CHAPTER 20

Models of flow pattern and mass distribution

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1 Introduction

Mohid is an open source model developed at the Technical University of Lisbon (IST) (available free for download at www.mohid.com under the GPL license). The first version of Mohid, dating from 1986, was a two-dimensional barotropic hydrodynamic model. Two decades of research made Mohid evolve into a three-dimensional baroclinic hydrodynamic numerical model, coupled with models of transport and water properties capable of simulating a wide range of natural phenomena and perturbations in ecosystems of anthropogenic origin.

2 Mohid overview

Mohid is written in FORTRAN 95, using the Object Oriented (OO) programming paradigm [1]. Given that OO allowed the creation of a modular architecture, it is more correct to describe Mohid as a system where diverse numerical models communicate. Depending on each specific problem different models are used, making it possible to match the problem domain with the best set of models available in the Mohid system.

There is also a framework to use whenever it is decided that a model should join the Mohid system. Mohid's framework, which is beyond the scope of the present text, presents programming rules, how to use and develop new application programming interfaces and describes output and input file formats.

Mohid is a three-tier system, the bottom most being the hydrodynamic model, the middle tier being the transport models and the top tier being water quality models. The hydrodynamic model provides the transport models with a velocity field. Water quality models run on top of both hydrodynamic and transport models, being space and time independent. Looking at the Mohid system from another perspective, it is possible to view it as a framework providing:

- velocity fields;
- transport mechanisms;
- interfaces to 'plug in' water property models.

The most important requirement for a water property model to be 'pluggable' is to be time and space independent. An example of time independence is that phytoplankton do not need to know

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that it is springtime; there is a set of physical conditions (temperature, light, nutrients, etc.) that triggers the spring bloom.

3 Finite volumes

Mohid uses a finite volume approach [2–4] to discretize equations. In this approach the discrete form of the governing equations is applied macroscopically to a cell control volume. A general conservation law for a scalar U, with sources Q in a control volume Ω is then written as:

$$\partial_t \int_\Omega U d\Omega + \oint_S \vec{F} d\vec{S} = \int_\Omega Q d\Omega. \tag{1}$$

where $\vec{F}$ are the fluxes of the scalar through the surface $\vec{S}$ embedding the volume. Discretizing eqn (1) in a cell control volume Ω_j where U_j is defined, eqn (2) is obtained:

$$\partial_t (U_j \Omega_j) + \sum_{\text{faces}} \vec{F} \cdot \vec{S} = Q_j \Omega_j. \tag{2}$$

In this way the procedure for solving the equations is independent of cell geometry. Cells can have any shape with only some constraints – the computational mesh must be regular – because only fluxes among cell faces are required [3, 5]. Therefore, a complete separation between physical variables and geometry is achieved [6]. As volumes can vary during a run, geometry is updated in every time step after computing flow properties. Moreover, spatial coordinates are independent, meaning that different geometry types can be chosen for each dimension, e.g. Cartesian or curvilinear coordinates can be used in the horizontal dimensions and a generic vertical coordinate with several sub-domains can be used in the vertical. This general vertical coordinate allows minimizing errors if compared with some classical vertical coordinates (Cartesian, sigma, isopycnal) as pointed out by Martins *et al.* [4].

4 Boundaries

Mohid's main input is the domain bathymetry. Bathymetric data can be stored in any regular grid, with independent variable spacing along the X and Y directions. Every grid point has a corresponding depth. The horizontal coordinates can be supplied in a variety of coordinates systems; the most commonly used are metric and geographic coordinates.

Open boundaries arise from the necessity of confining the domain to the study area. Variables values must be introduced in such a way that information about what is happening outside the domain is guaranteed to enter the domain, so that the solution inside the domain is not corrupted. Waves generated inside the domain should be allowed to go out.

5 Hydrodynamic model

Mohid's hydrodynamic module solves the three-dimensional incompressible flow primitive equations. Hydrostatic equilibrium is assumed as well as Boussinesq and Reynolds approximations. The density is obtained from salinity and temperature fields, which are transported by the water property module. The equations solved by Mohid are respectively the equation of mass (3) and the equation of momentum conservation (4):

$$\frac{\partial}{\partial t} \int_V \rho dV = -\oint_A \rho (\vec{v} \cdot \vec{n}) dA, \tag{3}$$

and

$$\frac{\partial}{\partial t}\int_V \vec{v}dV = -\oint_A \vec{v}(\vec{v}\cdot\vec{n})dA + \oint_A \upsilon_T \frac{\partial(\vec{v})}{\partial n}dA - g\oint_A (\eta - z)\cdot\overrightarrow{n_{xy}}dA$$
$$-g\oint_A \left(\int_z^\eta \frac{\rho-\rho_0}{\rho_0}dz\right)\cdot\overrightarrow{n_{xy}}dA - \oint_A p_{\text{atm}}\overrightarrow{n_{xy}}dA + \int_V 2\vec{\Omega}\times\vec{v}dV. \tag{4}$$

In eqns (3) and (4) $\vec{v}$ is the horizontal velocity (v_x, v_y), η is the free surface height, $\upsilon_T = (\upsilon_x, \upsilon_y, \upsilon_z)$ is the turbulent viscosity and $\vec{n} = (n_x, n_y, n_z)$ is the normal to surface A. A is the surface that encircles the control volume V. Ω is the rotation velocity of Earth. ρ is the water density and ρ_0 is the reference water density. g is the acceleration due to gravity and p_{atm} is the atmospheric pressure.

Equation (3) is used to compute both the free surface and the vertical velocity. Equation (4) provides horizontal velocity.

5.1 Turbulence

Turbulence is obtained by multiplying the turbulent viscosity υ_T by the velocity gradient. The horizontal turbulent viscosity υ_H can be either uniform or a function of the velocity gradient (5) according to Smagorinsky [7].

$$\upsilon_H = C\Delta x\Delta y\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)^2 \Big/ 2 + \left(\frac{\partial v}{\partial y}\right)^2\right]^{1/2}. \tag{5}$$

The vertical turbulent viscosity can be computed in three different manners: empirical solutions, mixing length and models of one or two equations.

Taking advantage of the modularity of the Mohid system, the GOTM (General Ocean Turbulence Model – Buchard *et al.* [8]) was coupled to it. GOTM is widely used in a variety of situations and maintained by an active community spread all over the world. This model encompasses the vast majority of the turbulence formulations.

6 Transport models

A transport model is necessary if a property is not evenly distributed. There are two types of mathematical formulations on top of which to build a transport model: Eulerian transport models and Lagrangian transport models.

A Lagrangian transport model follows specific water masses (or objects). For instance, suppose you send an SOS message in a bottle; if you follow the bottle along its path you are using a Lagrangian approach.

In an Eulerian approach there is a mesh (usually) fixed in time. The computation of a given property in each time-step is the result of a mass balance. For instance, suppose that at time step t there is a concentration of suspended sediments in a given cell of the mesh; at $t + 1$ the concentration will be the previous concentration (assuming not all water was renovated) balanced by its inflow and outflow.

6.1 Lagrangian transport model

Lagrangian transport models are very useful to simulate localized processes with sharp gradients (submarine outfalls, sediment erosion due to dredging works, hydrodynamic calibration, oil dispersion, etc.).

Mohid's Lagrangian module uses the concept of tracer. The most important property of a tracer is its position (x, y, z). For a physicist a tracer can be a water mass, for a geologist it can be a sediment particle or a group of sediment particles and for a chemist it can be a molecule or a group of molecules. A biologist can spot phytoplankton cells in a tracer (at the bottom of the food chain) as well as a shark (at the top of the food chain), which means that a model of this kind can simulate a wide spectrum of processes.

Tracers' movements can be influenced by the velocity field from the hydrodynamic module, by the wind from the surface module, by the spreading velocity from oil dispersion module and by random velocity.

At the present stage the model is able to simulate oil dispersion, water quality evolution and sediment transport. To simulate oil dispersion the Lagrangian module interacts with the oil dispersion module. To simulate water quality evolution in time the Lagrangian module is a client of the water quality module. Sediment transport can be associated directly with the tracers using the concept of settling velocity.

Another feature of the Lagrangian transport model is its ability to calculate residence times. This can be very useful when studying the exchange of water masses in bays or estuaries.

6.1.1 Tracer concept

As referred to above, the Mohid's Lagrangian module uses the tracer concept. Tracers are characterized by their three spatial coordinates, volume and a list of properties (each with a given concentration). At every time step each tracer performs a random movement.

The tracers are 'born' at origins. Tracers that belong to the same origin have the same list of properties and use the same parameters for random walk.

6.1.2 Tracer movement

Usually the mean velocity is the major factor influencing particle movement. Spatial coordinates are given by the definition of velocity:

$$\frac{dx_i}{dt} = u_i(x_i, t), \tag{6}$$

where u stands for mean velocity and x for particle position.

The Lagrangian module allows several tracer trajectory computations for each hydrodynamic time step.

6.1.3 Turbulent diffusion

Turbulent transport is responsible for dispersion. The effect of an eddy over a particle depends on the ratio between eddy size and particle size. An eddy bigger than the particle makes it move at random, as explained in Fig. 1. An eddy smaller than the particle causes entrainment of matter into the particle, increasing its volume and mass according to environmental concentration, as shown in Fig. 2.

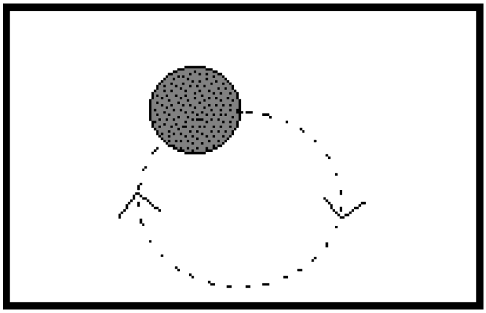

Figure 1: Random movement forced by an eddy larger than the particle.

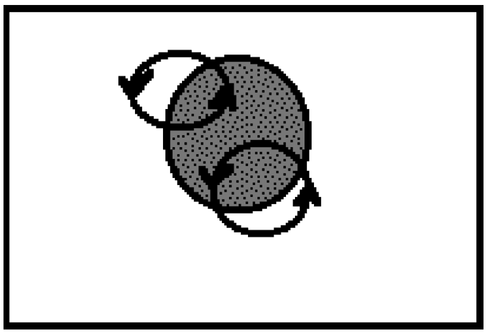

Figure 2: Random movement forced by an eddy smaller than the particle.

6.2 Eulerian transport model

The Eulerian transport model solves the integral version of the equation governing the evolution of a generic quantity P inside a control volume V:

$$\frac{\partial}{\partial t}\int_V P dV = -\oint_A \vec{F} \cdot dA + \text{Sources} - \text{Sinks}. \tag{7}$$

A is the surface neighbouring the control volume. The surface integral of $\vec{F}$ is the flux of P through A. This flux has an advective component and a diffusive component. Sources and sinks are solved by the water properties models coupled to Mohid.

The Eulrerian transport model uses the velocity field computed by the hydrodynamic model. Advective phenomena are computed by multiplying the water fluxes at each surface of the control volume by the property's concentration. Diffusive phenomena are computed using central differences. The Eulerian model uses an algorithm that guarantees mass conservation of every property applying the continuity equation.

7 Numerical modelling of water properties

Above we discussed how Mohid deals with mass transport, either using Lagrangian or Eulerian approaches. Often it is necessary to model properties, e.g. faecal coliform (sewage systems), oil (resulting from oil spills) and biogeochemical cycles. Sinks and sources of non-conservative properties are modelled using zero-dimensional formulations (geometry-independent).

7.1 Water quality model

Efforts towards ecological modelling are being made in most countries where water quality management is a major concern. Most new generation models tend to become much more biologically and chemically diversified than earlier models, as it is now largely recognized that there is no way to simulate in sufficient detail the ecosystem behaviour without an in-depth treatment of the full cycle of organic matter.

The first ecological model coupled to the Mohid system in 1999 [9] is adapted from EPA [10] and pertains to the category of ecosystem simulations models, i.e. sets of conservation equations describing as adequately as possible the working and the interrelationships of real ecosystem components. It is not correct to say that the model describes the lower trophic levels with great accuracy. In fact the microbial loop that plays a determinant role in water systems in the recycling processes of organic waste is very simplified in this first model.

A second ecological model was coupled in 2006 [11]. This model has a decoupled carbon–nutrient dynamics with explicit parameterization of carbon, nitrogen, phosphorus, silica and oxygen cycles. It considers two major groups of producers in the system, diatoms and autotrophic flagellates, and also the dynamics of the microbial loop and several organic matter components. All living and organic matter compartments of the model have variable stoichiometry. Synthesis of chlorophyll is simulated according to the scheme proposed by Geider *et al.* [12], allowing for a temporal and spatial variation of C:Chla ratios in producer populations.

Both ecological models have a zero-dimensional formulation, meaning both can be used with the Lagrangian or the Eulerian transport model, depending on the characteristics of the problem to be solved.

8 Mohid's results

Hydrodynamic fields are the bottom most layer of results produced by Mohid. Every other result is built on top of hydrodynamics, be it wave braking or some transport phenomena. Some results from previous uses of the Mohid system are shown to illustrate models of flow pattern and mass distribution.

8.1 Tagus operational model

IST runs an operational model of the Tagus estuary, Europe's largest estuary. Operational models provide historical and real-time observations and daily predictions of several atmospheric and water conditions of hydrodynamic and biogeochemical properties, both from numerical models and field data. Figure 3 shows Tagus' velocity field, accessed via Google Earth (www.mohid.com/tejo-op/ModOperacional_Tejo.kmz), superimposed with dissolved oxygen superficial concentration. These results are obtained using the Eulerian transport model to calculate advection and diffusion processes and the water quality model to compute local consumption and exchanges with the atmosphere.

Before the widespread use of computers and numerical models, laboratorial analysis of air and water samples, scattered in time and space, provided a discrete image of monitored systems. It is now possible to use automatic acquisition systems (for instance measuring currents and salinity)

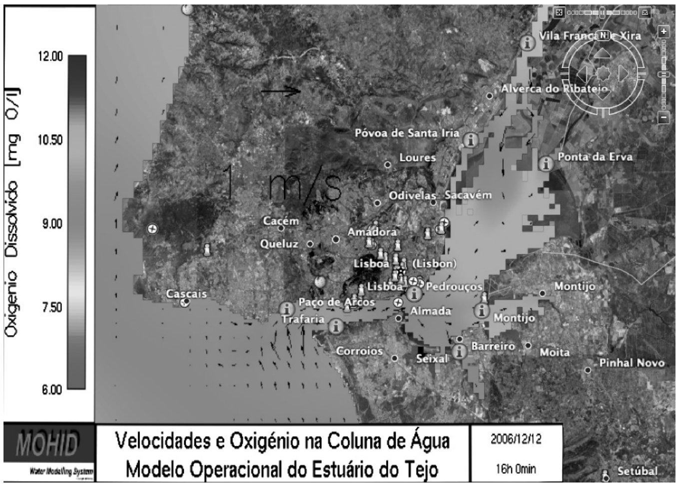

Figure 3: Tagus operational model's results accessed via Google Earth.

and remote sensing from equipment in satellites and planes (for instance for water level or chlorophyll). Numerical models are the best way to fill in field data gaps in space and time. Results from numerical models are inherently continuous and, consequently, more user friendly.

Numerical models used by an operational model are constantly validated by field data and, on the other hand, field data are used as a model input in order to produce forecasts.

Operational models are also used to produce scenarios, making it easy to study extreme natural conditions and the consequences of anthropogenic activities. Operational models are decision support tools that help in reacting to catastrophes and program activities.

8.2 Sediment transport

Lagrangian analysis of transport phenomena is used in two contexts: to simulate properties with sharp gradients and to track particles movements.

In the following example Lagrangian tracers were used to study sediment transport at Nazaré Canyon (off Portugal) [13].

Lagrangian tracers were used to simulate bottom sediments (Figs 4 and 5), highlighting erosion and deposition areas and tracking the advective transport of particles. To these particles, a critical shear erosion, critical shear deposition and a settling velocity is attributed. In this particular case several boxes of particles were distributed along a submarine canyon and adjacent shelf. Figure 4 shows the initial distribution of particles. Each box has a distinct colour so that it is possible to follow each group of particles. In Fig. 5 we can observe their position 11 days after. Lagrangian tracers may be used to simulate transport of sediments, pollutants, chemical particles or even contaminators.

9 Conclusions

Models of flow pattern and mass distribution can be viewed as a framework where different models can be coupled. Mohid provides velocity fields and transport mechanisms. Water properties (ecological values, sediments, oil, etc.) use models that are time and space independent. An

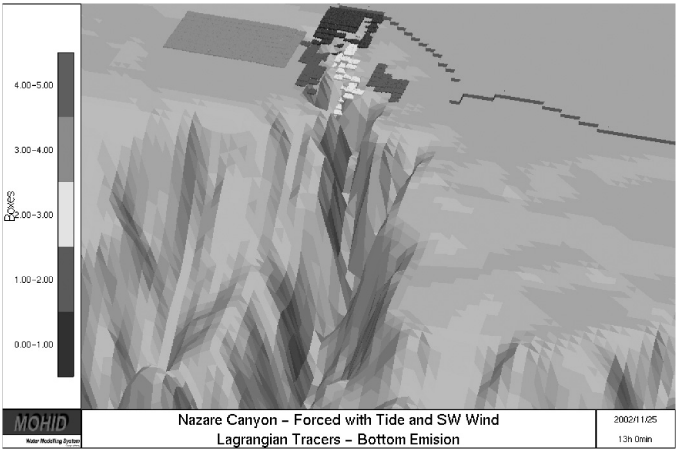

Figure 4: Sediment transport at Nazaré Canyon – day 1.

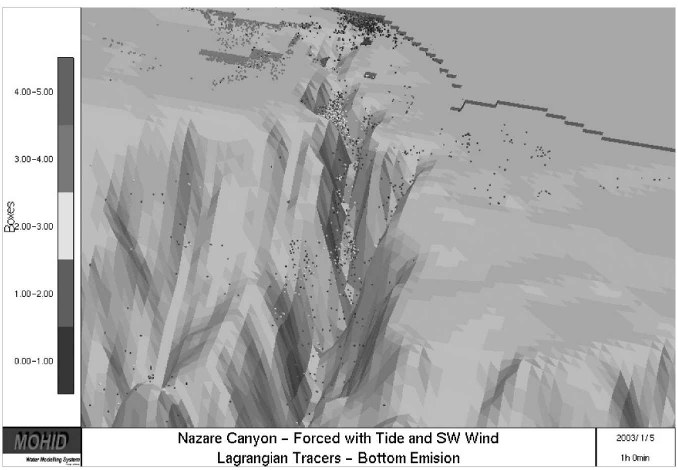

Figure 5: Sediment transport at Nazaré Canyon – day 11.

example of time independence is that phytoplankton do not need to know that it is springtime; there is a set of physical conditions (temperature, light, nutrients, etc.) that triggers the spring bloom. In addition, phytoplankton do not know whether it is in Africa or Europe.

The strength of this type of model relies in the loose coupling of the three tiers that compose it. There is a high level of abstraction in the way each sub-model relates with each other, for instance, hydrodynamic results are always the same, and run exactly the same way, regardless of how many water properties are modelled.

Models of flow pattern and mass distribution are very complex and require a large amount of computational power. The use of models of flow pattern and mass distribution is highly recommendable whenever advective/diffusive processes are important. Transport phenomena take a non-negligible role wherever strong gradients are present, as for instance in an oil spill.

Models should only be plugged into a model of flow pattern and mass distribution after being fully developed. In the early stages of model development a system of flow pattern and mass distribution may prove far too complex.

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