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<th>DEVELOPMENT AND APPLICATION OF THE ENVIRONMENTAL HYDRODYNAMIC 3D MODEL FOR COMPUTATION AND FORECASTING OF OIL POLLUTIONS IN COASTAL MARINE ENVIRONMENT</th>
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Abstract:
Oil spill in the marine environment has been simulated as multiphase: oil slick thickness on the water surface, dissolved, emulsified and particulate in the water column and in the bottom sediment. The three-dimensional hydro-environmental model could simulate full advection and dispersion processes of all these oil phases in the realistic marine conditions. The hydro-environmental sub-model provides temperature, salinity and current structure, water level, and suspended matter concentration. These variables will be used in the oil pollution sub-model simulating the advection and diffusion processes for all oil spill phases in the water and bottom sediment. This sub-model includes two-dimensional (2D) model for surface oil slick, dissolved and particulate oil in the bottom sediment and three-dimensional (3D) model for the dissolved, emulsified and particulate in the water column.

Preliminary result for the surface oil spill shows that the model could be used to simulate and predict the spreading of oil spilled on the sea and to evaluate the potential damages to marine environment, including application of the oil combating elements, such as chemical dispersants and booms.

Keywords: Coastal marine environment, Environmental hydrodynamic 3D model, Oil pollution

1. Introduction
The present of oil in the sea is mainly due the results of accidents in the sea. The computation and forecasting and the displacement of oil in the sea environment are very difficult due to the different phases of oil: oil slick, dissolved oil, emulsions, particulate oil in water and bottom sediment. The previous models for oil slick are built on the basis of applying the semi-impirical formulas, developing integrated with the marine dynamic models. In practice, the Euler approach is traditional in hydrodynamics and the Lagrange approach is used in studying the oil slick spreading trajectories.

In the future, the Euler approach will become more and more popular due to the demand of combining the dynamic equations of polluted substances transportation with the thermal hydrodynamic model. Using of similar techniques as in thermo-hydrodynamics allows us to enhance the modeling capability of water qualities as well as the precision of the environment studies in general. The integration of the dynamic principles and the experimental data opens up the possibility of application of the model to several marine environment problems.

Based on the study of the dynamic principles of interactions of oil phases and the environment compound, we can build the dynamic model of oil compound as well as the marine environment.

2. The dynamical relations between the oil phases in the marine environment.
As presented above, there are four phases in the marine environment: oil slick, emulsion, particulate and dissolved oil. Among those, the oil slick only exists on the sea surface and the there remaining phases exist in the water column. In the sediment, there are only two phases: the dissolved and particulate oil (Fig. 1)
The transportation and degradation of oil in the environment are governed by the physical, chemical and biological processes. It also depends on the properties of the oil and the hydrodynamical, meteorological, and environmental conditions. These processes include: advection, turbulent diffusion, spreading, evaporation, dissolution, emulsification, hydrolysis, oxidation, biodegradation, and sedimentation [6,8].

When the oil spill begins over the sea, it spreads to make a thin oil slick. The transportation of the oil slick depends mainly on the advection and turbulent diffusion by the wind and currents. In this dispersion process, the oil slick also changes its form. The lighter oils tend to evaporate, the dissolvable oils blend into water, the under-water oils will be emulsified and transported as oil droplets. The emulsification or water-in-oil process depend on turbulences and often appears a couple of days after the oil spill. They tend to form several thin films and will be very sticky when transferred to the shoreline. As time goes by these thin films will stick together to form a thick mousse. The heavier oils can combine with the suspended sediment and go down to the bottom and be biodegraded by the bacteria. The oil slick and particles have relatively small contact area compare to their volume therefore their degradation process is quite slow.

3. Dynamics of the transformation and displacement processes of the oil phases in marine environment.

The dynamics of the oil phases is established based on the principle of matter transformation as well as the diffusion advection process and matter transformation process.

In the static condition, the amount of oils on the sea is correlative to the thickness of the oil slick. The change in the thickness of the oil slick is influenced by three processes: evaporation, emulsification, dissolution into the under water. The speed of the emulsification and dissolution processes depend on the concentration of the oil phases $C_e$ and $C_d$ respectively, and the thickness of the mixed layer $z_m$. The transformation ability of the oil phases depends on the density of the oil slick $\rho_o$ and the saturation concentration of the lighter oil $C^*$. All these processes will lead to the decreasing of the amount of oil and the thickness of the oil slick and there exists no reverse dynamical process.

This leads to a result: for the marine environment under the oil slick, there is an incoming source of oils which exhibits in the corresponding increasing.

At the same time, from the water environment there will be an exchange flux of oils to the bottom sediment,
the direction of this flux depends on the difference between the concentration of the dissolved and particulate oils in the water \((C_d, C_p)\) and in the bed sediment \((C_{db}, C_{pb})\) respectively.

The transformation of the oil phases mainly happen in the water and bottom sediment.

All the oils, water layer in the emulsion (water-in-oil or oil-in-water) and dissolved oils have the tendency to transform into particulate due to the present of the suspended matters in the water. This process depends on the difference in concentration of the oil phases and the concentration of the suspended matters \(S_w\), where the suspended matters can be of natural or artificial origin due to using the oil dispersant substances.

Therefore this transformation process is the same as a source of making particulate oils in water.

A similar process can be applied to two main oil phases in the bottom sediment which are particulate oils and dissolved oils.

This means that certain amount of dissolved oils will be transformed into particulate oils.

In the natural condition of sea environment with the present of the dynamical phenomenons such as wave, current, advection, convection and dispersion will play a crucial role to the transformation rules as well as the distribution displacement of oils in the oil slick, water column, bottom and shoreline sediment.

4. Mathematical model for oil displacement in sea environment

Since the transformation, advection and diffusion of oils in each environment are different, we need to build a system of models for each environment which related to each other through the boundary conditions. In this case we can introduce the system of models for oil slick, oil-in-water environment and bottom sediment.

a. Model for oil slick on sea surface

Though there are many formulas, we can use the equation of thickness variation of oil slick based on the generalization of the diffusion advection process and the exchange process between oil slick and air, and water through the evaporation of lighter oils and the emulsification as well as the dissolution of the heavier oils.

\[
\frac{\partial h}{\partial t} + \nabla (h \nabla) - \nabla (D \nabla h) = Q
\]

(1)

This equation is constructed based on the principle of conservation of mass for the moving oil slick [4,6]. The loss rate due to evaporation, emulsification and dissolution in water \((Q)\) is expressed in the function:

\[
Q = -k_v h - k_{ev} (a_{ev} \rho_o - C_o) \frac{Z_m}{\rho_o} - k_{dv} (a_{dv} C_o - C_d) \frac{Z_m}{\rho_o}
\]

(2)

In equation 1, the diffusion advection process only happen on the horizontal direction and are described through the operator: \(\nabla = \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j}\).

The velocity in the advection factor consists of two components: the general regular current and the wind-driven current. Where the wind-driven current can be computed according to the wind speed with the coefficient approximately 3%:

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There are many ways to evaluate the horizontal diffusion coefficient \( D \), however we choose the following \([5]\):

\[
D = \frac{\rho f h}{\rho_f} \tag{4}
\]

where \( f \) is the friction coefficient between oil slick and surface water.

Therefore the model for thickness variation of the oil slick can be solved through the impact of wind field and current on the sea surface.

This is a 2D model with the initial condition of the oil slick is given by the thickness \( h \). In addition to the boundary condition for the oil slick at the shoreline and sea open boundaries, the model requiired the concentration of oil emulsion \( C_e \) and oil dissolution \( C_d \) in the water layer which contact with the oil slick. This are the conditions associated to the model of oil in water environment.

**b. Model for oils in the water environment (whole water column)**

For the whole water column, the 3D model of the marine environmental components \([1-3]\) which apply for three different oil phases related to each other by the laws of dynamics and diffusion-advection:

\[
\frac{\partial C_i}{\partial t} + \nabla (C_i \vec{v}_i) - \nabla (D_i \nabla C_i) = Q_i \tag{5}
\]

with:

\[
\vec{v}_i = \frac{\partial}{\partial x} \vec{v} + \frac{\partial}{\partial y} \vec{F} + \frac{\partial}{\partial z} k \quad \vec{v}_i = \vec{v}_e + w_i k; \quad i = e, d, p
\]

Where the velocity \( (\vec{v}_i) \) consists of the current velocity \( (\vec{v}_e) \) and the setting velocity \( (w_i) \) of the corresponding oil phases. \( D_i \) is the diffusion coefficient of the oil phases in water environment. The oil concentration variables \( C_e \) and \( C_d \) are measured in \( g\text{-oil}/m^3 \) and the variable \( C_p \) is measured in \( g\text{-oil/kg-sediment} \).

According to the law of dynamical transformation, the production and destruction of each phases are specified by the corresponding expression:

\[
Q_e = -k_e S_w \left( a_e C_e - C_p \right) \tag{6}
\]

\[
Q_d = -k_d S_w \left( a_d C_d - C_p \right) \tag{7}
\]

\[
Q_p = k_e \left( a_e C_e - C_p \right) + k_d \left( a_d C_d - C_p \right) \tag{8}
\]

So we obtain a set of equations for the oil models in the system of 3D thermo-hydrodynamical environmental models MDEC which have been previously developed and applied.

A similar equation for the suspended matters is also combined with the equations of oil phases to allow us solve all the water environment variables.

To implement this model, an important problem is to deal with the boundary conditions in the water.
environment.

As explained above, on the interface between water and oil slick, the flux of emulsion oil going into water depends on the amount of present emulsion $C_e$.

$$ FLS_e = k_e \left( a_e \rho_o - C_e \right). \quad (9) $$

The flux of dissolution oil depends on the correlation between present concentration and saturation concentration of the lighter oil phase.

$$ FLS_d = k_d \left( a_d C_r - C_d \right). \quad (10) $$

For the interface between water and sediment, the exchange oil flux depends on the difference between the concentration of oils in sediment and the near-bottom water layer.

$$ FLB_d = -k_d \left( a_d C_d - C_d \right), \quad (11) $$

$$ FLB_p = -k_p \left( a_p C_p - C_p \right). \quad (12) $$

This is also the relation between model of oils in water environment and in the bottom sediment.

c. Model of oils in the bottom sediment

We assume that the bottom sediment layer which contains the oil phases is not significant, so their concentration can be taken as the average of the thickness of the surface sediment $(b)$. So we can build the model of oil in the sediment with the laws of dynamical transformation mainly between dissolved oil and particulate oil. The horizontal advection and diffusion process will play a key role so this is a 2D model:

$$ \frac{\partial C_{sb}}{\partial t} + \nabla (C_{sb} v_{ib}) - \nabla (D_{sb} \nabla C_{sb}) = Q_{sb} \quad (13) $$

In this model, the velocity of the bed sediment can be specified through the bed flux or dynamic velocity $v_{ib}$.

The production and destruction rates get from the transformation and exchange flux through the water-sediment interface:

$$ Q_{sb} = -k'_{d} \rho_s \left( a'_{d} C_{sb} - C_{pb} \right) - k_{d} \left( a_{sb} C_{sb} - C_{d} \right) \frac{z_b}{b}, \quad (14) $$

$$ Q_{pb} = k'_{d} \left( a'_{d} C_{sb} - C_{pb} \right) - k_{pb} \left( a_{pb} C_{pb} - C_{r} \right) \frac{S_w z_b}{\rho_s (1 - \phi) b}. \quad (15) $$

Where $S_w$ is the concentration of suspended sediment in the water and $\phi$ is the spongyness of the bed sediment.

In these formulas, the concentration $C_{sb}$ is measured in $g$-oil/m$^3$ and $C_{pb}$ is measured in g-oil/kg-sediment. In using formulae (14), (15), we assume that the oil exchange process between water and bed only happens in the active boundary layers include the lower boundary of water $Z_b$ and the upper boundary of sediment $b$.

So we obtain a system of three models for the oil slick, oil in water column and in the bottom sediment environments. Since these models are related to each other through the boundary conditions, we can solve independently when these conditions are given.
The thermo-hydrodynamical model MDEC will provide the hydrodynamical factors such as current, wave, water density, bottom stress for the implementation of the models. By combining all 4 models, we can give an apprehensive solution to the oil spreading problem in marine environment and create a environmental-ecological model which can fulfill the forecasting, impact assessment and oil spill recovery task.

5. The method for implement of the combining model between hydrodynamics and oil spreading in the coastal marine environment.

It is well-known that, the construction and development of the 3D marine hydrodynamic models allow us to discribe, in a quite accuracy way, the current, temperature, salinity fields and other environmental components for the whole water layer. So the system of models should be based on the 3D thermal hydrodynamical models with model for each particular environment that contains oils.

The marine thermo-hydrodynamical models can provide the characteristics for the 2D model of oil slick on sea surface (1). Since the evaporation process only happens to the lighter oils, so the evaporation coefficient is chosen to guarantee that the evaporation process will end in the right moment. As the emulsification only happens after certain time, the oil-emulsion exchange coefficient will be parameterized as a function of time. The thickness of the mixed layer will be chosen in the experimental process. The system combining the concentration of dissolved oils and emulsion in water is the result of the implementation of the 3D model for oils in the water environment.

The 3D model for oils in water environment is implemented for the scalar variables \( C_e, C_d \) and \( C_p \) as in the 3D model of the environmental components in the 3D model of MDEC. As the dynamical process of oil phase transformation depends on the concentration of suspended matters, in the implementation steps, in addition to the environmental variables above we need to supplement other variables. The surface boundary conditions for the oil phases are only applied for the areas that have oil flicks on the surface. For the combining model using the oil concentration in the bottom, the boundary conditions will be obtained by carrying out model for oils in the bottom sediment.

The 2D model will be constructed and implemented in order to compute the horizontal distribution of two oil phases: dissolved oils and emulsion in the bottom sediment.

So in addition to the combining thermo-hydrodynamical model for oil phases applied to whole water column which provides the three dimensional distribution of the environmental factors, oil concentrations, the 2D models for oil slick and oils in the bottom sediment give us the wide horizontal distribution of the thickness of oil slicks on sea surface and oil concentration in sea bed. This approach has been developed and implemented in the problem of suspended and bed load sediment transport.

6. The results of the implementation of the model

The system of the MDEC model had been applied to simulate the hydrodynamical, suspended matter and environmental components included oil in the Hai Phong esuary and coastal area. As in the case for Halong Bay, the simulated fields of the water circulation and water level show mostly well for as very commplicated coastal and estuarine condition as combined river- air-sea interaction. Fig. 2 show the the total surface water circulation filed for two different wind condition according monsoon in the case study region.
For the oil sub-model, the testing of the model is carried out by using the parameters which originated in the work of Tkalich and ctv [3]. The obtained results for the spreading of oil slick show that the model has been successfully simulate in time and shape of the oil spill as in the classical models as well as in reality [5]. Fig.3 shows the positions of the oil slick after 6, 12, 18 and 30 hours in the case of SE wind for the source of oil spill in the region between Doson and Cathai. In this case the oil slick is transformed in shape for the ellipse on the wide, offshore region to the strip shape in the nearshore region.

In the case of NE wind, the oil slick is quickly approached the Doson-Haiphong shoreline, where there is strong nearshore current (Fig.4).
Fig. 4. Distributions of the thickness of oil slick on sea surface after 6(a), 12(b), 24(c) and 30(d) hours in the NE wind.

For the oil phases in the water environment, though the concentrations of each component are different, the distribution regions of them have similar shape and the result is the gathering of oils in the Cat Hai area and the Bach Dang estuary. Fig. 5. shows the diagrams of the distribution of particulate concentration in water at depth of 0.5 m and similarly for oil slick in the SE wind field at 06, 24 hours.

Fig 5. Distribution of concentration particulate in water (depth 0.5m) after 6(a), 24(b), hours in the SE direction wind.

In the case of NE wind, the oils also had the tendency to approach the Hai Phong-Do Son shoreline and extend the affected area in the East-West direction (Fig. 6.)

Fig 6. Distribution of concentration of particulate oils in water (depth 0.5m) after 6(a), 24(b) hours in the NE wind.

The amount of oils particulate in the bottom sediment increases as time goes by and the position has relatively small variation compare to oils in water and oil slick (Fig. 7.)
7. Conclusion

The preliminary results for the combined system of 2D, 3D environmental, hydrodynamical, for the hypothetical case of oil spill at sea show the ability to forecast a comprehensive impact of the oil phases to the sea and nearshore environment in the natural weathering condition as well as using the oil dispersant materials. By making more comprehensive experimental tests for several oil spill cases, this system of models can be developed and applied, together with the recovery strategies, for the case of oil pollution sources in water or sea bed. This system of models also allow to integrate with models of ecological components and water quality therefore open up the applications in monitoring and forecasting coastal and marine environment.

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