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## A cross-scale numerical modeling system for management support of oil spill accidents

Alberto Azevedo<sup>a,\*</sup>, Anabela Oliveira<sup>a</sup>, André B. Fortunato<sup>a</sup>, Joseph Zhang<sup>b</sup>, António M. Baptista<sup>c</sup>

<sup>a</sup> National Laboratory for Civil Engineering, Av. do Brasil 101, 1700-066 Lisbon, Portugal

<sup>b</sup> Center for Coastal Resources Management, Virginia Institute of Marine Science, 1375 Greates Road, P.O. Box 1346, Gloucester Point, VA 23062, USA

<sup>c</sup> NSF Science & Technology Center for Coastal Margin Observation & Prediction, Oregon Health and Science University, 3181 SW Sam Jackson Park Road, Portland, OR 97239-3098, USA

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### ABSTRACT

A flexible 2D/3D oil spill modeling system addressing the distinct nature of the surface and water column fluids, major oil weathering and improved retention/reposition processes in coastal zones is presented. The system integrates hydrodynamic, transport and oil weathering modules, which can be combined to offer different-complexity descriptions as required by applications across the river-to-ocean continuum. Features include accounting for different composition and reology in the surface and water column mixtures, as well as spreading, evaporation, water-in-oil emulsification, shoreline retention, dispersion and dissolution. The use of unstructured grids provides flexibility and efficiency in handling spills in complex geometries and across scales. The use of high-order Eulerian–Lagrangian methods allows for computational efficiency and for handling key processes in ways consistent with their distinct mathematical nature and time scales. The modeling system is tested through a suite of synthetic, laboratory and realistic-domain benchmarks, which demonstrate robust handling of key processes and of 2D/3D couplings. The application of the modeling system to a spill scenario at the entrance of a port in a coastal lagoon illustrates the power of the approach to represent spills that occur in coastal regions with complex boundaries and bathymetry.

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### 1. Introduction

The minimization of the economical and environmental impacts of oil spills in coastal zones is a major concern worldwide. According to The International Tanker Owners Pollution Federation Limited statistics, 85% of the spills are smaller than 7 tons, and the number of those over 700 tons has decreased significantly during the last three decades (ITOPF, 2008). However, large spills are responsible for most of the oil spilled annually (Albaigés et al., 2006; Azevedo et al., 2009), and they have major environmental and economical consequences.

Due to improvements in numerical methods and advances in computers, modeling systems are becoming useful to forecast the fate of oil spills and to assist in combat and contingency planning for these type of environmental catastrophes. A typical modeling system combines a hydrodynamic model, a transport model and an oil weathering model, either through soft coupling (e.g. Beegle-Krause, 2001) or through full integration of all modules (e.g. Singaas, 1998; ASA, 2004; Tkalich, 2006; Guo and Wang,

2009). Reviews of the state-of-the-art of oil spill modeling have been provided by Spaulding (1988), ASCE (1996), Reed et al. (1999), Lehr (2001) and Foreman et al. (2005).

Oil spill models can range from simple trajectory models, that only account for advection, to three-dimensional transport (Fernandes, 2001; Tkalich, 2006; Guo and Wang, 2009) and fate models (Lehr et al., 2000) that might include the simulation of response actions and the estimation of biological effects (ASA, 2004, 2008). Most oil spill models consider the surface and water column oil as a simple tracer, disregarding the reology differences between the two distinct types of oil mixtures. These models only consider the transfer rates between the two layers, without the actual 3D representation of the oil phases.

Oil processes have been described mathematically with very different degrees of complexity (e.g., compare the formulation of Stiver and Mackay (1984) with the formulation of Fingas (2004) for evaporation). Some important processes are still often ignored, including the interaction between the water and the shoreline (or the coastal structures). For instance, models OILMAP (Spaulding et al., 1992; ASA, 2004) and COZOL (Reed et al., 1988; Howlett and Jayko, 1998) are among the most complete currently available, yet they fail to represent retention/reposition of oil in intertidal areas.

\* Corresponding author. Tel.: +351 21 844 3758; fax: +351 21 844 3016.  
E-mail address: [aazevedo@lnec.pt](mailto:aazevedo@lnec.pt) (A. Azevedo).

The majority of current oil spill models are particle-tracking models, which are simple to apply and have low computational requirements (ASA, 2004; Fernandes, 2001; Beegle-Krause, 2001). These Lagrangian approaches are very attractive when oil droplets are used to represent the oil at sea or when strong concentration gradients are present, but they fail to adequately represent complex transformation processes, as errors accumulate in the two-way mapping from particle's mass to concentrations. By contrast, Eulerian models are very efficient in diffusion-dominated problems and complex domains due to the use of a fixed grid, and can better represent complex transformation processes. However, the computational costs of Eulerian models tend to be high, mostly due to the need to couple the transport and chemical kinetic equations with the hydrodynamic models. Many Eulerian models (Tklich, 2006; Guo and Wang, 2009) are this better used in conjunction with High Performance Computing clusters.

An alternative to the Lagrangian or Eulerian methods most often used in oil spill models are Eulerian–Lagrangian methods (ELMs). ELMs (Baptista, 1978) solve advection in a Lagrangian framework through the Backward Method of Characteristics, while solving other processes in a fixed grid. ELMs tend to be computationally effective as they minimize stability constraints on time steps, an attractive feature that needs to be balanced against the fact that most ELMs are not inherently mass conservative. Various flow, transport and water quality models (Wood and Baptista, 1992; Celia et al., 1990; Zhang and Baptista, 2008; Rodrigues et al., 2011) have successfully used ELMs. Of relevance to oil spills, many of these models have combined ELMs with unstructured grids, to achieve maximum flexibility in handling processes across a broad range of both time and space scales.

This paper presents a flexible and integrated modeling system that couples a 3D hydrodynamic model and a flexible 2D/3D oil spill model, to enable the simulation of spills occurring across estuarine-to-oceanic scales. VOILS (Vela-Oil-Selfe) was developed through the hard coupling of the 2D ELM transport model VELA (Oliveira et al., 2000; Oliveira and Fortunato, 2002), the new oil weathering processes model described herein and the circulation model SELFE (Zhang and Baptista, 2008). The degree of complexity of the simulation are all customizable by the user, who has control over the choice of surface slick only versus 3D water column representations, over the processes specifically accounted for, and over the formulations used to describe various processes. Unstructured grids are used to discretize the domain in the horizontal, and ELMs are used for both circulation and oil transport. High-accuracy schemes are used for the tracking of the characteristic lines and for the evaluation of the integrals at the feet of the characteristic lines, to enable good mass balance (Oliveira and Baptista, 1995, 1998; Oliveira et al., 2000). The formulation for shoreline retention/release of oil explicitly accounts for the dynamics of intertidal areas.

Details of the modeling system are described in Section 2. Benchmark tests, ranging from controlled analytical solutions to a spill scenario at the entrance of a port are presented in Section 3, to illustrate the soundness of the underlying methods and the robustness and computational efficiency of the modeling system. Section 4 offers a synthesis and major conclusions.

## 2. Modeling system description

### 2.1. General approach

VOILS handles the surface slick and the water column differently, explicitly recognizing the different nature of the fluids involved (Fig. 1). The model considers the surface slick to be essentially composed by oil, and solves a 2D transport equation for the slick thickness as per Tklich (2006). By contrast, the fate

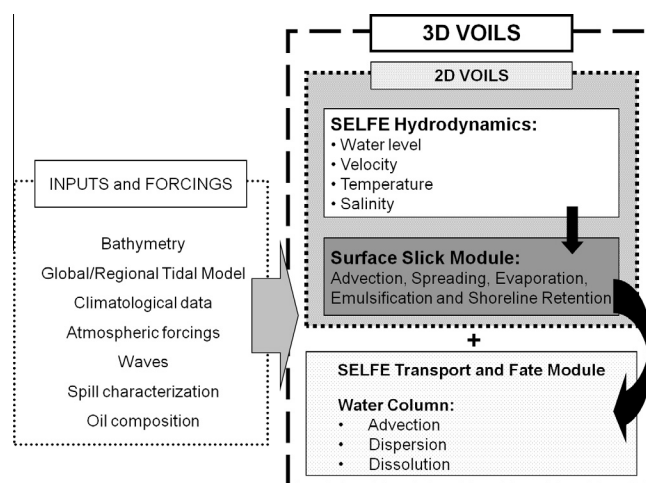


Fig. 1. 2D/3D VOILS scheme.

of the lower-concentration oil present in the water column is described by solving the 3D transport equation for oil concentration.

The separate treatment of the surface layer and the water column contributes to the flexibility of VOILS, which can be used in 2D (henceforth, 2D-VOILS) or 3D. 2D-VOILS solves the surface slick dynamics using decoupled hydrodynamic forcing (in the form of surface velocities) derived from any compatible circulation model, such as SELFE (Zhang and Baptista, 2008) or ELCIRC (Zhang et al., 2004). In 3D mode, the oil spill model is fully coupled to SELFE and the two layers (surface and water column) are solved independently. SELFE starts by solving the hydrodynamics and provides the elevations and velocity fields to the oil model for the surface layer (2D-VOILS). Then, the transport, source and sink terms are calculated and the fluxes of oil to the water column are provided to the tracer transport module in SELFE, which solves the transport of the oil in the water column. Kinetic relations between tracers (i.e., dispersed and dissolved oil are treated in the water column as two distinct tracers) are solved in the oil weathering module and passed to the 3D transport module in SELFE.

The computational time is highly dependent on the physical set-up (chosen processes and formulations), the number of nodes of the horizontal grid and the vertical layers, the details of the backtracking scheme, among other factors. For a common set-up, 2D-VOILS may take 3.5 h to simulate 2 days with a horizontal grid of 42,000 nodes and a time step of 15 min using an Intel Xeon CPU E5606 with 2.13 GHz. By contrast, the 3D version takes 8 h for the same horizontal grid and 7 vertical layers and a consistent set-up. The increase of the number of vertical layers from 7 to 11 can change the simulation period to 14 h.

### 2.2. The 2D Eulerian–Lagrangian oil slick model

2D-VOILS can be used to simulate surface oil transport and weathering forced by a 2D or 3D circulation field. The 2D-VOILS model consists in the coupling of the VELA transport model (Oliveira et al., 2000; Oliveira and Fortunato, 2002), adapted for the conservation of oil, with an oil weathering module. The oil weathering module includes the most relevant processes that occur during an oil spill event at the scale of days to weeks: spreading, evaporation, water-in-oil emulsification, shoreline retention, dispersion and dissolution. This module is coupled to the advection–diffusion processes through the source and sink terms. In 2D-VOILS the slick thickness is determined by solving an advection–diffusion equation that simulates oil dynamics at the sea surface (Tklich, 2006):

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