A SPH MODEL FOR PREDICTION OF OIL SLICK DIAMETER IN THE GRAVITY-INERTIAL SPREADING PHASE

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Abstract. This paper presents the implementation of the SPH Lagrangian method for the prediction of the oil slick diameter in the gravity-inertial spreading. Computer codes that predict the slick diameter generally use hybrid models (Eulerian-Lagrangian), and simulations start from the end of the first phase (gravity-inertial), in which the oil slick diameter is given by Fay's equations [1, 2]. Fay adjusted curves to oil spreading experimental data on a calm sea condition aiming to estimate the oil slick diameter as a time function, after the spill occurrence. The mathematical modelling in this work is based on the Navier-Stokes equations, for incompressible Newtonian fluids. In the boundary treatment, a model for the collisions between the particles has been used, with the definition of an energy restitution coefficient [10]. At the end of the first stage of the spill, the numerical results obtained by SPH simulations show agreement with the solution obtained from Fay's equations.

1   INTRODUCTION

The spreading is due to the pollutant's tendency to flow over itself. It's the most significant transport process in the first few hours of the spill. Its understanding and quantification are of great importance to the preservation of the environment.

The curves adjusted by Fay [1,2] to oil spreading experimental data are still used in prediction models for oil slick reaching. The researcher estimated the oil slick diameter based on mathematical equations, dividing the phenomenon in three distinct stages, in which the gravitational, inertial and viscous forces and superficial tension are held accountable for the movement of the oil over the water. The shear stress on the surface of the oil was not considered due to the wind action, the advective forces and the turbulent diffusion. Due to the inexistence of winds, currents and waves, the oil spread in a circular shape, in a displacement that presented radial symmetry. Field data was employed in the attainment of proportionality coefficients for the equations proposed in the three stages of the spreading. It is known that the oil spreading, in real-life conditions, cannot be fully explained by these equations; however, through modifications, like considering the shear effects caused by the wind on the surface of the oil

(which explain the elliptical shape of the oil slick in an actual spreading), the equations can be applied nowadays.

The first stage of the oil spreading is not usually taken into consideration in the numerical study of the phenomenon because it is very short (about an hour for a 10,000 ton oil spill – according to Fay's results, [1]). An estimate of the oil slick diameter at the end of this stage, which is necessary for algorithms that simulate the longer lasting stage of the spreading (gravity-viscous), is, in general, obtained with a prediction based on Fay's adjusted curves to experimental data. Most of the software are hybrids and utilize meshes (in the Eulerian modelling of the water) and particles in the discretization of the oil. The prediction of the oil particle's position over time is based on the solution of Langevin's equation, according to reference [3]. However, the employment of Eulerian modelling in the simulation of oil on the water surface is not a good choice, for the need of updating meshes (remeshing), after each numerical iteration, making the process expensive and complicated.

During the last few years, the meshless Lagrangian methods have been more and more employed. The particle methods are included in this category, providing stable and accurate numerical solutions to integral equations or partial differential equations. The Smoothed Particle Hydrodynamics method is an alternative to the solution of problems modelled by the equations of conservation of mass, momentum balance and energy transport.

Particle methods, which address the spreading problem with a Lagrangian view for the two phases involved (oil and water), are incipient in the scientific study of spreading. Violeau [4] and Yang and Liu [5] presented their model and results employing this approach to the study of oil spill containment using floating devices.

The present work presents the implementation of a purely Lagrangian particle model, based on the equations of conservation of mass and momentum balance for the oil, in a calm sea condition. The Smoothed Particle Hydrodynamics (SPH) method is employed in the solution of those equations. The study is directed towards the understanding of the first stage of the spreading (gravity-inertial), independent of the other physical and chemical processes that occur during the spill, presented in references [6,7]. Employment of purely Lagrangian methods in the diameter prediction of the oil slick can not be found in literature. An algorithm was developed and implemented, using Fortran Language, and the numerical results were verified with the curves adjusted by Fay.

This paper is organized in sections as follows. In Section 2, the Lagrangian mathematical modelling employed in this work is briefly presented. Section 3 presents the methodology of the prediction of the oil slick diameter in the gravity-inertial spreading of oil and numerical aspects. The results and discussion of the results are in Section 4. Finally, the conclusions of this study are presented in Section 5.

2 SMOOTHED PARTICLE HYDRODYNAMICS (SPH) METHOD

Originally, the SPH method was developed in the end of the 70s of the 20th century, by Lucy [8] and Gingold and Monaghan [9], for the modelling of astrophysics phenomena. After some time, it was employed in the field of solid and fluid mechanics with a wide range of applications, due to its ability to incorporate the complexity of physical problems. Especially due to the complex geometries involving free surface fluids and fluid-structure interaction, the method has attracted a great number of researches.

For the solution of conservation differential equations, the SPH method discretizes the domain in a finite number of particles. The values of the physical properties in the reference particles are obtained by the interpolation of the properties of neighbouring particles with the use of smoothing functions (kernels). The particles are delimited by an influence domain (at a maximum distance $\mathrm{k}h$ from the fixed particle considered) that defines an area of influence in which there is the contribution of the neighbouring particles to approach the physical property in the reference particle.

In the SPH method, different kernels can be used, and so that they are considered suitable for interpolation, it is necessary that each one follows certain properties: smoothness, positivity, symmetry, convergence, decay, compact support, and normalization within the domain of influence. Common kernels used in the interpolations are presented in [10].

SPH provides approximations to the physical properties (such as density), gradients (such as pressure gradients), divergents (such as velocity divergents) and Laplacians (such as temperature and velocity Laplacians) related to fluid flow, with a second order error.

2.1 SPH Approximations for the Conservation Equations

Modelling of fluid flows and energy transport is performed by the conservation (mass and energy) and momentum balance equations. For an incompressible Newtonian fluid, the Navier-Stokes equations are employed. Table 1 shows the SPH approximations for these equations, written in a Lagrangian description, Eqs. (1)–(3).

Table 1. Differential Equations and SPH Approximations

Differential Equation (Continuum)	SPH Approximation (Domain discretised by particles)	
Mass conservation: $$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \mathbf{v}$$	$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = \sum_{b=1}^{n} m_b \mathbf{v}_{ab} \cdot \nabla W\left(X_a - X_b, h\right)$$	(1)
Momentum balance: $$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} + \upsilon \nabla^2 \mathbf{v} + \mathbf{g}$$	$$\frac{\mathrm{d}\mathbf{v}_a}{\mathrm{d}t} = \sum_{b=1}^{n} m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla W\left(X_a - X_b, h\right) +$$ $$+ 2\upsilon_a \sum_{b=1}^{n} \frac{m_b}{\rho_b} \mathbf{v}_{ab} \frac{(X_a - X_b)}{\left|X_a - X_b\right|^2} \cdot \nabla W\left(X_a - X_b, h\right) + \mathbf{g}$$	(2)
Energy conservation: $$\frac{\mathrm{d}e}{\mathrm{d}t} = \frac{1}{\rho}\left(-P\nabla \cdot \mathbf{v} + \varepsilon_\mathrm{v} + \nabla \cdot \mathbf{q} + q_H\right)$$	$$\frac{\mathrm{d}e_a}{\mathrm{d}t} = \frac{1}{\rho}\left[-P_a \sum_{b=1}^{n} m_b \mathbf{v}_{ab} \cdot \nabla W\left(X_a - X_b, h\right) + \right.$$ $$\left. + \varepsilon_\mathrm{v} + \nabla \cdot \mathbf{q} + q_H \right]$$	(3)

where ρ is the fluid density, t is the time, ∇ is the mathematical vector operator nabla, $\mathbf{v}$ is the fluid velocity, $\mathbf{g}$ is the acceleration due to gravity, υ is the kinematic fluid viscosity, P is the absolute pressure, e is the specific internal energy, ε_v is the energy dissipation per unit volume, $\mathbf{q}$ is the conduction heat flux, q_H is the heat generated by other sources per unit volume, W is the kernel, X is the particle spatial position, h is the support radius, a and b are subscripts that refer to fixed and neighbouring particles, respectively and $\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b$.

2.2 Consistency

In the SPH method, the consistency depends not only on the function approximation employed but also on the influence domain, the number of particles, and their distribution within the domain. If the influence domain is continuous and complete, there is a uniform distribution of particles inside it, and the support radius has been properly defined, the conditions for the consistencies of zeroth and first orders are met due to the properties of normalization and symmetry of the kernel. The influence of the support radius in the approximations obtained by SPH therefore needs to be properly analysed [11].

In regions near the boundaries, the truncation of the influence domain occurs, leading to less accuracy in approximations. This phenomenon is known as particle inconsistency.
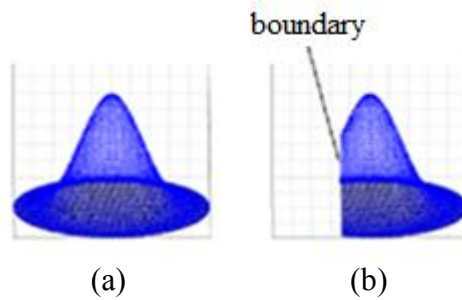

Figure 1. Influence domain: (a) complete and (b) incomplete or truncated.
It is possible see that the kernel is not defined in a whole domain.

Chen et al. [12] proposed the application of the Corrected Smoothed Particle Method (CSPM) for the particles inconsistency treatment, by introducing a correction factor. The particle density is corrected from the use of given expression in Eq. (4):

$$\rho_a^* = \sum_{b=1}^{n} m_b W(X_a - X_b, h) \left/ \sum_{b=1}^{n} W(X_a - X_b, h) \frac{m_b}{\rho_b} \right. \tag{4}$$

where ρ_a^* is the corrected density of the particle.

Similar expressions are obtained for the pressure gradient Cartesian components [10].

2.3 Numerical aspects of SPH for dynamic fluid flows

2.3.1 Variable Smoothing Length

The length of the influence domain is very important in the SPH method. It influences the efficiency of the calculations and the accuracy of the solutions. If the length of the influence domain is too small or too large, the results will not be consistent with the studied physical problem. The need to apply support radius compensation occurs, for example, in the simulation of dam breaking. In this work the following form correction proposed in [13]:

$$\frac{Dh}{Dt} = -\frac{1}{n_d}\frac{h}{\rho}\frac{D\rho}{Dt} \tag{5}$$

where n_d is the number of domain dimensions.

2.3.2 Artificial Viscosity

The transformation of kinetic energy into heat takes place in problems involving mainly shock waves and needs to be measured, which does not happen when Eqs. (1)-(3) are employed. The artificial viscosity application in the simulations aims to avoid numerical instabilities and the interpenetration between particles [13]. The formulation used is shown in Eq. (6):

$$\pi_{ab} = \begin{cases} \dfrac{-\alpha_\pi \chi_{ab} c_{ab} + \beta_\pi \chi_{ab}^2}{\rho_{ab}}, & (\mathbf{v}_a - \mathbf{v}_b)\cdot(X_a - X_b) < 0, \\ 0, & (\mathbf{v}_a - \mathbf{v}_b)\cdot(X_a - X_b) \geq 0. \end{cases} \tag{6}$$

$$\chi_{ab} = \frac{h_{ab}(\mathbf{v}_a - \mathbf{v}_b)\cdot(X_a - X_b)}{|X_a - X_b|^2 + 0{,}01\varphi^2}, \quad c_{ab} = \frac{c_a + c_b}{2} \quad , \quad \rho_{ab} = \frac{\rho_a + \rho_b}{2} \quad , \quad h_{ab} = \frac{h_a + h_b}{2}.$$

where π_{ab} is the artificial viscosity, α_π and β_π are coefficients used in the calculation of artificial viscosity, c_a and c_b are the velocities of sound in the fixed and neighbouring particles, respectively, h_a and h_b are the support radii of the fixed and neighbouring particles, respectively, φ^2 is a factor that prevents numerical differences when two particles approach one another. The factor φ^2 was set to $0.01h_{ab}^2$.

The term related to artificial viscosity is added to the terms of pressure in the SPH approximations for the momentum balance and energy conservation equations.

2.3.3 Temporal Integration

The Euler method (First Order Runge-Kutta) was employed in the update of particle properties over time. The integration stability depends on the time period choice. The CFL (Courant-Friedrichs-Lewy condition) numeric stability criterion was applied to guarantee the convergence of the results [14].

2.3.4 Boundary Conditions

In this work, the geometrical boundary conditions have been implemented. The collisions of the particles of fluid against the solid walls (considered as being well-defined planes) have been studied. The inter-particle collisions were not considered.

An algorithm for the study of collisions and trajectories of the particles that collide against the solid walls of the domain has been implemented. After the temporal integration and obtaining of the position of the center of mass of each fluid particle by the SPH method (in the situation in which there are not walls delimiting the domain), the collision algorithm, based on mathematical and geometry fundaments, brought the particles back into the domain. This is based on the fact that the fluid particles could not escape the domain due to the presence of the predefined geometrical planes. The degree of elasticity of the collisions was measured by a coefficient of restitution of kinetic energy (CR).

When a collision of a particle against a plane was detected, and the particle's velocity was obtained by the SPH method, there was a correction of the magnitude of its velocity component perpendicular to the collision plane, immediately after the impact as follows [10]:

$$(v_{col})_i \; = \; CR \; \times \; (v_p)_i \tag{7}$$

where $(v_p)_i$ and $(v_{col})_i$ are the magnitude of the particle's velocity component perpendicular to the collision plane at the i direction, before and after the collision, respectively; $i \in (x, y)$.

After the collision, the sense of the particle's velocity component and mass centre coordinate perpendicular to the wall is altered. The sense and magnitude of the velocity component parallel to the wall remains unaltered.

The coordinate of the particle's mass centre perpendicular to the plane is corrected, as show Eq. (8).

$$(C_f)_i = (C_1)_i + (1.00 + CR)(r - d) \tag{8}$$

where:

$(C_1)_i$ and $(C_f)_i$ and   are the coordinates of the mass centre position at the time instant $(t_o + \Delta t)$ and after the reflection, respectively,

r is the particle radius,

d is the distance between the particle's mass centre and the collision plane.

Figure 2 shows the initial and final mass centres positions (C_o and C_f) after colliding successively with two planes (A and B) in a numerical iteration. The point C_1 is the final position that would be achieved by the particle mass center if there were no walls delimiting the field.
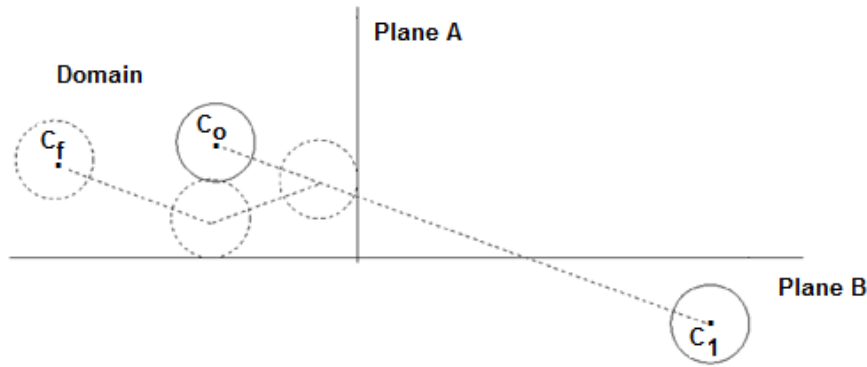
Figure 2. Collisions experienced by a particle in a time step.

3 PREDICTION OF OIL SLICK DIAMETER IN THE GRAVITY-INERTIAL SPREADING

3.1 Mathematical modelling and computer code

Fay [1, 2] adjusted curves to experimental data of the spreading of oil, considering a calm sea condition. These adjusted curves, defined for idealized theoretical conditions are still used, with some modifications. Mass losses, shear on the surface of the oil (caused by the wind), the advective forces and the turbulent diffusion were were not considered. After performing a physical analysis of the forces acting on the oil, he divided the process in three stages. In the first stage, the action of the gravity force predominates as driving, balanced by the force of inertia, resistant to movement. This stage has its duration as a function of the volume of the spilled oil, being called gravity-inertial spreading. The expression adjusted by Fay to the experimental results is presented by Eq. (8):

$$D = 2k_1 \left(\Delta_w g V t^2 \right)^{\frac{1}{4}} \tag{8}$$

$$\Delta_w = \frac{\rho_w - \rho_o}{\rho_w} \tag{9}$$

where D is the oil slick diameter, ρ_w is the water density, ρ_o is the oil density, g is the magnitude of the gravitational acceleration, V is the volume of the oil spilled, $k_1 = 1.14$.

This stage of the spreading lasts until the time instant t_f given by Eq. (10):

$$t_f = \left(\frac{h_o}{g \Delta_w} \right)^{\frac{1}{2}} \tag{10}$$

where h_o is the initial oil height.

The initial movement of the spilled oil is analogous to that of a dam break [15]. The mass conservation and momentum balance equations, Eqs. (1) and (2), have been employed to obtain the solution using the SPH method. This solution is verified by comparison with the results from Fay's equation.

3.2 Computational Geometry, Initial and Boundary Conditions

The simulated domain consisted of a tank with a 20-meter length, 20-meter width and 1.5-meter height, with a water level of 0.50 meters, and an oil volume initially disposed, in the centre, in the form of a cylinder with a height and diameter of 1 meter. Figure 3 presents the tank and the initial particle disposition.

The study was carried out with a small volume of oil, which caused the first stage of the spreading to be short. A bigger volume of oil was used in Fay's experiments; however, there are no restrictions in his work regarding the volume of the oil spill and the use of his adjusted curves in the prediction of the oil slick diameter, making this research feasible, especially due to the specifications of the available hardware.

A bi-dimensional analysis of the problem was carried out. A longitudinal section of the volume was studied (Fig. 4). Figure 5 shows an upper view of the spreading and circular shape of the oil slick spreading on calm sea condition.

The oil particle positions along the horizontal direction were monitored at each numerical iteration. The initial lateral distance between the centres of mass of the particles was 2.00×10^{-2} m, being employed in the discretization of the domain 2,500 oil particles and 26,000 water particles (density of 1,000 kg/m^3 e absolute viscosity of 1.00×10^{-3} Pa.s). The oil was considered a homogeneous, uniform and isotropic fluid. The simulations were carried out for light-weight oil, with a density of 850.00 kg/m^3 and absolute viscosity of 3.32×10^{-3} Pa.s. The time period employed in all simulations, defined by the CFL stability criterion was 1.41×10^{-4} s. The water particles remained still during the simulations. Tait equation has been employed in predicting the dynamic pressure field of oil [16]. The modified pressure concept has been implemented [17]. The duration of the spreading in its first stage, obtained by Eq. (10) was 0.82 s, with a total of 5,815 numerical iterations.

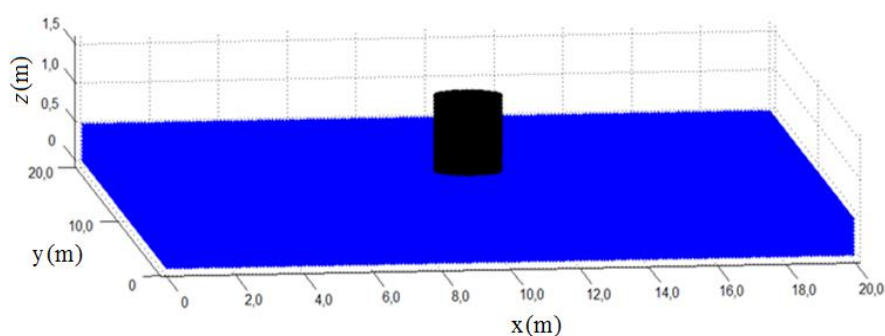A rigid plane was established, at water level, where the oil spreading occurred.
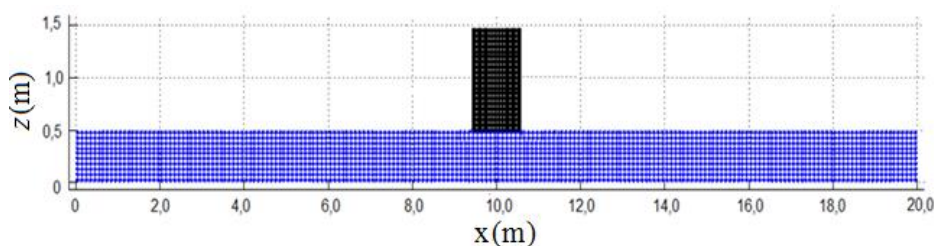

Figure 3. Simulated geometry.

Figure 4. Longitudinal section of the oil at the initial time instant.
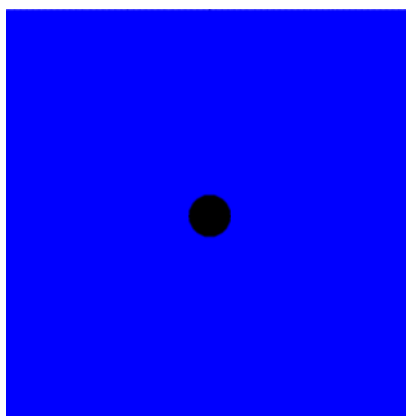

Figure 5. Upper view: the circular shape of the oil slick spreading on calm sea condition.

3.3 Numerical Simulations

In the simulations that were carried out, artificial viscosity was employed (with the coefficients $\alpha_\pi = 0.30$ and $\beta_\pi = 0.00$), a renormalization of the density of the oil was applied, the Tait equation was employed to predict the dynamic pressure fields of the oil (with the parameter B worth $0,85 \times 10^5$ Pa), a correction of the pressure gradients was made, the interpolations were carried out with the cubic spline kernel, the support radius varied over time, the boundary conditions were chosen (a plane fixed at water level) and the collisions against the boundaries were established as a result of the employment of energy restitution coefficients, temporal integration carried out by the Euler method.

After obtaining the velocity fields of the oil particles using the SPH method, the collisions that occurred against the horizontal plane defined at water level were detected with the analysis of the water particle trajectories. The direction of the velocity components of the particles that collided remained the same, however the sense of the vertical velocities of the particles changed. The sense of the velocity component in the x-axis remained unchanged. The positions of the particles' mass centres after the shocks also were corrected.

The oil particle evolution was monitored during the simulation. With the employment of radial symmetry, at each iteration, the circumferences were established with the radii defined by the longest horizontal distance between the positions of the oil particles and the position of the centre of the tank (10.00 m; 10.00 m; 0.50 m).

4 RESULTS AND DISCUSSION

In the beginning of the simulation using the SPH method, there was a bigger resistance to the oil movement with all the coefficients of restitution employed until the time period reached 0.04 s (Figure 7). In this time period, the oil slick diameter showed a tendency to remain constant. After this time period, the oil slick expanded until an inflection point in the curve (plotted in red) at around 0.12 s. From this moment until the end of the simulation, a positive growth rate was observed for the oil slick diameter.

Table 2 presents the oil slick diameters obtained by the SPH method (with the coefficient of restitution receiving values from 0.70 to 0.92) and by Fay's equation. The difference between the results is also presented.

Table 2. Oil Slick Diameter at the end of the Gravity-Inertial Stage

CR	Oil slick diameter (m)		Difference between the diameters - ΔD (m)
	SPH	Fay	
0.70	2.2583	3.0971	0.8388
0.80	2.2703	3.0971	0.8268
0.90	2.9824	3.0971	0.1147
0.92	3.0980	3.0971	-0.0009

It was verified that results obtained for the oil slick diameter obtained by the SPH method converged to results provided by the Fay's equation, as the CR increased. When the energy restitution coefficient reached 0.92, the results were coincident at the end of first stage of spreading. Figure 6 shows the agreement between the results (SPH and Fay's equation), at the end of the gravity-inertial phase, when using the CR with a value of 0.92.
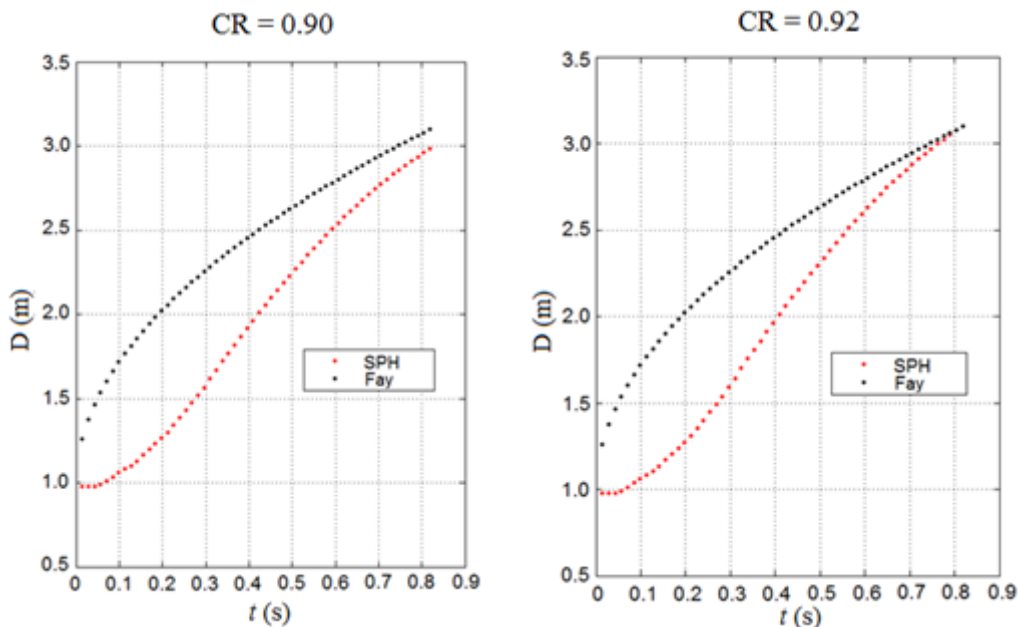

Figure 6. Evolution of the oil slick in the first stage of spreading.

The convergence of the numerical results (comparing to Fay's equation solution) occurred for low energy dissipation, but that needed to be correctly defined so that the correct diameter value was reached at the end of the first stage of the spreading.

Aiming to measure the computational efficiency, the CPU (central processing unit) processing time was measured. Table 3 presents the time period for different coefficients of restitution of energy, maintaining the same conditions and parameters for all simulations. All the simulations were carried out using Linux operating system, Intel i5-2450M processor (second generation) and 8 GB memory. The description of the sequential computational algorithm used in simulations is in [18].

Table 3. CPU processing time for different energy restitution coefficients

CR	CPU processing time
0.70	6 h 5 min 6 s
0.80	5 h 46 min 19 s
0.90	5 h 44 min 4 s
0.92	5h 43 min 31 s

5   CONCLUSIONS

In this work, with the employment of the Lagrangian SPH method in the discretization of the energy conservation and momentum balance equations, consistent numerical results were reached, in agreement with Fay's results, for the prediction of the oil slick diameter of light-weight oil, at the end of the first stage of the spreading.

The mathematical model used Navier-Stokes equations for Newtonian and incompressible fluids. While choosing the boundary conditions, a plane was fixed at water level and the coefficients of restitution of kinetic energy were employed to measure the interface effect on the oil movement. The energy restitution coefficient reflects the percentage of energy dissipated during the collision of the particle against the plane. The calibration of the proposed numerical model was done according to values attributed to the restitution coefficient (CR). Simulations were carried out for light-weight oil and, after employing different coefficients, a result for the oil slick diameter, in agreement with the solution of Fay's was obtained for a CR equal to 0.92.

The algorithm employed is capable of obtaining a solution for the first stage of the oil spreading, becoming a new tool to be used in the researches. For other types of oil, with specific physical properties (density, viscosity) another value for the coefficient of restitution can be found, so that there is an agreement between the oil slick diameter (found using the SPH method and Fay's equation) at the end of the gravity-inertial stage.

The numerical result obtained is important, for the oil slick diameter found is an input entry for the gravity-viscous stage simulation, the longest and the one that causes the greatest environmental impacts, not needing to employ Fay's adjusted curves for its prediction anymore.

The employed model, in its first stage, shows itself as a promising tool and can also be used in the study of the subsequent stages of oil spreading on a calm sea. It can be applied to real-life conditions (in which there are winds, currents and waves) with the attribution of the physical properties of the external agents to the particles that discretize the domain.

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