with sea water. The main characteristics of oil change are their magnetism at the first step and direct interaction of physical, chemical and biological disappearance of dispersion. In this paper evaporation, emulsification, dispersion into the water column and changes in viscosity, density model discussed for physiochemical processes that occur after oil spill. These processes are interdependent on each other and coupled ordinary differential equations (ODE) formed, solved using polymath software. The results predicted by computer simulation, were quite well for emulsification, evaporation and viscosity seems to be consistent under normal atmosphere.

Introduction:

Oil spills pose serious threats to environmental and ecological approach. Today's population becomes more and more dependent on petroleum and its products. Obvious the necessity, of using super-tankers to ship crude oils is clearly going to keep increasing. As emergency events, oil spills do not provide ideal conditions for experimentation and hypothesis testing. Clean up is properly more interested in mediating the environmental damage from the oil then in providing resources and information to on-scene scientists. The oil spill modeling data from laboratories and pilot spills are smaller in magnitudes than actual accidental spills. Previous studies revels that algorithm used in spill models are often quite straightforward and try to catch only the combined behavior of the oil slick, ignoring finer scale processes. The transport and fate of spilled oil in sea water control by physio-chemical and bio-chemical processes. This process divided into diffusion, surface spreading, evaporation, emulsification, photo-oxidation and biodegradation. The fraction of the oil is change from the time of spill interact with water. Light fraction evaporate from surface interaction while water soluble components dissolve in the water and immiscible components become emulsified and dispersed in the use of small droplets. The formation of oil - water emulsion depends upon the behavior of waves in marine. In some cases, the oil droplets interact to sediments particles of the river and eventually set on the sea bed for slow bacterial degradation process.

Literature Review:

There have been several review papers summarizing the extensive literature on oil spill modeling. Many spill models assume an empirically based wind and wave induced component for the drift of a slick. Elliot (2000) uses a random walk technique in the vertical as well as the horizontal direction and suggests that the angle between the wind and wind driven component of drift is small, effectively zero. Sebastiao (1995) proposed a numerical model for the simulation of the physiochemical weathering of an oil spill at sea as a result of the coupled action of the oil drop entrainment mechanism as it relates to the position of numerous individual particles. Spaulding (1996) reported an integrated environment monitoring and modeling system called COASTMAP linked with OILMAP to provide a fully operational, real time system that allows prediction of circulation, winds and oil trajectory for estuarine and costal sea areas .Riazi (1999) presented a semi analytical model to estimate the amount of oil disappeared from an oil spill floating on seawater surface. The model estimates area, volume and composition of oil spill versus time.

Buranapratheprat (2008) suggests that the movement of oil in the sea surface comes from several forces and the trajectory is dominantly directed net force in that position and time. The model takes into account the affect of stokes drift and tidal current along with some background current. Varlamov (2000) developed an oil spill model applicable to the simulation of initial stages of oil spill evolution processes, taking into consideration the fact that mainly physical and chemical processes immediately following the spill regulate the oil weathering. Korotenko (2001) developed a 3D hybrid flow model to predict the dispersal of oil pollution in coastal waters. The transport module of the model takes predetermined current and turbulent diffusivities. Gin (2001) developed an oil spill-food chain model to assess the probable impacts of oil spill on several key marine organisms. The model gives temporal and spatial estimates of concentration of hydrocarbons accumulated by marine organisms. Fay (2002) presented a comprehensive model for predicting the dynamics of spill from LNG and oil product tankers. They reported the spill volume, discharge rate and duration are significant determinants of spill behavior. Brenner discussed modelling and simulation of the oxygen-sag model and demonstrate the potential benefits of the application of user friendly numerical software packages in environmental engineering education and practice. The simulation is used to obtain the profiles of oxygen concentration, oxygen deficit, as well as de-oxygenation and re-oxygenation rates as function of distance for a steady river velocity. Simulations are carried out for various organic loads and ambient temperatures.

Modeling for fate of Oil Spill

Mathematical modeling for fate of oil spill depends up on spreading mechanism, evaporation, emulsification, dispersion of crude oil.

1. Spreading Mechanism: When oil intact with waters it quickly reaches the water temperature. The spreading of oil shall take place only if the pour point of crude oil is less than the ambient sea water temperature. Crude oils with high wax content will have a high pour point and those materials will solidify either immediately or shortly after the spillage. The spreading model realized to be in three phases each determined by the dominant spreading and retarding forces involved. The first phase is the gravity inertial spreading which lasts for few minutes except for large spills. The third phase the tension, viscous phase occurs when the slick may be dispersed or broken into separate slicks. The second phase in which gravity viscous spreading considered mainly for the simulation of spreading. On the basis, of gravity and viscous formulation the rate of change of surface area for oil spill models that have many variables changing simultaneously. The rate of spreading calculated by

$$\frac{dA}{dt} = K_1 \ A^{1/3}[V/A]^{4/3} \tag{1.1}$$

2. Evaporation: It is primary initial process that is involved in the removal of oil from sea. The rate of evaporation contro by the physio-chemical properties of the oil and increases with spreading, high water temperature, strong winds and rough weather conditions. The loss of light fractions of the crude through evaporation results in increased density and viscosity

while the volume of spill decreases. Commonly two methods are use to determine the evaporation rate the pseudo components approach and the analytical approach .But here dimensionless termed (E) as fraction evaporated used.

$$F_E = 1/_C * [\ln P + \ln C * Ke * t + 1/P] \quad (2.1)$$

The initial vapor pressure P in atmosphere at the temperature T is calculated as $\ln P = 10.6 * (1 - T/T1)$ (2.2)

For a crude oils $C = 1158.9 * API^{-1.1435}$ (2.3)

$$T = 542.6 - 30.275 * API + 1.565 * API^2 - 0.03439 * API^3 + 0.00026 * API^4 \quad (2.4)$$

The oil loss due to evaporation measured in term of volume decrease expressed as:

$$V(t) = V_0 - \Delta F_E * V_0 \quad (2.5)$$

$$\frac{dv}{dt} = -v_0 * \frac{dF_E}{dt} \quad (2.6)$$

3 Emulsification: It involves the dispersion of water droplets into the oil medium. It generally is affected by the amount of surfactant present in the spilled oil. The ability of crude oil to form emulsion is related to the level of asphaltenes in the oil and the stability of emulsion is related to the presence of wax crystals. The emulsification results in a large increase in volume, significant increase in the density and very large increase in viscosity.

$$Y = C_3 * [1 - e^{-2*10^{-6}} (1+w)^2 * t/C_3] \quad (3.1)$$

Mousse formation leads to an increase in viscosity which can be calculated by the Mooney Equation:

$$\mu = \mu_0 * e^{[2.5*\frac{Y}{1-C_3*Y}]} \quad (3.2)$$

$$\mu_0 = 224 * \sqrt{Q} \quad (3.3)$$

Evaporation also leads to increase in viscosity which can be obtained from

$$\mu = \mu_0 * e^{[C_4 * F_E]} \quad (3.4)$$

4. Dispersion of crude oil: It occurs through formation of oil droplets which go into the water column. Evaporation and rate of natural dispersion largely determine the life of an oil slick on the sea surface. Natural dispersion reduces the volume at the surface and reduces the evaporation loss, but does not lead to any changes in the physiochemical property of the spilled oil. Natural dispersion is the result of three separate process, the initial process of globulation where oil droplets are formed from the lick as a result of breaking waves, the process of dispersion where the oil droplets are transported into the water column due to the energy supplied by the breaking waves and rising forces, and the process of coalescence of the oil droplets with the slick. The fraction of oil dispersed or entrained in the water column is calculated as a lost fraction of the sea surface oil per hour given by

$$D = D_a * D_b \quad (4.1)$$

$$D_a = 0.11(W+1)^2 \quad (4.2)$$

$$D_b = (1 + 50 * \mu^{0.5} * \delta * s_T)^{-1} \quad (4.3)$$

5. Formulation of mathematical model for the fate of oil spill: When oil spill does occur at the sea the various process as mentioned above happen simultaneously. These variables depend on each other and can be described by a set of differential equations that can be solved by numerical software polymath. The model considers the fate of the surface oil and does not consider the dispersion aspects. The effect of wind and currents in the advection of the slick is also not taken into account.

Equation (2.1) is incorporated in differential form as eqn (5.1) and eqn (1) is used as it is. Equation (3.1) is also incorporated in differential form to give eqn (5.3). The volume of oil spill found in equation (5.4) by combination eqn (2.5) & eqn (2.6) using limit $\Delta t \to 0$. The viscosity equation is obtained by adding the eqn (2.5) and eqn (2.6) which give change in viscosity due to mousse formation and evaporation loss to the environment. This is given by equation (5.5). Hence five ordinary differential equations able to describe the system:

$$\frac{dF_E}{dt} = K_E * e^{[10.6(1-\frac{T}{T_1}) - F_E * C]} \quad (5.1)$$

$$\frac{dA}{dt} = K_1 A^{1/3} [V/A]^{4/3} \quad (5.2)$$

$$\frac{dY}{dt} = 2.0 * 10^{-6} (W+1)^2 * (1 - Y/C_3) \quad (5.3)$$

$$\frac{dv}{dt} = -v_0 * \frac{dF_E}{dt} - D * V \quad (5.4)$$

$$\frac{d\mu}{dt} = C_4 * \mu * \frac{dF_E}{dt} + \frac{2.5*\mu}{(1-C_3*Y)^2} * \frac{dY}{dt} \quad (5.5)$$

Results & Discussion: Following the ODE representing in the previous section for the various processes of the fate of oil spill. It can be coded and tested using a mathematical software package Polymath that requires very little technical coding effort. After testing each of the modules separately, they are combined into one program using a mathematical software package.

Table 1: POLYMATH Model for the fate of oil spill

No.	Equation # Comment
1.	d(Fe)/d(t) = Ke* K1 # Fraction evaporated
2.	d(A)/d(t) = K1*A^(0.3) *V^(1.34) # Spreading of Oil spill in water
3.	d(Y)/d(t) = 2*10^(-6)*(W+1)^2*(1-Y/C3) # Fractional water content
4.	d(V)/d(t) = -V0*Ke*K1-D*V # Loss of Volume for oil spill
5.	d(u)/d(t) = C4*u*Ke*K1+2.5*u/1-C3*Y*2.0*10^(-6)*(W+1)^2*(1-Y/C3) # Viscosity of oil spill
6.	K1=exp((10.6*(1-T/T1))-(Fe*C)) # Auxiliary eqn of No.1
7.	T = 542.6-30.275*API+1.565*API^2-0.03439*API^3 # Initial boiling temperature (K)
8.	C = 1158.9*API^(-1.1435) # Auxiliary eqn of No.1
9.	D = Da*Db # Spill diameter (m)
10.	Da = 0.11*(W+1)^2 # Fraction of sea surface oil dispersed per hour
11.	Db = (1+50*u^0.5*p*st)^(-1) # Faction of dispersed oil not returning to surface
12.	API = 32 # Crude oil of depend the source of reservoir
13.	T1 = 295 # Ambient temperature (K)
14.	W # Wind speed (m/s)
15.	C3 = 0.7 # Crude oils and heavy fuels.
16.	C4 # values oil varies between 1 and 10 depends upon source
17.	V # Volume of spill (m3)
18.	p # Slick thickness(cm)
19.	st # Oil water interracial tension (dyne/cm-1)
20.	K1 # Constant with default value of 150s-1
21.	Q# Asphaltenes Content (%)

1 Evaporation: To simulate the effect of API, the basic equation of evaporation was solved using three values of (32,33 and 34 depend upon the source of crude oil) for the same data presented in fig. 1. This resulted in the solution of the problem for three different API values of 0.42 to 0.61. This simulation represents the same ambient & initial boiling temperature and mass transfer coefficient that API of crude oil may the preliminary parameter to study the evaporation. POLYMATH graphical output given in Figure 1 shows fraction evaporated curves (as a function of time) for the three different crude oils, where the fraction evaporated increases with the increase of API. Initially amount of fraction evaporated increase exponentially (auxiliary eqn 1 in table 1) later it become linear and does not change with the change its symmetry. It shows API produces the dominant effect at an initial stage of evaporation, at end of evaporation process amount of evaporation become constant.

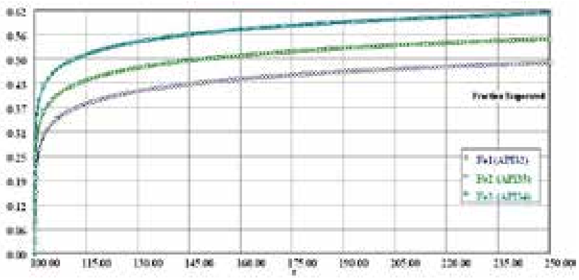

Figure1: Fraction Evaporated: Simulation result of Fraction of oil evaporated API 32, 33 & API 34. The horizontal axis is fraction of oil evaporated as function of time on vertical axis

2. Emulsification: Wind speed is a very important parameter to determine the fate of oil spill in water that involves physiochemical processes especially in emulsification. This is a basic parameter (eqn 3 in Table1) demonstrating how the rates of the change fractional water content with wind speed. This information is shown clearly in Figure. 2, which demonstrates the higher wind speed, higher the fractional water content. For simulate the effect of wind speed , the basic equation as mentioned in Table 1 was solved using four values of (3,4,5 and 6 m/s) depend upon the marine conditions. The result shows an initial exponential increase of the fractional water content (Y) and also an increase with respect to time (t). At the saturation point, the wind speed effect become constant as shown in fig.2. The saturation values reaches up to 0.62 at wind speed 6m/s.

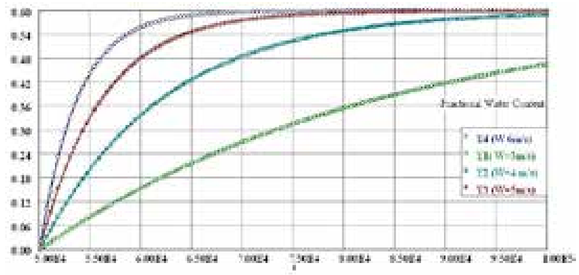

Figure 2: Fractional Water Content: Simulated result of Fractional water content for different wind speed. The horizontal axis is fractional water content having different wind velocities in ocean as function of time on vertical axis

3. Viscosity: It is crucial parameter to analyze the fate of oil spill, because evaporation affects the viscosity as mentioned by Mousse and Mooney (eqn 3.2 & 3.4). Viscosity (u) model equation (eqn 5 in Table1) has dependency on Fe and Y parameters. The combined effect of evaporation and emulsification on viscosity results in a significant change in viscosity in the oil spill. Viscosity profile (as a function of time) using the same data presented in Figure 3. This figure demonstrates

nicely the significant decrease of the viscosity of oil spill caused by the increase of time. The changes caused in viscosity during the warmer months of the summer can be simulated. The negative values of viscosity in fig 3 reflect the decrease in viscosity with time, while fractional water content for given data remains the same.

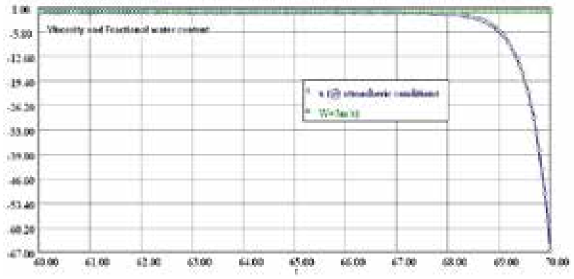

Figure 3: Fractional Water Content & Viscosity: Simulated results of Fractional water content and viscosity at constant wind speed (3m/s). The horizontal axis is fractional water content and viscosity as function of time on vertical axis

Conclusion: The plots for the evaporative and water content curve show good model predictions, but the initial rate of water incorporation, variation in environment conditions, particularly wind speed deviates the simulated result from experimental result. In case of viscosity, a fair agreement was found between the model and the experimental data but an overestimation is predicted during most of the spill. This is probably due to the viscosity equation which includes the effect of both evaporation and emulsification in the calculation for viscosity. Hence it can be concluded that the algorithm produces satisfactory results although more experimental data are still needed for a better validation.

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