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Offshore petroleum pollution compared numerically via algorithm tests and computation solutions

Daniel Constantino Zacharias [a,*], Karina Fernandes Oliveira Rezende [b], Adalgiza Fornaro [a]

[a] *Departamento de Ciências Atmosféricas, Instituto de Astronomia, Geofísica e Ciências Atmosféricas, Universidade de São Paulo, IAG/USP, Rua do Matão, 1226, São Paulo, SP, 05508-090, Brazil*

[b] *Departamento de Biologia Celular e do Desenvolvimento, Instituto de Ciências Biomédicas Universidade de São Paulo, ICB/USP, Avenida Professor Lineu Prestes, 1524, São Paulo, SP, 05508-900, Brazil*

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ABSTRACT

This work aims at using oil transport and weathering models available in literature, and compare them numerically, by developing algorithms of Lagrangian particles for oil spilled on the ocean surface. This is the first step in the development of a new model for oil spills in the Brazilian Atlantic Ocean, comparing it with two reference models developed by the National Oceanic and Atmospheric Administration (NOAA) and distributed by the Environmental Protection Agency (EPA). The results, in this work, were subject to statistical tests, which showed good compatibility between the new and reference models. The code was tested on the southeast coast of Brazil under different meteorological and oceanic conditions. The modeling results of the physical and chemical transformations related to the oil weathering presented very similar results, even for completely different formulations. Similar results were also obtained for the transport and trajectory of the oil slick, whereas slick size varied greatly according to different turbulence parameters assumed for the water-oil-air interface layer. All the models analyzed presented very similar results for all analyzed effects, being considered reliable to describe the oil slick trajectory and weathering.

1. Introduction

The oil and gas consumption recorded over the last decades resulted in the increase in extraction, refining and transport of fossil fuels (Lardner and Zodiatis, 2017; Alves et al., 2014, 2015; 2016) and consequently, there is a higher risk of environmental accidents in maritime areas (Milani et al., 2000).

Efficient performance for the spilled oil removal depends on the knowledge of the slick size formed (to dimension the required containment) and on the ability to predict the spilled oil behavior in the short and long term (Huang, 1983). For this, the transport and oil degradation models can be used in both the preventive and corrective aspects, as they allow simulating hypothetical situations and, from these hypotheses, enable action plans to face possible future accidents (preventive action) or simulate real-time conditions of an accident in progress and, therefore, trigger the most effective countermeasures to contain the slick (corrective action).

Ferreira et al. (2003) state that modeling has become an important tood in defining an area likely to be target of an accidental offshore oil spill. The spilled offshore oil transportation and destination are mostly managed, in a short period, by processes of transport and physical-chemical transformation and, in a long period, by processes of biological degradation, according to the local oceanic and atmospheric conditions.

The physicochemical changes in the oil start when the lighter fractions of the spill are evaporated, small oil droplets disperse in the water column (entrainment of the oil in the water below the slick), emulsions are formed (entrainment of marine water in the oil, being stabilized in the presence of asphaltenes) and inorganic components are dissolved (Shen et al., 1987).

The models of oil spill transport and degradation by Lagrangean particle propose to numerically represent the physical-chemical effects acting on a continuous oil slick using a large number of discrete particles (Alves et al., 2015, 2016). In contrast, our study aims to test and evaluate recent models available in literature, such as those by Wang (Wang et al., 2005), Zadeh (Zadeh and Hejazi, 2012) and Stringari (Stringari et al., 2013). Wang and Zadeh based their work on similar premises in weathering, but describe the slick movement differently, while Stringari

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* Corresponding author.
E-mail addresses: daniel.zacharias@iag.usp.br (D.C. Zacharias), karinaforezende@yahoo.com.br (K.F.O. Rezende), adalgiza.fornaro@iag.usp.br (A. Fornaro).

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Table 1
Principal equations of the physical-chemical models used in this study.

	Wang et al. (2005)	Zadeh and Hejazi (2012)	Stringari et al. (2013)
Advection	$\vec{V_S} = \alpha_W D\vec{V_W} + \alpha_C \vec{V_C}$	$\overline{v} = \left(u_x + \frac{\tau_x^w}{C_f}, u_y + \frac{\tau_y^w}{C_f}\right)$	$U_{Ai} = k_c U_c + k_w U_w$
Spreading	$L_e = 1,39\left(\frac{\Delta g A^2 t^{\frac{3}{2}}}{\nu^{-\frac{1}{2}}}\right)^{\frac{1}{4}}$	$L_{min} = 53,76\ \Delta^{\frac{1}{3}}\ V^{\frac{1}{3}}\ t^{\frac{1}{4}} L_{máx} = L_{mín} + 0,95\ U^{4/3} t^{3/4}$	$D_x = \frac{\pi k_2^2}{16\sqrt{t}}\left(\frac{\Delta g V^2}{v_w^2}\right)^{1/3} U_{Si} = R_1\ cos\ (2\pi\ R_2)\sqrt{\frac{2D_x}{\Delta t}}$
Diffusion	$\vec{V} \acute{=} \left(\left(\frac{4E_T}{\delta t}\right)^{0,5}\right) R_n e^{i\theta}$	$R_h = \frac{\partial h}{\partial t} + \overline{\nabla}(h\overline{v}) - \overline{\nabla}(D\overline{\nabla}h)D = g\Delta h^2 C_f^{-1}$	$\Delta S_D = R_1\ \sqrt{12\ \Delta t\ D_x} U_{Di} = \Delta S_D\ cos\ (2\pi\ R_2)$
Evaporation	$F_V = \frac{\left[LnP_0 + Ln\left(CK_E t + \frac{1}{P0}\right)\right]}{C}$	$F_e = C_{Fe}\ \ln(K_{As}\ exp(C_{F0}) + 1\ )$	$\frac{dF_e}{dt} = K_{Fe}\ exp\left(A - \frac{B}{T} C_T\right)$
Emulsification	$Y_W = \frac{(1 - e^{-K_A K_B (1+V_W)^2 t})}{K_B}$	$F_W = K_B\ (1 - e^{-K_A (1+V_w)^2 t/K_B})$	$\frac{dF_w}{dt} = K_{Fw}\left(1 - \frac{F_w}{F_w^{final}}\right)$

represents the weathering differently from the other two. The algorithm results were compared and validated with GNOME (NOAA, 2012) and ADIOS2 (NOAA, 1994) in their most current and revised versions (Lehr et al., 2002).

Thus, the objective of this work is to develop algorithms based on three models already consolidated and available for use in literature, and compare the results, enabling in this way to detect the main points and as well as opportunities to upgrade our new oil slicks drift and weathering model. This paper presents the first step for a new Brazilian oil spilled model called STFM (Spill, Transport and Fate Model), focusing the six main processes of oil spill development and deterioration on the ocean surface: advection, mechanical/gravitational spreading, turbulent diffusion, evaporation, emulsification and dispersion (Table 1).

1.1. *Advection*

Advection, the transport of the oil slick by wind, waves, and sea currents, is essential to describe the oil slick spread on the ocean surface, determining all the areas affected by the spill, from its origin to its final destination. Since this process is dependent on wind, current and fluctuation capacity (given the oil density), it can occur on both the sea surface and the sea layers, beneath the surface (Huang, 1983).

1.2. *Mechanical spreading*

Spreading, basically the first environmental effect of the oil slick and its formation, is one of the most important process correctly describing the development of oil spills. It consists of a balance of forces between the gravity which causes the slick to spread, makes it thinner, and increases the area, and the viscosity which acts to keep it as cohesive as possible. The adequate knowledge of the oil slick spread is essential to control the extension of the contaminated area, as well as due to its influence on the rate of weathering processes such as evaporation, dissolution, photo-oxidation and biodegradation (Huang, 1983).

1.3. *Turbulent diffusion*

Turbulent diffusion is the mass transport within the oil slick through random and chaotic movements arising from the shear internal movements to the fluid itself when moving in turbulent flow. In the models, the spatial and temporal resolution processes smaller than the scales used are parameterized as turbulent diffusion and resolved from equations of random principle (Wang et al., 2005). A coefficient of diffusivity (Zadeh and Hejazi, 2012) is the most common approach to describe both the turbulent diffusion and also to represent the turbulence in these models.

1.4. *Evaporation*

Evaporation, the major process in the oil weathering, affects mainly the lighter components, being also the main responsible for the natural oil spilled removal on the ocean surface. The oil evaporation rate is assumed as a kinetic function of first order obtained from the spill area, wind speed, vapor pressure and temperature (Huang, 1983). The analytical methods for oil evaporation have been the most used in the oil slick spill and formation models, although considering several simplifications (Reed et al., 1999).

1.5. *Emulsification*

The emulsification described in this study is the gradual inflow of seawater droplets into the spilled oil, forming a new stable system. The emulsion is a mixture between two immiscible liquids, in which one of them (in this case seawater) penetrates in the form of small droplets inside the other (in this case the oil spilled), forming a stable mixture (Fingas and Fieldhouse, 2004).

As the chemical composition varies greatly, not all oils emulsify, and still several crude oils only form emulsions after a certain period of evaporation. In all cases, once the emulsification is started, the process follows practically uninterrupted until the saturation limit of the slick, being the content of waxes, resins and asphaltenes determinants for the slick emulsification (Lehr et al., 2002).

1.6. *Sinking*

Oil sinking represents not only an important part of the oil spill fate, but also a process which provokes significant pollution on coastlines. This process starts with increased specific gravity of the oil after weathering, followed by moving downward and adherence of the smallest drops to particulate matter with densities higher than the water and finally, sinks. (Huang, 1983). In a first stage, heavy compounds whose densities are higher than those of the sea water sink to the inside water column which usually happens due to the adhesion of particles or organic matter from the sea water to the oil slick. The oil-particulate aggregate increases the velocity of oil heavy compounds downwards until they are settled as part of the ocean bottom (Li et al., 2016). Twenty years after the Exxon-Valdez spill, the population of sea otters in the region still presents sequels and chronic effects due to the existence of residual oil fractions on the seabed (Monson et al., 2011).

Important studies on the sinking oil effects enabled, for the first time ever, bathymetric, oceanographic, geological and anthropogenic data to produce hazard maps for the Eastern Mediterranean Sea (Lardner and Zodiatis, 2017; Alves et al., 2014, 2015; 2016). The results of these studies will be tested on the oil spill that occurred in Salamina Island, Athens coast, in September 2017, as the region will be suffering the effects of this spill for the years to come.

2. Material and methods

We applied the proposed and already established models (Stringari et al., 2013; Wang et al., 2005; Zadeh and Hejazi, 2012), writing algorithms to test the equations, comparing the results with those obtained by GNOME (NOAA, 2012) and ADIOS2 (NOAA, 1994) in their most updated