MODELLING COASTAL SYSTEMS: THE MOHID WATER NUMERICAL LAB

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1 THE MOHID MODELLING SYSTEM

MOHID Water is a numerical model included in MOHID Water Modelling System (Braunschweig et al. 2004), an integrated water modelling software that can be used to simulate water bodies, porous media flow and infiltration, and watersheds (http://www.mohid.com). Over the past years MOHID Water has been used to simulate a variety of processes and scales in marine systems. This chapter presents a brief record of these applications, along with a description of the transport processes simulated by the MOHID system and its modelling philosophy. MOHID Water is the latest version of MOHID long set of evolutions which started back in 1985. Since then, a continuous development effort of new features has been maintained. Model updates and improvements have been made available on a regular basis and used in the framework of many research and engineering projects. Initially, MOHID was a two-dimensional tidal model written in FORTRAN 77 (Neves 1985). This version also gave the present name to the model, which derives from the Portuguese abbreviation of ”MOdelo HIDrodinámico” (Hydrodynamic Model). Traditionally known as a hydrodynamic model, it was first used to study estuaries and coastal areas using a classical finite-differences approach. Further developments included a 3D setup and the addition of baroclinic effects (Santos 1995), and full discretization to a finite volumes approach, allowing the use of generic vertical coordinates (Martins 2000).

A substantial increase in the number of users has occurred since the model was made available on Internet, backed up by an online user forum. Model robustness in hydrodynamics set the basis for the development and coupling of a transport model, including fine sediment transport (Cancino and Neves 1999). This development also allowed the coupling of a water quality (eutrophication) module (Portela 1996, Miranda 1999, Pina 2001, Saraiva et al. 2007) which increased the variety of model applications and transformed the model into a fully integrated tool. In time, the increase of MOHID programmers and users proved to be unsustainable due to the multidisciplinary nature of the endeavour and to FORTRAN 77 language limitations. So it was necessary to establish a methodology which allowed reusing the code systematically and improving its robustness. The model was restructured and converted to ANSI FORTRAN 95, profiting from its new features such as the ability to use object oriented programming methods. This migration began in 1998, implementing object oriented features as described by Decyk et al. (1997) with significant changes in code organization (Miranda et al 2000), leading to an object oriented model for surface water bodies which integrates different scales and processes (Leitão 2003). The object oriented strategy proved to be reliable and robust, though it has increased the code and the execution time twofold or threefold, depending on the nature of the applications (Miranda et al. 2000). Presently the MOHID development is a relatively straightforward task due to the use of this philosophy.

2 APPLICATION EXAMPLES

MOHID Water has been applied in numerous studies, integrating a wide variety of processes and scales. Among the recent applications to marine systems we find:

- Estuaries: Sado estuary, Portugal (Martins et al. 2001); Tagus estuary, Portugal (Leitão et al. 2003, Braunschweig et al. 2003, Mateus 2006); Guadiana, Portugal (Saraiva et al. 2007);
- Coastal lagoons: Ria de Aveiro (Trancoso et al. 2005, Vaz et al. 2007); Ria Formosa (Silva et al. 2002), Óbidos (Silva et al. 2005);
- Coastal areas: Ria de Pontevedra; Spain (Villarreal et al. 2002), Brazilian Coast (Leitão et al. 2004), Nazare Canyon, Portugal; Galician coast (Carracedo et al. 2006, Fig. 1);
- Oceans: Cadiz Gulf, Spain (Leitão et al. 2005), Iberian West Coast (Coelho et al. 2002, Santos et al. 2005).

Some of these modelling studies focused only on hydrodynamic processes: Cadiz gulf circulation (Leitão et al. 2005); Poleward current (Coelho et al. 2002); Barotropic 3D flows in an estuary (Martins et al. 2001) and in a costal lagoon (Silva et al. 2002); Baroclinic 3D flow in an estuary (Leitão 2003) and in a Galician Ria (Villarreal et al. 2002); Waves and currents interaction effect on the sea level in a coastal lagoon (Silva et al. 2005); Non hydrostatic processes associated with internal waves (Theias 2005). Some studies were also focused on the dynamics of fine sediment: In the Western Scheldt and Gironde estuaries (Cancino and Neves 1999); Dredge material contaminated with release in a coastal area off-shore of the Santos estuary (Leitão et al. 2004); The effect of internal tides on fine sediment transports in the Nazare Canyon, located on the Portuguese coast. Other studies focused on water quality issues: The Prestige oil spill (Carracedo et al. 2006); Influence of nutrient loads in Portuguese estuaries (Saraiva et al. 2007); Modelling of Macroalgae in a shallow temperate estuary (Trancoso et al. 2005); Modelling phytoplankton dynamics in the Tagus estuary, Portugal (Mateus 2006); A methodology to estimate renewal time scales in estuaries applied to the Tagus Estuary case (Braunschweig et al. 2003).

3 TRANSPORT PROCESSES

Transport processes play a key role in marine environments and so one main goal of MOHID is to simulate them accurately. This modelling system simulates the transport processes of momentum, mass and heat in the water column, and the vertical transport of mass in the sediment column. Mass can be transported in the dissolved phase and the particulate phase, both in the water and the sediment columns (Figure 2). The particulate matter tends to be adsorbed to the fine sediments. The fine sediments settle at the water-sediment interface (fluff layer). They can be eroded or undergo a consolidation process; if they are consolidated the adsorbed particulate matter can be transferred to the dissolved phase and be dispersed in the sediment column by diffusion processes (Figure 2). The accurate simulation of hydrodynamic and fine sediments dynamics is critical for modelling the transport of water properties (e.g. primary producers, particulate and dissolved organic matter, oxygen, etc.) controlling in a relevant way the biogeochemical variability of the marine systems. MOHID simulates the hydrodynamic processes in the water column using a eulerian referential. However, the transport of mass and heat can be done using a eulerian or a lagrangian referential. The fine sediments dynamic can be divided into two major compartments: the water column and the sediment column. In the first the transport is highly 3D in nature, while in the second the transport is mainly in the vertical direction.

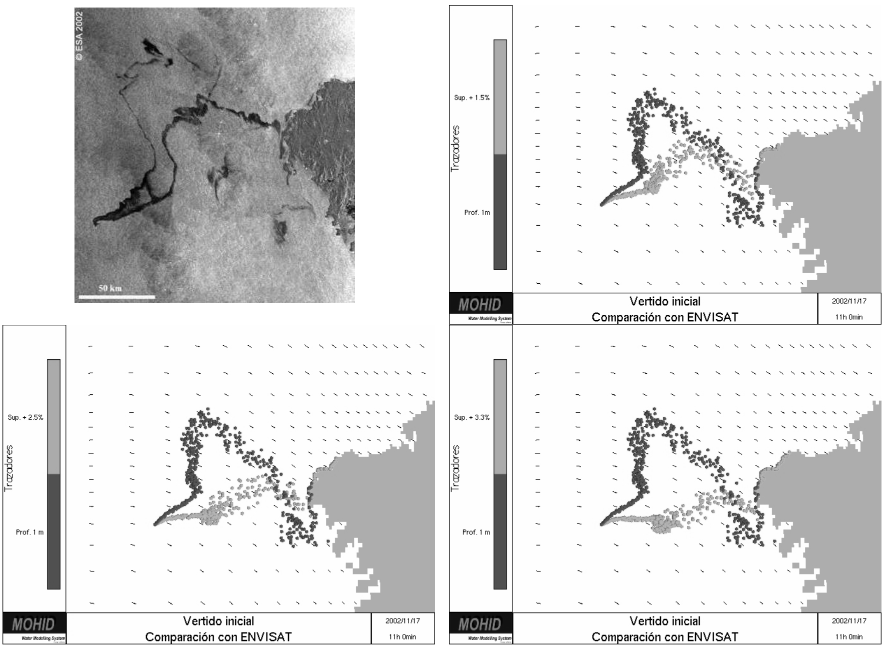

FIGURE 1: *Lagrangian particles are released at different depths: surface particles (dark grey), 1 m depth particles (light grey). Surface particles are directly dragged by wind with a velocity proportional to the wind velocity in a percentage of (b) 1.5%, (c) 2.5%, (d) 3.3%. Results are compared with an ENVISAT satellite image (a) taken on November 17th (adapted from Carracedo et al. 2006).*

3.1 Eulerian referential

MOHID is able to simulate in an Eulerian referential (fixed grid) the transport processes of momentum, mass and heat in the water column. The evolution of the non-turbulent flow properties (hydrodynamics) is computed using the Navier-Stokes equations for a rotating fluid. The geophysical fluid is constrained to the hydrostatic and the Boussinesq approximations, as a practical result of dimensional analysis. The spatial discretization is done using a finite-volumes approach (Martins et al. 2001) similar to Chu and Fan's (2004) method. MOHID also solves a seawater density non-linear state equation, depending on pressure, salinity and potential temperature using the algorithm of Millero and Poisson (1981). The system uses a structured grid: an Arakawa C grid type in the horizontal and a generic vertical coordinate with the possibility to choose different types of discretizations (e.g. z-level, sigma and double-sigma coordinates). A "partial step" approach is recommended for bottom layer discretization for z-level vertical discretization in 3D models. This methodology is better than the traditional "full step" or "staircase" approach. Adcroft et al. (1997) show that this approach minimizes the traditional problems associated with the staircase topography of z-level models ("staircase noise"). The baroclinic pressure gradient term is always calculated using a z-level approach, with a linear interpolation, to minimize spurious pressure-gradients (Kliem and Pietrzak 1999).

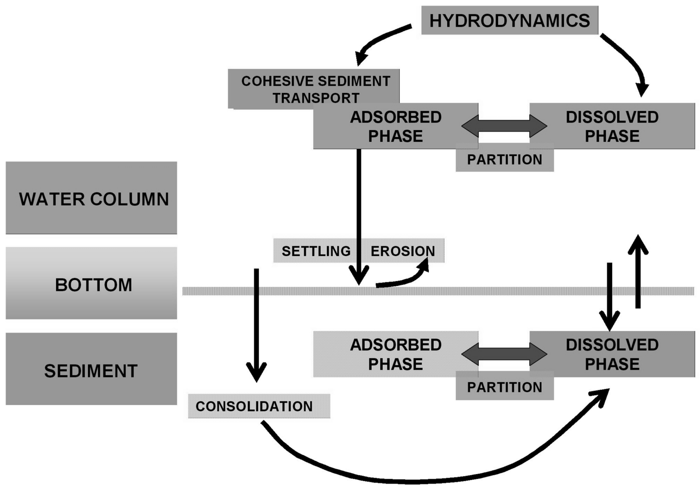

FIGURE 2: *Transport processes model by MOHID.*

The temporal discretization is done using an alternate direction semi-implicit (ADI) method for the 2D mass balance equation (used to compute the SSH). For the 3D momentum (zonal and meridional velocities), heat and salt balance equations in the vertical direction are computed implicitly while the horizontal directions are calculated explicitly. The advection of momentum, heat and salt is computed using a total variation diminishing (TVD) scheme with a Superbee limiter. A biharmonic filter for the velocities is used to dissipate high frequency noise in applications where the dissipation rate is low (e.g. open ocean applications). The advantage of this methodology, relatively to the Fickian diffusion, lies in its ability to dissipate the high-frequency processes without significantly changing the lower frequency processes. To calculate the turbulent vertical mixing, the GOTM (Burchard 2002) code is embedded in MOHID. The parametrization proposed by Canuto et al. (2001) is used by default in the MOHID system. Finally, the hydrodynamic model can be forced with tide, momentum and atmospheric heat fluxes, wind waves and fresh water discharges.

3.2 Open boundary

To prescribe coherent open boundary conditions (OBC), good external data are mandatory (Blayo and Debreu 2005). There are several sources of external solutions for coastal applications. Several global tidal solutions became very common approximately 15 years ago (e.g. CSR4, FES2004, GOT00.2, NAO. 99b, TPXO6.2). The MOHID system has the necessary software tools to generate the external solution from the FES2004 tidal SSH atlases (Lyard et al. 2006). Pre-operational models have been made available over the last years (Mercator, HYCOM-US, Topaz and FOAM), providing a best estimate on the current state of the ocean low frequency processes. The MOHID system also has the necessary software to use the Mercator and HYCOM-US for external solutions and initial conditions (Leitão et al. 2005). The MOHID system allows the user to construct a tree of one-way nested models with no limitations on the number of nesting levels from a software perspective (Braunschweig et al. 2004). By default, for each nesting level the external data for the OBC is the upper level in the MOHID nesting system. However, the user can add another solution linearly to the upper nesting levels. This nesting capability allows overlapping different scales in an efficient way to study local processes.

3.3 Lagrangian referential

Mohid can simulate the transport of mass (dissolved and particulate) in the water column using a lagrangian approach (Leitão 1996). The velocities of lagrangian particles at any point in space are calculated with a linear interpolation between the points of the hydrodynamic model grid. Turbulent transport is responsible for dispersion. The effect of eddies on particles depends on the ratio between eddies and particle size. Eddies bigger than the particles make them move at random. On the other hand, eddies smaller than the particles cause entrainment of matter into the particle, increasing its volume and mass according to the environment concentration. The random movement is calculated following the procedure proposed by Allen (1982). The random displacement is calculated using the mixing length and the standard deviation of the turbulent velocity component, as given by the turbulence closure of the hydrodynamic model. Particles retain the velocity during the necessary time to perform the random movement, which is dependent on the local turbulent mixing length (Leitão 1996). It is also possible to associate to the particle the main processes of the fine sediments dynamics described below: settling velocity, adsorption/desorption, deposition and erosion.

3.4 Fine sediments in the water column

Particulate properties transported in the water column are governed by a 3D advection-diffusion equation where the vertical advection includes the particle settling velocity. Two different approaches are followed to compute settling: a constant settling velocity and a settling velocity dependent of fine sediment concentration. In the first case, each particulate can have its specific and constant settling velocity, which can be derived from literature (depending on its size and biogeochemical characteristics). The latter approach, however, needs some considerations. Since the settling velocity algorithm was developed for fine sediment modelling, it raises the question of how the settling velocity of particulates with other properties can be computed. The model assumes the same velocity as for the fine sediment settling velocity, therefore reinforcing the importance of fine sediments in the distribution and fate of the adsorbed contaminants fraction. The algorithm follows a formulation widely used in literature (e.g. Mehta 1988), where the general correlations for the settling velocity in the flocculation range are:

$$W_S = K_1 C^m \quad for \quad C < C_{HS} \tag{1}$$

and in the hindered settling range:

$$W_S = K_1 C_{HS}^m \left[1.0 - K_2 \left(C - C_{HS}\right)\right]^{m_1} \quad for \quad C > C_{HS} \tag{2}$$

where W_S ($m\ s^{-1}$) is the settling velocity, C ($kg\ m^{-3}$) is the concentration, and the subscript HS refers to the onset of the hindered settling (of about 2 to 5 $kg\ m^{-3}$). The coefficients K_1 ($m^4\ kg^{-1}\ s^{-1}$) and K_2 ($m^3\ kg^{-1}$) depend on the mineralogy of the mud and the exponents m and m1 depend on particle size and shape.

3.4.1 Adsorption/Desorption

Adsorption and desorption are considered as a reaction process, that can be included in the sinks and sources terms of the transport equation. This reaction involves the dissolved and the particulate phases of the contaminant being simulated, where the two phases tend to an equilibrium, which is given by a partition coefficient. The equilibrium can be described by the following system of equations (Hayter and Pakala 1989):

$$\frac{\partial C_d}{\partial t} = k \left(D\% \times C_p - P\% \times C_d\right) \tag{3}$$

$$\frac{\partial C_p}{\partial t} = k \left(P\% \times C_d - D\% \times C_p\right) \tag{4}$$

where C_p and C_d are the particulate and dissolved contaminant concentrations respectively; k (s^{-1}) is the equilibrium kinetic rate for adsorption-desorption between dissolved and particulate phase; D% is the dissolved contaminant fraction; and P% the particulate contaminant fraction. The kinetic constant defines the rate at which the two phases tend to equilibrium. To account for the fact that, in the presence of low suspended matter concentrations, the adsorption process is less likely to occur (the probability of a contaminant ion to collide with a particle is lower), a direct relation between the kinetic rate and the suspended particulate matter was implemented:

$$\begin{cases} k = k_{ref} \cdot \frac{C_{SPM}}{C_{SPMreference}} & for \quad \frac{C_{SPM}}{C_{SPMreference}} < 1 \\ k = k_{ref} & for \quad \frac{C_{SPM}}{C_{SPMreference}} \geq 1 \end{cases} \tag{5}$$

where C_{SPM} is the concentration of the suspended particulate matter approximately equal to the fine sediment concentration. The k_{ref} is the kinetic rate for a C_{SPM} of reference ($C_{SPMreference}$).

3.5 Water-sediment interface model

The water sediment interface model also known as fluff layer computes and manages boundary conditions for the water column and sediment compartments.

3.5.1 Fine sediments fluxes

For fine sediments at the bottom, a flux term, F_b (mass of sediment per unit bed area per unit time) can be defined, corresponding to a source or sink for the suspended particulate matter in conditions of erosion or deposition, respectively. Consequently, at the bottom:

$$F_b = F_E - F_D \tag{6}$$

where F_E and F_D are respectively the erosion and deposition fluxes. It is assumed that, when bottom shear stress is smaller than a critical value for deposition, there is addition of matter to the bottom, and, when the bottom shear is higher than a critical value, erosion occurs. Between those values, erosion and deposition balance each other. The erosion algorithm used is based on the classical approach of Partheniades (1965). Erosion occurs when the bottom shear stress exceeds the threshold of erosion. The flux of eroded matter is given by:

$$\begin{cases} F_E = E\left(\frac{\tau}{\tau_E} - 1\right) & for \quad \tau_b > \tau_{CSE} \\ F_E = 0 & for \quad \tau_b < \tau_{CSE} \end{cases} \tag{7}$$

where τ is the bed shear stress, τ_{CSE} is a critical shear stress for erosion and E is the erosion parameter ($kg\ m^{-2}\ s^{-1}$). This erosion algorithm is computed at the sediment-water interface. If this layer is eroded, erosion occurs from the underlying sediment layer, which has a higher level of compaction, therefore increasing the erosion shear stress thresholds. This is obtained by defining τ_{CSE} as depth dependent, reflecting the increasing resistance of the sediment to be eroded as scouring reaches deeper layers. Wave induced shear stress can also be computed by the model by a linear wave theory, given wave characteristics such as wave period and wave significant height. Estuarine local waves can be important in terms of sediment resuspension, especially in shallow water where the wave stresses effect reaches the sediment bed. Pina (2001) presents a detailed description on the formulation implemented in the model. On the other hand, the deposition flux can be defined as:

$$F_D = -p(W_S C)_b \tag{8}$$

where p is the probability of sediment particles to settle down on the bed; W_S is near-bed the settling velocity; and C the near-bed fine sediment concentration. The probability of deposition (Krone 1962), can be defined as:

$$p = (1 - \frac{\tau_b}{\tau_{CSD}}) \tag{9}$$

where τ_b (Pa) and τ_{CSD} (Pa) are the bottom shear stress and the critical shear stress for deposition respectively. This concept reflects the fact that the deposition of flocks is controlled by near-bed turbulence. For a flock to stick to the bed, gravitational forces must be strong enough to withstand the near bed shear stress. The deposition algorithm (Krone 1962), like the erosion algorithm, is based on the assumption that deposition and erosion never occur simultaneously, i.e., a particle reaching the bottom has a probability of remaining there that ranges from 0 to 1 as the bottom shear stress varies between its upper limit for deposition and zero respectively. Deposition is calculated as the product of the settling flux and the probability of a particle to remain on the bed:

$$\begin{cases} F_D = (CW_S)_B(1 - \frac{\tau}{\tau_{CSD}}) & for \quad \tau_b < \tau_{CSD} \\ F_D = 0 & for \quad \tau_b > \tau_{CSD} \end{cases} \tag{10}$$

The critical shear stress for deposition depends mainly on the size of the flocks. Bigger flocks have a higher probability of remaining on the bed than smaller flocks. As only a single characteristic class of fine sediment is considered in the model, parameters must be calibrated, starting from reference values found in literature, in order to achieve good approximations in the final results. Consolidation is considered to occur in recently deposited sediments at the sediment-water interface and is modelled as a sediment flux, $F_{consolidation}$ (kg_{sed} m^{-2} s^{-1}), between the fluff layer and the first sediment layer at a certain rate, $k_{consolidation}$ (s^{-1}), dependent on the sediment mass per unit of surface area deposited at the fluff layer. It is assumed that consolidation only occurs when shear stress (τ_b) is lower than the critical shear stress for deposition (τ_{CSD}):

$$\begin{cases} F_{consolidation} = 0 & for \quad \tau_b > \tau_{CSD} \\ F_{consolidation} = M_{sediment} \cdot k_{consolidation} & for \quad \tau_b < \tau_{CSD} \end{cases} \tag{11}$$

This consolidation flux is one of the governing processes for particulate contaminant fractions to enter the sediment compartment.

3.5.2 Particulate properties fluxes

Particulate properties fluxes at the sediment-water interface depend on erosion and on consolidation processes. As the erosion algorithm was developed specifically for fine sediment modelling, when computing other particulate properties fluxes at the bed, the erosion rate parameter cannot be the same. Thus, a specific proportionality factor for the erosion constant is computed, E_{prop}, for each property, relating the quantity of property ($M_{property}$ in $kg_{property}$ m^{-2}) to the quantity of fine sediment deposited in the bed ($M_{sediment}$ in kg_{sed} m^{-2}). The particulate property erosion flux is then computed similarly to fine sediments but with a specific E_{prop}:

$$E_{prop} = E\left(\frac{M_{property}}{M_{sediment}}\right) \tag{12}$$

In this way, critical shear stress values are considered equal for all particulate properties, with the specific erosion constant being the differentiating factor. When consolidation occurs a similar algorithm is followed, relating the sediment consolidation flux to the particulate property deposited mass. Thus, the property consolidation flux (F^{prop}) can be computed with the following expression:

$$F^{prop}_{consolidation} = F^{sediment}_{consolidation}\left(\frac{M_{property}}{M_{sediment}}\right) \tag{13}$$

3.5.3 Dissolved properties

Dissolved properties fluxes across the water-sediment interface depend both on erosion / consolidation processes and on concentration gradients between the water column lower layer and on the interstitial water of the sediment upper layer. As stated before, when the fluff layer is active (i.e. there are recently deposited sediments on the bed), interstitial water between those sediment particles is not considered. Thus, when erosion occurs there is no dissolved properties influx from the fluff layer to the water column. The interstitial water in the sediments upper layers (containing solutes such as dissolved contaminant fractions, nutrients, etc) is flushed to the water column when consolidated sediment is eroded (upper sediment compartment layer). On the other hand, when consolidation occurs, water overlying the sediment bed becomes part of the sediment interstitial water. These processes constitute an additional flux of solutes to and from the water and sediment columns. Thus, a water flux (F^{water} in $m^3\ s^{-1}$) can be computed, corresponding to the amount of porewater dragged along with the eroded sediments or to the amount of overlying water captured in the consolidation process:

$$F^{water}_{erosion/consolidation} = F_{erosion/consolidation} \cdot A \cdot \phi_k \cdot \frac{1}{\rho_{sed} \cdot (1 - \phi_{kn})} \tag{14}$$

where, $F_{erosion/consolidation}$ is the fine sediment flux ($kg_{sed}\ m^{-2}\ s^{-1}$) between the sediment-water interface and the sediments' upper layer, ϕ_{kn} is the porosity in the upper (k=n) sediment layer, ρ_{sed} is the sediment dry density ($kg_{sed}\ m^{-3}_{sed}$) and A is the area (m^2) of the sediment-water interface. Respectively, solute fluxes are given by:

$$F^{solute}_{erosion/consolidation} = \frac{F^{water}_{erosion/consolidation} \cdot C^{solute}}{A} \tag{15}$$

where C is solutes' concentration ($kg\ m^{-3}_{water}$) in the sediment upper layer or in the water column bottom layer, depending on the type of flux (erosion or consolidation). As mentioned above, the concentration gradients between the water column bottom layer and the sediment surface layer can also produce a mass flux through the sediment-water interface. Solutes in a turbulent flow can be transported by a mean advective flux, turbulent diffusion and molecular diffusion. It is usually considered that solutes diffusion coefficient is equal to the fluids turbulent viscosity, which are usually several orders of magnitude higher. Nonetheless, when approaching the sediment bed water flow is reduced, and the same is true of turbulent motion, leading to an increase in the importance of molecular diffusion relative to the turbulent one. Thus, a sub-diffusive layer (Boudreau 1997) is formed, where a linear concentration gradient can be considered, and a diffusive flux, $F_{diffusive}$ ($kg_{solute}\ m^{-2}\ s^{-1}$), can be computed representing the rate at which this gradient tends to be eliminated:

$$F_{diffusive} = \frac{D_{molecular}}{\delta} \cdot A \cdot (C_{water} - C_{intertidal}) \tag{16}$$

in which $D_{molecular}$ is the molecular diffusion coefficient ($m^2\ s^{-1}$), and δ (m) is the sub-diffusive boundary layer thickness, which is dependent on near-bed turbulence:

$$\delta = \frac{2 \cdot \nu_{water}}{u_+} \tag{17}$$

where ν_{water} is the water kinematic viscosity ($m^2\ s^{-1}$) and u_+ is near-bed shear velocity ($m\ s^{-1}$).

4 SEDIMENT COLUMN MODEL

The sediment compartment consists of saturated porous media, formed by sediments and by water that fills the interstices between the sediments. Properties in this compartment can either be dissolved (in the porewater), or particulate (adsorbed on to sediments). The sediment-water interface handles processes occurring between the water and the sediment column. Since it is very difficult to define physically, this interface really is an abstraction. In the model it can be seen as a thin sediment layer (fluff-layer) with transient characteristics, depending basically on temporal scales associated with hydrodynamics and transport in the water column, namely erosion and deposition. This layer has a separation function, which allows dissociating processes that occur on the sediment deposit, at a very slow scale, "filtering" the high frequencies of erosion/deposition fluxes that shape it, therefore leading to consolidation. Dissolved properties can be produced in the interface but their mass is not part of it, becoming part of the water column by means of a boundary condition flux. Contrastingly, particulate properties are part of the sediment-water interface. This can be the case when sediment deposition occurs but the sediment is not yet consolidated. Thus, a particulate property deposited mass is tracked in order to know how much of is available when erosion conditions occur. Following this concept, it is considered that dissolved properties can exchange fluxes directly between the water column and the sediment interstitial water. In erosion conditions, if this transient layer is completely eroded, then scouring takes place from the sediment compartment upper layer, where consolidated sediment is present. When this happens, interstitial water is entrained along with the sediment, constituting a flux to the water column. In the same way, when the fluff-layer consolidates and becomes part of the sediment column there is an input of overlying water (and its properties) to the sediment compartment. The sediment column model is a set of 1D vertical models defined below the 3D water column model (Figure 3). Both models share the same horizontal discretization, but compute independent vertical coordinates. Adsorption and desorption processes are simulated with a similar approach as in the water column.

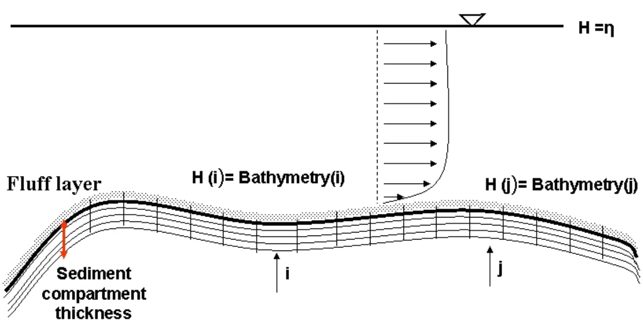

FIGURE 3: *Sediment compartment discretization.*

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