Numerical modeling of oil spill drifts for management of risks in continental waters

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Abstract

The application of the European Water Framework Directive and the monitoring obligation on water quality for human consumption and industrial activities create a need for water quality evaluation and monitoring systems. The Migr'Hycar research project was initiated to provide decisional tools, and fulfil operational needs, for risks connected to oil spill drifts in continental waters.

Within the framework of the Migr'Hycar project, a new 2-D numerical oil spill model has been developed by combining Lagrangian and Eulerian methods. The Lagrangian model describes the transport of an oil spill near the surface. This model simulates the major processes acting on the spilled oil. Though generally considered as a minor process, dissolution is important from the point of view of toxicity. To model dissolved oil in water, a Eulerian advection-diffusion model is used. The fraction of dissolved oil is represented by a passive Eulerian scalar and its quantity directly depends on the dissolved mass of particles.

In parallel with model development, experiments on the behaviour of hydrocarbons have been carried out in an artificial river facility in Berlin, which is part of the German federal environment agency (UBA). After spilling refined commercial products into an artificial channel, the aim of these experiments was to study the drift of the oil spill and the dissolution in the water column. Experimental results on situations with controlled conditions will allow the quality of the numerical predictions to be confirmed and validated.

Keywords: modelling, oil spill, continental waters, dissolution, evaporation, hybrid model, two-dimensional.

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1 Introduction

The European Water Framework Directive (WFD) together with the requirement to monitor water resources for drinking as well as leisure and industrial purposes, have substantially increased the demand for water-quality evaluation and monitoring systems.

Although in almost half of all instances of contamination, the exact cause is never determined, oil spills can be due to human error, accidental or voluntary discharge of cargo residues, domestic or industrial tank overflow, leakage from fuel stations, traffic accidents, fire, etc.

When faced with hydrocarbon contamination of inland waterways, authorities and other organizations can seldom call on dedicated decision-making tools to intervene in an effective way.

Whereas considerable management and monitoring resources are rapidly deployed for off- or inshore incidents, the more frequent occurrence of continental water pollution is dealt with using relatively modest means. A limited grasp of the nature and magnitude of such events often renders both industry and government powerless in controlling their impact.

The MIGR'HYCAR research project (www.migrhycar.com) was initiated to provide decisional tools, and fulfil operational needs, for risks connected to oil spill drifts in continental waters (rivers, lakes, estuaries). These tools are meant to be used in the decision-making process after an oil spill pollution and/or as reference tools to study scenarios of potential impacts of pollutions on a given site. The Migr'hycar consortium has been organized to closely match project objectives and comprises modelling technology developers (EDF, Saint-Venant Laboratory for Hydraulics, VEOLIA), researchers with long-standing experience of hydrocarbon physicochemical behaviour (Agribusiness laboratory LCA, CEDRE), engineering consultants liaising closely with local and regional authorities (SOGREAH), two water intake operators directly concerned with project-related issues and well experienced in applying protective warning systems (EDF, VEOLIA), and a major player in the oil industry (TOTAL). The consortium has therefore the expertise required to develop a surface-water risk monitoring and prevention system against oil spillage contamination.

In this study, a two-dimensional trajectory and fate hybrid model is developed to simulate the process of advection, turbulent diffusion, evaporation and dissolution in the water column. Then, the developed model has been applied to simulate oil spill in the Gironde estuary and in an artificial river.

In section 2 we briefly describe the conceptual model. In section 3 we deal with the main physical phenomena and show how they are modelled. Finally, our first results and validation cases are described in section 4.

2 Conceptual model

Within the framework of the Migr'Hycar project, a new 2-D numerical oil spill model has been developed using TELEMAC-2D software.

TELEMAC-2D is part of a computational suite, the TELEMAC system. This offers all the modules required for 2D and 3D numerical simulations in hydrodynamics (currents and waves), sediment transport and water quality.

TELEMAC-2D was developed by the National Hydraulics and Environment Laboratory (Laboratoire National d'Hydraulique et Environnement – LNHE) of the Research and Development Directorate of the French Electricity Board (EDF-DRD), in association with other research institutes.

The TELEMAC-2D code solves depth-averaged free surface flow equations as know as non-linear shallow water equations, as derived first by Barré de Saint-Venant in 1871. The main results at each node of the computational mesh are the water depth and the depth-averaged velocity components. The main application of TELEMAC-2D is free-surface maritime or river hydraulics modelling.

Recently published models for oil spills couple Lagrangian and Eulerian approaches (Guo and Wang [1]; Suh [2]; Nagheeby and Kaladoozan [3]).

The hybrid oil spill model we introduce here combines an Eulerian and a Lagrangian approach. It is new due to the fact that the Lagrangian model describes the transport of an oil spill near the surface. The oil slick is represented by a large set of small hydrocarbon particles. Each particle has an area, a mass, its element number, its barycentric coordinates in this element, etc., associated to it. This model allows the main processes that act on the spilled oil: advection, effect of wind, diffusion, evaporation, dissolution, to be simulated. Though generally considered as a minor process, dissolution is important from the point of view of toxicity. To model dissolved oil in water, a Eulerian advection-diffusion model is used. The fraction of dissolved oil is represented by a passive Eulerian scalar and its quantity directly depends on the dissolved mass of particles.

3 Physical process

When an oil spill occurs, the slick moves due to advection and diffusion phenomena. At the same time, the mass of the oil slick changes because of evaporation and dissolution. Therefore, these fate and transport oil spill process described in the following paragraph need to be included in the oil spill model.

3.1 Advection

3.1.1 In 2D: free surface velocity evaluated

As explained above, TELEMAC-2D solves the depth-averaged free surface flow equations. Therefore, in order to calculate the surface slick displacement, we need to evaluate the surface velocity using the depth-averaged velocity. The hypothesis of logarithmic profile for the vertical velocity has been made in order to estimate the surface velocity. In fact, we calculate the averaged velocity by integrating the logarithmic profile. A function of the mean velocity, the surface velocity and the friction velocity is deduced. We specify the friction velocity at the bottom thanks to the friction coefficient. In this way the following relation for the surface velocity is obtained:

$$\bar{u}(h) = \langle \bar{u} \rangle \cdot \left(1 + \frac{1}{\kappa} \sqrt{\frac{Cf}{2}} \right) \tag{1}$$

where $\bar{u}(h)$ is the surface velocity, $\langle \bar{u} \rangle$ is the depth-averaged velocity, κ is the Karman constant, Cf is the friction coefficient

3.1.2 Wind effect on the oil spill drift

We consider a float which moves due to wind and current. A solid body submersed in a fluid which moves with constant velocity is subjected to the following force:

$$F = \frac{1}{2} \rho \, S \, C_d \, \bar{u}^2 \tag{2}$$

where $\bar{u}$ is the fluid velocity, S is surface of the solid, ρ is density, C_d is the drag coefficient.

If the solid moves at velocity $\bar{v}$, it is necessary to replace the vector $\bar{u}$ by the vector $\bar{v} - \bar{u}$.

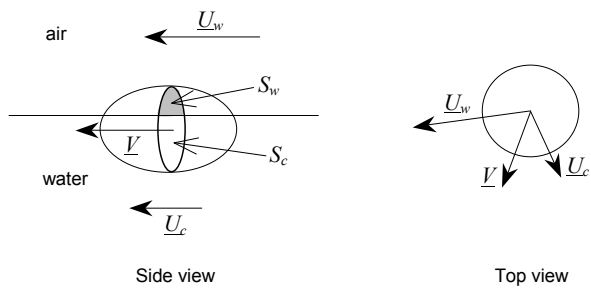

Figure 1: Forces acting on the float.

The float is subjected to wind and current. At steady state, Newton's second law allows us to write the following relationship:

$$\rho_w S_c C_{D,c} \left| \bar{v} - \bar{u}_c \right| \left(\bar{v} - \bar{u}_c \right) + \rho_a S_w C_{D,w} \left| \bar{v} - \bar{u}_w \right| \left(\bar{v} - \bar{u}_w \right) = 0 \tag{3}$$

where $\bar{v}$ is the body velocity, ρ_a is the air density , ρ_w is the water density, $C_{D,c}$ is the drag coefficient in the water, $C_{D,w}$ is the drag coefficient in the wind, S_w is surface of the solid in the wind, S_c is the surface of the solid in the water, $\bar{u}_c$ is the current velocity, $\bar{u}_w$ is the wind velocity

If the float velocity $\bar{v}$ is expressed in a basis formed by $\bar{u}_c$ and $\bar{u}_w$, which are known, a solvable system of equations is obtained. This system has the following solution:

$$\underline{V} = \frac{1}{1+\beta}\left(\underline{U}_c + \beta \underline{U}_v\right) \qquad \beta = \sqrt{\frac{\rho_a S_v C_{D,v}}{\rho_e S_c C_{D,c}}} \qquad \text{(4) and (5)}$$

The drag coefficient for a petroleum slick is a function of the area of the slick, so the drag coefficients $C_{D,c}$ and $C_{D,w}$ are equal. We thus obtain

$$\beta = \sqrt{\frac{\rho_a}{\rho_w}} = 0.036 \tag{6}$$

We can deduce that the oil spill transport induced by wind is 3.6 % of the wind velocity. A similar result is suggested by Reed *et al*. [4]. Thus, in light wind without breaking waves conditions, oil spill drift induced by wind is 3.5% of the wind velocity.

3.2 Diffusion

A drifting substance, for instance petroleum parcels submerged in a current, will diffuse. This diffusion is mostly induced by the turbulent flow. In order to take this phenomenon into account, a stochastic approach is adopted. The hypothesis of "white noise" is made in order to consider the random displacement of a petroleum parcel in water. This hypothesis allows us to define the particle displacement like a Markov process which means that each particle's displacement at each time step is independent of its displacements at previous time steps.

Contaminant dispersion is modelled using one governing equation, namely the Advection-Diffusion equation (Hervouet [5])

$$\frac{\partial hC}{\partial t} + \nabla \cdot (hCu) = \nabla \cdot \left(\frac{h\nu_t}{\sigma_c} \nabla C\right) \tag{7}$$

where h is the water depth, C the pollutant concentration, u the flow velocity, σ_c is the turbulent Schmidt number, ν_t is the turbulent viscosity

The turbulent Schmidt number can be set to $\sigma_c = 0.72$ (Issa *et al*. [6]).

A transformation will be applied to the Advection-Diffusion equation to obtain a Lagrangian equation:

The first step in this transformation is to interpret the concentration $C(X,t)$ as a probability $P(X,t)$ to find a particle at a location X at a time t. Then, using mass conservation, we develop and simplify the previous equation, which leads to

$$\frac{\partial P}{\partial t} = -\left(u - \frac{1}{h}\nabla\left(\frac{h\nu_t}{\sigma_c}\right)\right)\nabla P + \frac{\nu_t}{\sigma_c} \nabla \cdot \nabla P \tag{8}$$

This equation is called the Fokker Planck equation. The main benefit of having rewritten the equation in the form of the Fokker-Planck equation is that it is now possible to say that previous equation is equivalent to the Ito stochastic differential equation (Gardiner [7]):

$$X(t+\delta t) = X(t) + (u - \frac{1}{h}\nabla\frac{h\nu_t}{\sigma_c})\delta t + \sqrt{\frac{2\nu_t}{\sigma_c}\delta t}\cdot\xi(t) \quad (9)$$

where δt is the time step, $\xi(t)$ is a vector with independent, standardized random components.

3.3 Evaporation

Evaporation is the most important process that oil undergoes after spillage. In a few days, light crudes or refined products can lose up to 75% of their volume. An understanding of evaporation is important both from the practical viewpoint of cleaning up spills and for developing predictive models.

The evaporation model used is based on Stiver and Mackay's work [8]. An expression of the evaporated fraction is determined thanks to the molar flux expression of Mackay and Matsugu [9] and the thermodynamic equation:

$$dF_{evap} = \exp\left(\ln\left(\frac{P_a\nu}{RT}\right) + \frac{\Delta H}{RT_B}\left(1 - \frac{T_B}{T}\right)\right)\frac{k_{evap}S}{V_0}\,dt \quad (10)$$

where F_{evap} is the evaporated fraction, P_a is the atmospheric pressure, ν is the molar volume, R is the universal gas constant, T is the temperature, K_{diss} is the mass transfer coefficient, ΔH is the molar enthalpy, T_B is the boiling temperature.

With the previous expression, a pseudo-component approach is adopted.

In the pseudo-component approach crude oils and refined products are modelled as mixtures of discrete non-interacting components. Each pseudo component (PC) is treated as a single substance with an associated boiling temperature. Then distillation data is used to determine the properties of the PC's. The data are stored as pairs of values: the temperature of the distillate (T_i), and the fraction of component i in oil (F_i). The mass change of each particle component i at every time step is deduced:

$$mass_{compo(i)}(t+1) = mass_{compo(i)}(t) - \rho_0 k_{evap} S\cdot\exp\left(\ln\left(\frac{P_a\nu}{RT}\right) + \frac{\Delta H}{RT_{B(i)}}\left(1 - \frac{T_{B(i)}}{T}\right)\right)F(i)\cdot dt \quad (11)$$

3.4 Dissolution

Dissolution is an important phenomenon from a toxicological and environmental point of view, although it only accounts for a negligible fraction of the mass of the oil. In fact, the oil quantity concerned by this process is about 1% of the initial mass of oil.

The concentration of dissolved petroleum in the water column at time t as a function of concentration at time t-1 is given by the following relation:

$$C(t) = S + (C(t-1) - S)\exp(-\alpha\delta t) \tag{12}$$

where δt is the time step, S is the petroleum solubility in water, $\alpha = \frac{k_{diss} A_p}{V}$ (where k_{diss} is the mass transfer coefficient, A_p is the particle area, V is the node volume).

The order of magnitude of the dissolved mass transfer coefficient k_{diss} is of several cm/h (Shen and Yapa [10], Hibbs *et al*. [11]).

Thus, thanks to the relation which links mass with concentration, the mass loss at time t for each particle can be deduced:

$$m(t) - m(t-1) = (1 - \exp(-\alpha dt))(S - C(t-1)) \cdot V \tag{13}$$

In TELEMAC-2D each variable is defined on every node in the mesh. If we consider a particle (M1) inside an element, it is important to define the dissolved mass of the particle at each element node.

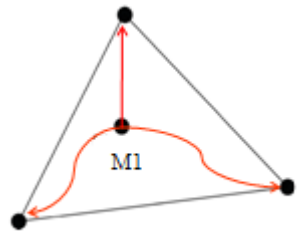

Figure 2: Particle M1 inside its element.

The coefficient α must be defined at each node i, for this we define the reduced particle area as

$$A_p \cdot SHP(i) = A_r(i) \tag{14}$$

where $SHP(i)$ is the barycentric coordinate at the node i, $A_r(i)$ is the reduced area at node i

An area is defined around each mesh node, according to a method defined in Hervouet [5]. The volume V is obtained by multiplying the node area by the depth of the node.

The previous steps allow the coefficient α_j to be calculated at each node of each element that contains a particle.

The dissolved mass of hydrocarbons in the water column is defined at each node by the following relation:

$$mass_{dissolved(j)}(t) = (1 - \exp(-\alpha_j dt))(S - C_j(t-1)) \cdot V_j \tag{15}$$

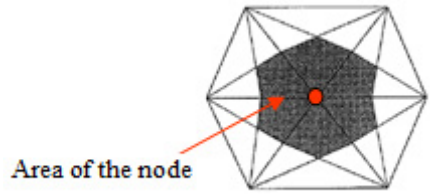

Figure 3: Area of mesh node.

The total amount of dissolved mass for each particle is:

$$mass_{totdissolved}(t) = \sum_{j=0}^{nb_{node}} mass_{dissolved(j)}(t) \tag{16}$$

A problem can occur if $mass_{totdissolved}$ is bigger than the mass of the particle. In this case, the dissolved mass needs to be multiplied by a coefficient:

$$Coefficient = \frac{mass_{particle(i)}}{\sum_{j=0}^{nb_{node}} mass_{dissolved(j)}(t)} \tag{17}$$

Thus, the quantity of tracer at the time step t, at node j, added by dissolution is defined as:

$$T_j(t) = T_j(t-1) + \frac{mass_{dissolved(j)}(t)}{V_j} \tag{18}$$

4 Results

4.1 Artificial river

4.1.1 Experimental process

Several experiments on the behaviour of hydrocarbons have been carried out at the Flieβ- und Stillgewässer Simulationsanlage (FSA) artificial river facility in Berlin, which is part of the German federal environment agency (UBA). Figure 4 shows a diagram of the artificial river.

After releasing refined commercial petroleum products into an artificial channel, the aim of these experiments was to study the drift of the oil spill and the dissolution in the water column. In fact, after releasing petroleum in the channel, a probe measures the petroleum content in the water column. When the probe detects a dissolved petroleum peak, a water sample is taken in order to determine the concentration of dissolved petroleum at this time. Figure 5 presents the result after releasing 10 ml of heavy fuel into the artificial river.

In this case, the water sample reveals a concentration of $36 \cdot 10^{-9}$ g/l of dissolved petroleum in the water column.

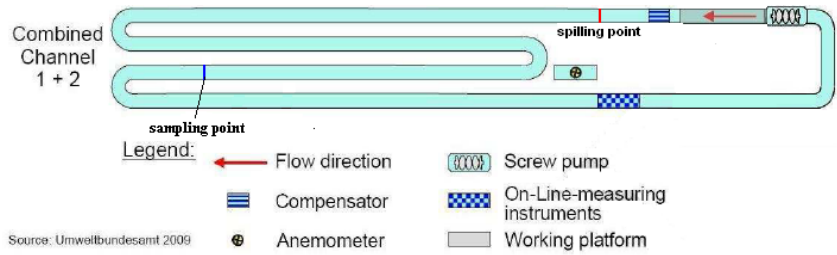

Figure 4: Sketch of the artificial river.

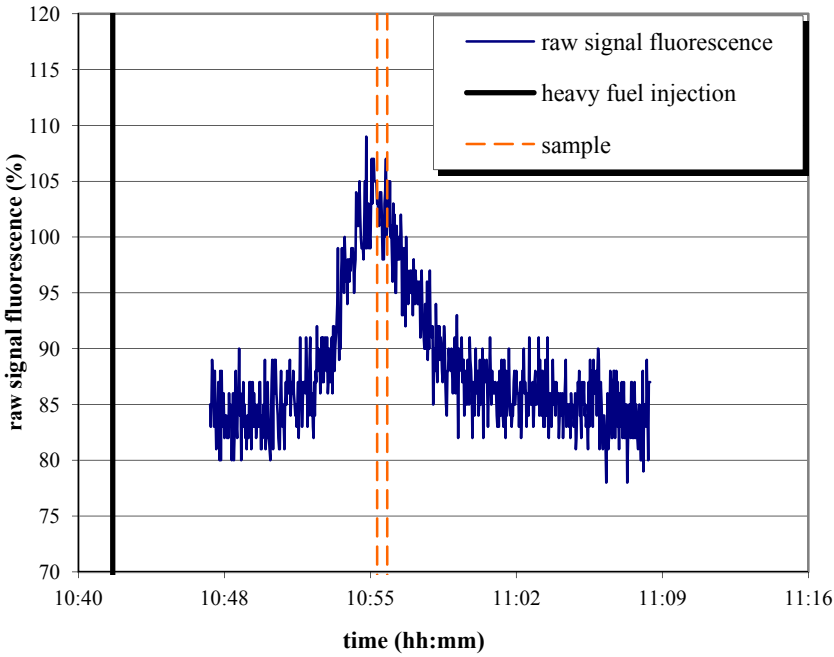

Figure 5: Fluorescence measurement of dissolved petroleum.

4.1.2 Modelling

To evaluate the hybrid oil spill model performance, a simulation is carried out with the same experimental conditions.

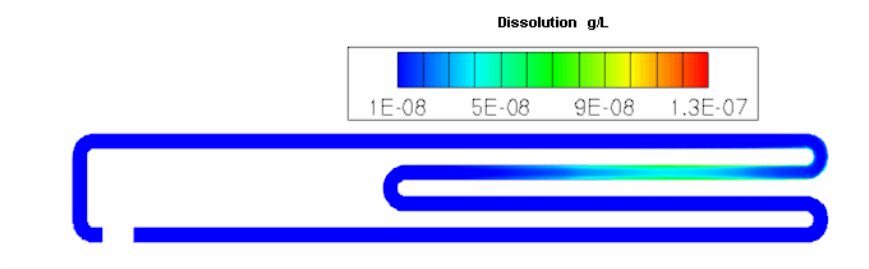

Figure 6: Simulation result in artificial river for heavy fuel.

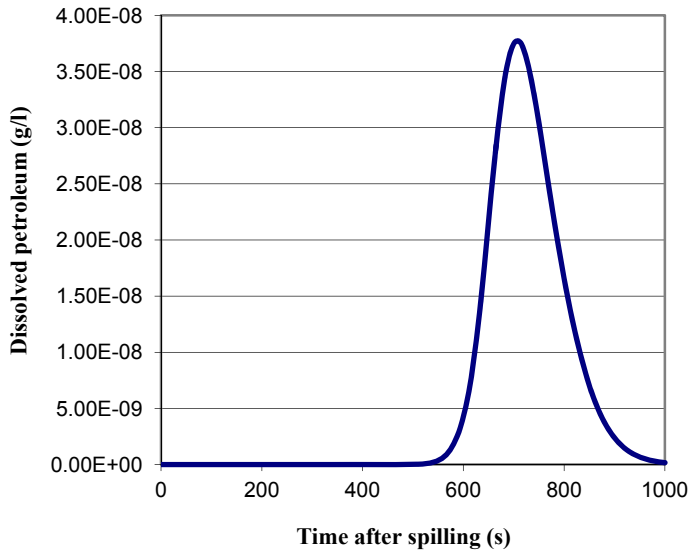

Figure 7: Dissolved heavy fuel in water column.

The simulation results are in agreement with the experimental results. In fact, the maximum value of dissolved petroleum in the water column occurs at 707 s after spilling in the numerical case whereas it occurs at 750 s for the experimental case which represents a difference of 5.7 percent. So, we can deduce that the transport is well modelled. Moreover, the dissolved hydrocarbons concentration in the water column has the same order of magnitude numerically and experimentally.

However, even if the numerical results are promising, a complementary study is necessary to validate the fate oil spill model.

4.2 Gironde estuary

Some water intake operators are located on the coast of Gironde estuary. An oil spill can have a strong impact on the management of these industries. So, it is important to be able to model accurately an oil spill which would occur in the estuary.

In the simulation presented in Figure 8, a hypothetical heavy fuel spill is considered to occur with an initial oil volume of 1 m^3. This oil spill is submitted to a north-west wind of 2 m/s. After one day, the shape of the slick is shown in Figure 8. The black dots represent the oil slick at the surface whereas the tracer represents the dissolution phenomenon in the water column. Even if the surface slick is not stranded, some heavy fuel reached the estuary coast. This phenomenon can have a strong impact for intake operators. So, it is important to follow up the dissolved oil in the water column and the surface slick for operational management of risks.

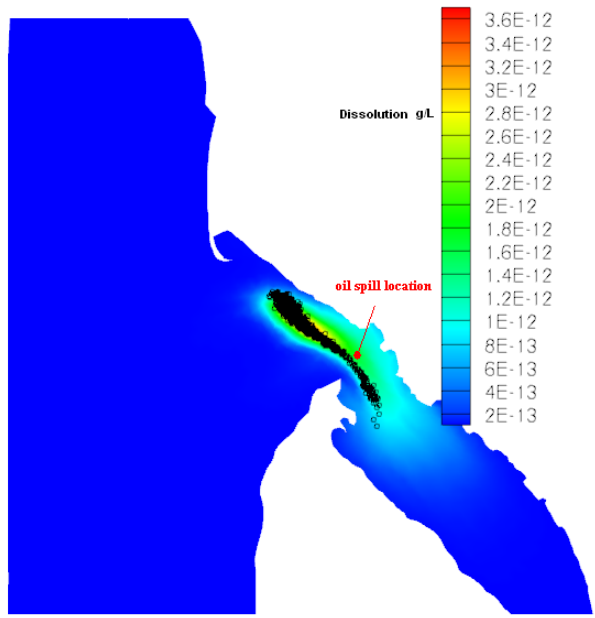

Figure 8: Simulation result of oil spill in Gironde estuary.

5 Conclusion

The hybrid model has been developed to simulate oil spill in continental waters. This model predicts the movement of an oil slick, the fate processes and the dissolution concentration of oil in the water column. This oil slick model has been coupled with the Telemac hydrodynamic model.

Verifications of the model were carried out by comparing numerical and experimental results. However, even if the numerical results are promising, a complementary study is necessary in order to validate the fate oil spill model. Application of the model to a case of oil spill in Gironde estuary exemplifies the capability of the model to deal with different phenomena.

The next steps of the work will consist of modelling the spreading of oil under the effect of gravity and surface tension. Then the model will be extended to full Navier-Stokes equations with Telemac-3D. An important step will be the adaptation to parallelism with domain decomposition.

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