RESEARCH PAPER

Optimization modeling of degradation processes in crude oil spilled on the sea surface considering the wind conditions

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ABSTRACT

The article describes an optimization model study of degradation processes in crude oil spilled on the sea surface considering the wind conditions. A new configuration of a simplified optimization model of the oil degradation process on the sea surface is proposed. Based on the proposed configuration, a simplified optimization model of oil degradation on the sea surface has been developed. The optimal relationship between the time dependence of the wind speed and the fractional volume of oil volatilization is established, at which the minimum fractional volume of oil dissolved in water is attained.

Key words: Degradation, hydrocarbons, modeling, optimization, fractional volume.

INTRODUCTION

The growing demand for hydrocarbon sources of energy in the modern world dictates the need to develop methods and increase the scale of oil and gas transportation. The marine transportation of crude oil in tankers or by pipelines is always associated with the risk of technogenic disasters, which inevitably result in the oil spills into the seas or oceans, which causes significant harm to the environment. Thus, the importance and relevance of model studies of the spilled oil mass transformation processes in the aquatic environment of seas and oceans is not in doubt. The oil mass located on the sea surface is degraded driven by various physical and biological factors that lead to the changes in density and viscosity of crude oil [1-3]. It is obvious that the study of oil degradation processes is important for planning measures to counteract harmful processes for marine flora and fauna in areas of such technogenic disasters.

Goals and objectives of the study

Freshly spilled oil forms an oil film on the sea surface, which is subjected to the following degradation processes:
- spread on the surface
- evaporation
- dissolution
- dispersion
- emulsification, etc.

These processes are integrated and occur in parallel over time. At the same time, creating a unified mathematical model that considers all of the above processes is the Herculean task of the environmental modeling, and this article aims to develop a simplified model of oil degradation, which takes into account only the first three processes of the above, i.e. spread on the surface, evaporation and dissolution.

Existing models of the considered oil degradation processes

The known mathematical models of oil degradation are often based on regional models of atmospheric dynamics, sea dynamics and wind waves. To calculate the area of the oil film for the case of a volley spill on a calm surface of sea waters, the J. Fay method is used [4]. In the model proposed in [5], a long-term oil spill is considered as the sum of a large number of instantaneous spills with regard to the spatial and temporal inhomogeneity of marine conditions. The authors [6] proposed a model based on the formal division of computational procedures into the processes of advection and the processes of environment state changes.

Without questioning the performance capabilities of the above and other similar models, let's note that we were not able to find an optimization model in the technical literature that enables to calculate optimal wind conditions that ensure minimal toxicity of sea waters in oil spills.

According to [7], the oil spill spread on the sea surface occurs in three stages:
- inertial-gravitational stage
- gravitational-viscous phase
- viscous surface tension.
- The longest is the gravitational-viscous stage, as a result of which the area of the oil spill (A) is determined by the following differential equation [7]:

$$\frac{dA}{dt} = \frac{k_{sp} \cdot V^{\frac{4}{3}}}{A},$$

Where:

V means the oil volume at the instant of time t, m³;

k_{sp} means the evaporation constant, 150 s⁻¹.

The evaporation process is the most important mechanism for oil removal from the sea surface. The evaporation rate is determined by the equation [8]:

$$\frac{dF_e}{dt} = \frac{K_{evp} \cdot A}{V_0} \cdot \left[a - \frac{\left(T_0 + T_g + F_e \right)}{T_{oil}} \right], \tag{1}$$

Where:

F_e means the volume of the evaporated oil fraction, %;

K_{evp} means the mass transfer coefficient in the evaporation process, m/s;

a, d – mean constants of the evaporation process;

T_0 means the initial oil boiling point;

T_g means the gradient of the oil distillation curve, K;

T_{oil} means the temperature of the spilled oil assumed to be equal to the temperature of the surface water.

At that, K_{evp} is determined by the following formula:

$$K_{evp} = 2.5 \cdot 10^{-3} W^{0.78}, \tag{2}$$

Where:

W means the wind speed at an altitude of 10 m (m/s);

Temperatures T_0 и T_g are determined as

$T_0 = 532.98 - 3.125$ API,

$T_g = 985.62 - 13.597$ API,

where API means API oil gravity (American Petroleum Institute).

It is obvious that the dissolution of oil in sea water leads to an increase in its toxicity. The amount of oil dissolved in water is determined by the following equation [9]:

$$\frac{dF_d}{dt} = K_{diss} A \left(\frac{S}{1000 \rho_{oil}} \right), \tag{3}$$

Where:

$$S = S_0 \cdot \exp\left(-12.0 \cdot F_e \right), \tag{4}$$

F_d means the fractional volume of oil dissolved in sea water, %;

K_{diss} means the mass transfer coefficient in the dissolution process, m/s;

S means the oil solubility at the instant of time t, g/m³;

S_0 means the initial oil solubility in water, g/m³;

ρ_{oil} means the initial oil density, kg/m³.

The simplified optimization model of the process of oil degradation on the sea surface

Contrary to the above model relationships of various degradation processes, this paper aims to develop a unified optimization model of the process of oil degradation on the sea surface. The essence of the optimization model can be formally stated as follows. Let's assume that there is a population X of interconnected partial oil degradation processes, defined as

$$X = \left\{ x_1(t); x_2(t); x_3(t); \right\},$$

where $x_i(t); i = \overline{1,3}$ means partial processes that determine the total oil degradation process.

It is required to determine the optimal relationship between processes $x_2(t)$ and $x_3(t)$, at which the following integral indicator can have the minimum value:

$$X_{1\text{int}} = \int_{T_0}^{T_f} x_1(t) dt,$$

Where:

T_0 means the fixed instant time of the oil spill;

T_f means the fixed instant time of the assessment.

With regard to the fact of increased toxicity of sea waters due to the dissolution of oil in water, the above-mentioned partial processes shall be defined as

$$x_1(t) = F_d(t).$$

$$x_2(t) = F_e(t).$$

$$x_3(t) = W(t).$$

Let's consider the issues of the proposed simplified model optimization.

Development of a simplified optimization model for oil degradation

With regard to the expressions (3) and (4), let's write:

$$\frac{dF_d}{dt} = \frac{K_{diss} A \cdot S_0 \exp\left(-12.0 \cdot F_e \right)}{1000 \rho_{oil}}. \tag{5}$$

Integrating (5), with regard to $F_e = F_e(t)$, $A = A(t)$, we obtain:

$$F_d = \int_0^{T_f} \frac{K_{diss} A \cdot S_0 \exp(-12.0 \cdot F_e)}{1000 \rho_{oil}} dt. \tag{6}$$

From expression (1) with regard to $A = A(t)$, we obtain:

$$A(t) = \frac{V_0}{K_{evp}} \cdot \left(\frac{dF_e}{dt}\right) \cdot \left[\frac{1}{a - \frac{b(T_0 + T_g \cdot F_e)}{T_{oil}}}\right]. \tag{7}$$

With regard to the expressions (6) and (7), we have:

$$F_d = \int_0^{T_f} \left\{\frac{K_{diss} \cdot S_0 \cdot V_0 \cdot \left(\frac{dF_e}{dt}\right) \cdot \exp(-12.6 \cdot F_e(t))}{1000 \rho_{oil} \cdot K_{evp}\left[a - \frac{b(T_0 + T_g \cdot F_e)}{T_{oil}}\right]}\right\} dt. \tag{8}$$

Let's take the following notation:

$$D\left(F_e(t), \frac{dF_e}{dt}\right) = \left\{\frac{K_{diss} \cdot S_0 \cdot V_0 \cdot \left(\frac{dF_e}{dt}\right) \cdot \exp(-12.6 \cdot F_e(t))}{1000 \rho_{oil} \cdot K_{evp}\left[a - \frac{b(T_0 + T_g \cdot F_e)}{T_{oil}}\right]}\right\}. \tag{9}$$

With regard to the expressions (2) and (9), the functional (8) can be written as follows:

$$F_d = \int_0^{T_f} \frac{D\left(F_e(t), \frac{dF_e}{dt}\right)}{2,5 \cdot 10^{-3} W(t)^{0.78}} dt. \tag{10}$$

Given the random nature of the wind speed change in time, we take the following model of $W(t)$:

$$\int_0^{T_f} W(t)\, dt = C; C = const. \tag{11}$$

Using expressions (10) and (11), we can compose a complete functional of unconditional variational optimization:

$$F_d = \int_0^{T_f} \frac{D\left(F_e(t), \frac{dF_e}{dt}\right)}{2.5 \cdot 10^{-3} W(t)^{0.78}} dt + \lambda \left[\int_0^{T_f} W(t)\, dt - C\right]. \tag{12}$$

Let's calculate the optimal function $W(t)$, at which $F_d \to$ min.

According to [10], the solution of this problem shall satisfy the condition:

$$\frac{d\left\{\frac{D\left(F_e(t), \frac{dF_e}{dt}\right)}{2.5 \cdot 10^{-3} W(t)^{0.78}} dt + \lambda\left[\int_0^{T_t} W(t) - C\right]\right\}}{dW(t)} = 0. \tag{13}$$

From expression (13), we obtain:

$$-0.78 \cdot 400 \cdot D\left(F_e(t), \frac{dF_e}{dt}\right)W(t)^{-1.78} + \lambda = 0. \tag{14}$$

From expression (14), we find:

$$W(t) = \int_0^{T_f} \frac{0.78 \cdot 400 \cdot D\left(F_e(t), \frac{dF_e}{dt}\right)}{\lambda}. \tag{15}$$

With regard to the expressions (11) and (15), it is possible to calculate the λ value using the formula (16). Let's denote the result of this calculation as $\lambda 0$:

$$\lambda_0 = \int_0^{T_f} \frac{0.78 \cdot 400 \cdot D\left(F_e(t), \frac{dF_e}{dt}\right)}{C} d(t). \tag{16}$$

With regard to the expressions (11) and (15), we obtain:

$$W(t) = \frac{D\left(F_e(t), \frac{dF_e}{dt}\right)}{\int_0^{T_f} D\left(F_e(t), \frac{dF_e}{dt}\right) d(t)}. \tag{17}$$

Using the expression (14), we can show that when solving the equation (17), the target functional (12) reaches a minimum. To do this, it is sufficient to calculate the second $W(t)$-derivative of the integrant in (12) and to make sure that it's positive.

Conclusion and findings

The proposed simplified optimization model of the degradation process of freshly spilled oil on the sea surface considers the effect of such processes as oil dissolution in water, evaporation of oil fractions and wind speed. It is obvious that consideration of all the affecting factors can lead to quite cumbersome mathematical calculations, the use of which is often difficult or impractical. The proposed optimization model did not consider such factors as dispersion, emulsification, wave effects, and water currents. These factors may be considered by introducing appropriate correction coefficients. In this paper, we obtained an analytical dependence of W(t) on indicators such as $F_e(t)$ and $F_e'(t)$, at which the fractional value of oil dissolved in water attains the minimum; this is equivalent to attaining the minimum toxicity of sea waters in the constructed model of oil degradation in the sea surface environment. The model proposed can be used in the development of software products to solve the environmental problems of ensuring the purity of sea waters.

In conclusion, let's formulate the main findings of the study.

1. A new approach to a simplified optimization model of the oil degradation process on the sea surface is proposed.
2. Based on the proposed approach, a simplified optimization model of the oil degradation process on the sea surface was developed.
3. The optimal relationship is determined between the time dependence of the wind speed and the fractional value of oil evaporation, at which the minimum fractional value of oil dissolved in water is attained.

Competing interests

The authors declare that there is no competing interest regarding the publication of this paper.

References

[1] Fingas V. F. Water-in-oil emulsions: formation and prediction. Journal of Petroleum Science Research. 2014;3(1):38–49.

[2] Azevedo A., Oliveira A., Fortunato A. B., Zhang J., Baptista A. M. A cross-scale numerical modeling system for management support of oil spill accidents. Marine Pollution Bulletin. 2014;80(1):132–147.

[3] Lehr W. J. Review of modeling procedures for oil spill weathering behavior. Advances in Ecological Sciences. 2001(9):51–90.

[4] Fay J. A. Physical processes in the spread of oil on a water surface. International Oil Spill Conference. American Petroleum Institute. 1971(1):463–467.

[5] Ovsienko S. N., Zatsepa S. N., Ivchenko A. A. The oil spills modelling and risk assessment of the environmental impact. Proceedings of State Oceanographic Institute. Modelirovanie razlivov nefti i ocenka riska vosdeistviya na okruzhayuschuyu sredu. |Trudy GOIN. 2005(209):248–271. (In Russ.)

[6] Stanovoy V. V., Lavrenov I. V., Neelov I. A. Modelling system for oil spills in the ice-infested seas. Problems of the Arctic and Antarctic. Sistema modelirovaniya razlivov nefti v ledovitykh moryakh. Problemy Arktiki i Antarktiki. 2007;3(77):7–16. (In Russ.)

[7] Sebastiao P., Soares C. G. Modeling the fate oil spills at sea. Spill Science & Technology. 1995;2(2):121–131.

[8] Stiver W., Mackay D. Evaporation rate of spills of hydrocarbons and petroleum mixtures. Environmental Science & Technology. 1984;18(11):834–840.

[9] Shen H. T., Yapa P. D., Wang D. S., Yang X. Q. A mathematical model for oil slick transport and mixing in rivers. Cold Regions Research and Engineering Lab. Hanover NH. 1993. No. CRREL-SR-93-21.

[10] Elsholz L. E. Differential equations and variational calculus. Differencialnye uravneniya i variacionnoe ischislenie. Moscow: Nauka Publ., 1974. 472 p. (In Russ.)