AN EULERIAN–LAGRANGIAN MODEL
FOR SEDIMENT TRANSPORT
IN ESTUARIES

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Aos meus pais

e ao Zé
There is a time for everything under the sun:
there is a time to grow,
there is a time to learn,
there is even a time for acknowledgment...

(adpt. Ecclesiastes)

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ABSTRACT

A depth–averaged model for the simulation of the fate of cohesive and non–cohesive sediments in estuaries, ELASED, is described and partially tested. The model was developed as a part of a computational structure for the integrated analysis of the dynamics and water–quality of coastal systems, ACE, which includes complementary circulation and water–quality models.

The formulation of the governing equations of ELASED relied on an extensive review of the current understanding of the main controlling mechanisms for sediment transport: hydraulic transport, aggregation and deposition, erosion, bottom consolidation, production (for organic sediments), and bioturbation (not included in the model). This review constituted a major part of the reported work, and is described in detail, together with a review of existing sediment transport models.

ELASED describes both the sediments suspended in the water–column (through an advection–dispersion– transformation equation) and the evolution of the bottom sediments (through an erosion–consolidation algorithm). Relevant features of the formulation include the recognition of the possible simultaneity of erosion and deposition, and the treatment of flocculation as a second–order reaction.

The solution of the governing equations is based on an Eulerian–Lagrangian method, that combines the Backwards Method of Characteristics (for advection) with the Finite Element Method (for dispersion, transformation, and bottom evolution). This numerical method has been very successfully applied to single,passive dissolved contaminants. This work contributes to the extension of the method to transport problems with multiple variables, and with water–column bottom–interaction.

ELASED was tested for two relatively simple situations: (a) a laboratory– scale rectangular channel, and (b) a field–scale rectangular channel with an expansion. In both cases, a steady flow was considered. Results are qualitatively consistent with what should be expected, but strongly suggest the need for a more realistic quantification of the various empirical coefficients intervening in the model.

Future work should concentrate on the application of ELASED to the analysis of actual estuaries, and be supported by field work and data analysis.

Keywords: Sediment Transport, Erosion, Deposition, Flocculation, Eulerian–Lagrangian methods, Finite–element methods, Estuaries.
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1. — INTRODUCTION

1.1 — Statement of the general problem

Generally surrounded by areas of large popational density and intense industrial activity, estuaries are used by man as natural harbors, and as natural disposal site of urban and industrial wastes. Very often they have been, indeed, the "waste treatment" facility of the big metropolis. In the second half of this century, primary and secondary treatment of urban and industrial effluents began to be implemented, reaching status of governmental disposition in the most developed countries. Simultaneously, legislation has been progressively approved to limit the use of potential contaminants. However, the environmental issue, and water–quality related standards in estuaries, are still very important targets of social concern due to: (a) — the lack of effective control over industrial discharges; (b) — the very low degradability, and inherent persistence of many contaminants used before their toxicity could be traced, or identified.

Besides waste disposals, estuaries receive river discharge, lateral runoff, and oceanic inputs. Sedimentary particles constitute the bulk of those inputs. Because of the mutual interaction between riverine discharge and tidal forcing, the circulation patterns in estuaries induce the deposition of large amounts of particles.

The development of extensive shoaling areas, filling navigation channels and docks, very often lead to inefficiency in the exploitation of harbor facilities, and traffic limitation in the navigation channel. These difficulties are overcome by removal of the deposited layers. Dredging operations are responsible for large controversy in the following aspects: economic — they are extremely expensive; land management — they require the use of adequate disposal sites for the dredged material; and, finally environmental — they may
reactivate, by resuspension of sediments, the chemical activity of toxic pollutants buried in deeper layers of the shoaling pools.

Toxic contaminants show strong affinity for sediments by means of water and surface chemistry processes: adsorption and desorption. In fact, trace metals, polychlorinated byphenyls – PCB's, polycyclic aromatic hydrocarbons – PAH's, and manmade organocompounds are readily scavenged from the water column, and incorporated into the particulate phase. The residence times of those pollutants, along with their potential for toxicity impact, in time and amplitude, greatly increase in the critical deposition areas of the estuary. Since heavy metals, PCB's, PAH's, and their metabolites present almost null, or very slow breakdown, deposition and resuspension of sediments behave as regulatory processes of the chemistry of the system, effectively controlling the availability of toxic substances to biota, and ultimately to man.

1.2 – Research objectives

The objective of this work is to develop a state-of-the-art model for sediment transport, that combines a rigorous and comprehensive description of the driving mechanisms, with an advanced numerical algorithm.

This model, ELASED – Eulerian–Lagrangian Analysis of Sediment Transport—, is the first sediment transport model to solve the advection–dispersion equation by an Eulerian–Lagrangian technique, very successfully applied to the transport of neutral substances in the recent past; and it is also, the first model of sediment transport that addresses explicitly, and as a whole, the aggregational mechanisms in the water-column, the eventual simultaneity of erosion and deposition, and the consolidation of bottom layers.
ELASED is a two–dimensional, depth averaged, finite–element model, that can be applied to cohesive and non–cohesive sediments. Flocculation is introduced by means of an analytical solution, whereas erosion and deposition are considered bottom boundary conditions. The consolidation algorithm consists on the use of a semi–empirical profile, whose shape is inferred from analysis of field data. The model is prepared to perform as an intermediate tool for future water–quality analysis.

Although some progress, in terms of an integrated simulation of the major phenomena involved in the dynamics of sedimentation, has been accomplished in this decade, the application of transport models to real estuaries still relies, very strongly, on the collection of field data. The quality of the results obtained is determinant on the ability of the model to simulate real mechanisms, and eventually on its potential to be managed as a predictive tool. Additional work of experimentation and calibration of the model will have to proceed, involving field surveys to collect data, and the development of reliable techniques of data analysis in a modeling perspective.

1.3 – Research Outline

The text is divided into five chapters, including the present Introduction.

In Chapter 2 we review the fundamental concepts and mechanisms associated with the dynamics of sediments in estuaries. Section 2.1 introduces the estuary as an individualized sedimentary environment. Section 2.2 provides the basic background on the characteristics of sediment particles. Section 2.3, which relies strongly on the work of Partheniades, Einstein, Krone, Mehta, and more recently, O'Melia, de Vriens, Westrich, Hayter and Luettich, discusses the dynamics of sediments. Hydraulic transport, erosion, deposition, and flocculation are treated with particular emphasis. Section 2.4 describes relevant aspects related to the fate of trace elements in estuaries. Among all possible
contaminants trace elements were chosen because they are largely used in industrial activities, most often out of control; because of their persistence, and easy penetration in the food chain, and finally, because highly toxic manmade compounds, as for example TBT, are also included in the group of trace elements.

Chapter 3 presents a general description of several sediment transport models, developed and applied in the current decade\textsuperscript{11,12,17,31,73,82,84}, which are among the best contributions to the development of sediment transport modeling.

Chapter 4 describes and tests ELASED, the new sediment transport model proposed. Section 4.1.1 presents the mathematical formulation of the model, whereas Section 4.1.2 discusses the numerical strategy used in its implementation. Section 4.3 describes the procedures of preliminary testing, and includes critical discussion of the results obtained. The problems tested are divided into two groups: (a): an attempt to simulate the recirculating flume experiments presented by Hayter in 1984; (b): an application to a simplified hypothetical "estuary" composed of a channel and an enlargement. The parameters used in case (b) were collected in the literature, and do not represent the real conditions of any estuary. However, this test was designed in the perspective of developing a better feeling of the difficulties involved in real-world applications.

Chapter 5 discusses the results obtained with this work, and identifies the objectives yet to reach: better handling of field data collection and analysis, reliability of the model as a predictive tool, and finally its applicability to water-quality problems.
2. — CONCEPTS AND MECHANISMS

"An estuary is a semi-enclosed coastal body of water, which has a free connection with the open sea, and within which sea water is measurably diluted with fresh water derived from land drainage". [Pritchard75]

2.1 — Estuaries as Sedimentary Environments

Typical estuaries behave as huge storage sinks of sedimentary particles. The main sources of sediments in estuaries are the river discharge, lateral runoff and waste disposals, as well as the oceanic contribution. The magnitude of the net input of sedimentary particles into the estuary is a function of the river transport capacity, available sediments supply, intensity of waves, long-shore currents and tidal action.

Besides river inflow, lateral runoff and waste disposals, marginal erosion and wind-blown sediments may also be important sources of sediments. Internal source is the in-situ production of biogenic particles as microbes, plants, fecal pellets, and calcium carbonate. Erosion and deposition occurring in the bottom layers of the estuary play role of source, or sink, as well. Suspended sediments escape the water-column by stable sedimentation, flushing, organic oxidation and biological cycling.

Estuarine bulk sediments are mainly constituted by relative coarse debris (150μm–300μm), fine sands, silts, clays, detritus, and microorganisms. The organic contents of sediments has a determinant role as an water-quality indicator, since the organic carbon contents regulates the uptake and release of trace metals and toxic organic
compounds. Organic matter is provided by the river input of sediments, runoff, wind–blown materials and essentially by waste disposals and biogenic activity.

The patterns of the flow circulation inside the estuary, as well as the nature and availability of sediments, are responsible for the distribution of the sediments by areas of predominant characteristics. The hydrodynamic circulation can be controlled either by the river or by the ocean. The development of extensive shoaling zones seawards is directly related to the predominance of riverine influence. As tidal and wave effects are dampened out by the impact of river discharge, marine sediments do not migrate towards the estuary, and the flow field is such that deltaic sedimentation regions begin to be established. When the circulation is dominated by astronomic factors, the placement and distribution of sedimentary particles, whatever is their origin, is determined by tides, waves or both simultaneously. If tides predominate, then fine sediments coat the shore—low velocity region—, and coarser sediments occupy the center of the estuary, where higher velocities occur. In a wave-dominated system, the reverse is true\(^4\). In general, the patterns of mixing and transport of sediments are variable from estuary to estuary, and for each estuary with the seasonal characteristics of the flow field.

As it has been previously discussed, the circulation inside the estuary is governed by fluvial discharges and tidal currents. Wind induced waves, density and oceanic currents can also be important, in consequence of local conditions.

Density currents are due to the difference of density between fresh and salt water, respectively 1.00 \(g/cm^3\) and 1.025 \(g/cm^3\) at 15\(^\circ\)C. Although density currents may also be originated by temperature differences between surficial and bottom waters in the estuary, their influence on the magnitude of velocities is generally assumed as negligible. The difference of density between saltwater and freshwater implies the stratification of the
water body, such that the latter overlies the denser saltwater. Whether this stratification is going to be important or not, it will depend on the ability of the hydrodynamic regime of currents in the estuary to generate the necessary turbulence, for the mixing of both water volumes.

When the magnitudes of tides and river discharge are small, the stratification is important and mixing happens either by diffusion or entrainment processes. The upper layer of relative freshwater moves downstream, towards the ocean, and the salt edge moves upstream along the river. The transport of the suspended particles in both layers follows the general trend of the fluid. There is a continuous interchange of particles, between the top layer and the saline water, by settling and entrainment. Particles in the bottom layer will also be submitted continuously to deposition and erosion.

The predominance of tidal flow over density currents is very characteristic of the geographic location of the estuary: in the occidental european coast, where tidal amplitudes reflect the upwelling effect of the Coriolis force in the Atlantic ocean, density currents are almost negligible; the opposite happens in the East coast of the USA due to reciprocal downwelling effects. Centrifugal forces that develop in the meanders of the estuary, and other potential generators of non-linear, non-periodic flows: strong winds, bottom roughness and topographic conditions, also contribute to the relevance of hydrodynamics in the overall estuarine circulation $^3,7,10,12,30$. The mixing that results from the combination of all processes referred above is highly heterogeneous, and zones of distinct mixing intensity are randomly spread in the domain.

During slack water and in regions of weak turbulence, the settling and deposition of particles are strongly favored. However, colloidal particles such as silts and clays, characterized by very small settling velocities, deposit only when they are already near the bottom. This is why, very fine sediments that are not rejected to the ocean have a long residence time in suspension, and the net input/output balance of sediments in estuaries
indicate that the water column plays a storage function in the overall sedimentary system.

The intensity of turbulence needed to keep a particle in suspension is less than the one that corresponds to its erosion from the bottom. Velocities that are sufficiently low to enhance deposition develop at very low water depths, near the bottom, originating the so-called fluffy zone, which is characterized by high concentrations of particles and high water contents. Until particles reach the fluffy zone, settling is directly dependent on the particles size. Coagulation and flocculation, which are aggregational processes regulated by the chemistry of the system, contribute to the increasing of the size of the particles and hence, to the increasing of settling velocity (Appendix A).

A zone of maximum turbidity usually forms in the region where the river discharge meets the tidal wave. Higher concentrations of sediments are found near the bottom and in the center of the cloud, decreasing radially in both directions: landward and seawards. The position of the cloud varies periodically with the propagation of the tides: it moves upstream with flood tide and downstream with ebb tide, and, for both situations with the season of the year. In the maximum turbidity zone, flocculation and deposition reach their largest activities in the estuary. Generally, the shoaling pools of estuaries always develop landward, which is related to the fact that the maximum turbidity zone do not reach the interface with the ocean.

The efflux of sediments in some estuaries, essentially the macro–tidal estuaries –Gironde, Amazon, Columbia–, is frequently dominated by the impact of the river discharge. When river discharges have large magnitudes, due to regular seasonal factors or to exceptional floods, the concentration of suspended matter in the water column goes up drastically. Since the net surface flow that is directed to the sea also increases, the amount of estuarial efflux is substantially augmented. Most estuaries behave as very efficient sedimentary traps for sediments, either because of flow deformation induced by the morphological characteristics of the estuary, which imply the decreasing of the magnitudes
of the velocities landward, or due to the storage effect of the water–column.

Seasonal changes in climate—temperature, precipitation, light intensity—are responsible for the alteration of the quality and quantity of sediment influx into the estuaries and the variability of chemical and biological activities.

Winter and Spring rains increase the river discharge, land flushing and consequently the sediment influx into the estuary. In summer, sediment load from the land diminishes dramatically as the weather becomes dry, and tidal influence in the overall circulation gets stronger. The sedimentological output of the estuary diminishes, since it is limited to the material kept in suspension by tidal turbulence and carried seaward during ebb. The final result will reflect the performance of both, marine and fluvial processes. The regime of the winds, through the wind–induced shear, may be responsible for the higher rates of resuspension of bottom deposited sediments, during late Fall, Winter and early Spring.

Seasonality is also associated to the intense biological activity of the estuary during spring and summer, as a consequence of temperature and light intensity changes. The production of diatoms, algae and other microbes at high rates improves the quality of sediments in solution by adsorption, feeding or excreting, biogenic processes that increase the density, size and aggregational suitability of the particles; the resistance to erosion of deposited fine grained material by burrowing and pelletization and the amount of organic matter in solution. During Summer, the occurrence of thermal stratification can be responsible for the decreasing of the sedimentation rate, due to the resistance to entrainment in the pycnocline.

The variability of the volumes of water contained inside the estuary influences the dilution and salinity, which are factors that play a major role in the chemistry and geochemistry of the system. As dilution decreases and salinity and organic contents increase in Summer, those variables require special attention in order to understand the fate of the estuary in that period of the year.
Due to the variability of river discharge and tidal influence, and diversity of biochemical environments, the definition of the upstream limit of the estuary is particularly important. Traditionally, this boundary has been defined according to hydrodynamic factors: as the section where mechanical tides influence is null —top of tidal prism—; or according to chemical and biochemical standards: as the section where the chlorinity falls below a standard value equal to 0.01 ppt\(^3\).

Based on the previous discussion, we identify four differentiated regions with completely different characteristics, but equally important in the overall behavior of the system: flood plain, intertidal flats, tidal channel and river channel (fig.2). A description of each region follows.

**Tidal–Channel** — This area is the main pathway of tides from and towards the sea. Intense turbulent flows, in deep tidal channels, transport essentially sand and other coarse debris, and so the bottom sediments consist of coarse non-cohesive materials. However, during slack water, silty and clayey mud may also be deposited\(^4\). The transport capacity of the flow in the tidal channel, and the nature and abundance of the sediments supply determine whether one or both of the fundamental types of sediments is present.

**River Channel** — River channel refers to the region of the estuary where the circulation is predominantly riverine. Unlike the flow in the tidal channel, the flow in the river channel is predominantly unidirectional. Long-term sedimentation net rates and bed configuration are different in both regions, but the nature of the basic processes involved is similar. The decision of taking these two channels separately relies on the characteristic is of the bottom sedimentary layers, the definition of the interface water—column/bottom and the magnitude of characteristics time—scales for erosion and deposition. Bioactivity is eventually irrelevant in both regions.
**Intertidal flats** – Intertidal flats are the regions of the estuary intermittently submerged due to the action of flood and ebb tides. Three different types can be analyzed: the high intertidal flats, usually submerged only during intense or spring tides; the low intertidal flats, periodically submerged according to the dynamics of normal tides propagation and, finally, the tidal marshes that differ from the formers mainly due to morphological and biological aspects. Tidal marshes fit well in the classification of intertidal flats because of the type of flow circulation; however, elsewhere in the estuary the biogeochemical processes are so important and complex, that they could justify, *per se*, the elaboration of a specific model. Consequently, tidal marshes will be subject of special treatment in this section.

High intertidal flats are the top borders of the water body as well as the tidal marshes boundaries. The sedimentary particles are mostly sand-sized. Some salt-tolerant grass may develop together with biogenic activity, although with very low intensity and impact. Low intertidal flats are characterized by intense bioturbation and the typical display of sediments is constituted by organoclays, clays, silts, fecal pellets, fine sands and other infaunal particulate.

Tidal marshes are vegetated saline intertidal flats. Both from an economical point of view, due to the existence of fisheries, crustaceous reefs and shrimp colonies, and from an ecological point of view, due to the rich variety of plants and microorganisms, tidal marshes constitute one of the areas of major interest in the estuary, and, yet they remain the least studied of all intertidal regions.

Tidal marshes have very complicated morphology and irregular topography. In the context of sedimentation, besides the physical impact of tides and overflows on erosion, saltation and deposition rates, additional components must be considered: the baffling effect of vegetation; sediment trapping due to coagulation —physiochemical flocculation of clays, formation of organoclays and pelletization of silts and clays$^2$; the erosional effect of
bioturbation on the loosening of fine bottom deposits during feeding and excreting activities, and, finally, the structural rearrangement of lower sedimentary layers caused by roots expansion and the already referred burrowing effect, which may indeed rework the entire sedimentary stratum layout (fig.3)

**Flood plain** — Flood plain is the area that, being external to the river main stem or the estuary itself, is invaded and submerged by water during floods. In the sense that floods may or may not be important for different estuaries, the consideration of the flood plain as part of the estuarial domain is dependent on the specificity of the areas to be studied. Its contribution for the global sediment discharge is reflected by the fast and strong increase of the load of sediments during flood events, which do not last long in terms of the usual time-scales of interest in transport modeling. However, the impact in the net sedimentary balance is not proportional to their duration. Indeed, the facie of some estuaries is dramatically changed during floods, not only because the input of material increases but also because the circulation patterns in the system are altered due to river discharge augmentation.

As it can be concluded from the analysis presented above, physical, chemical and biological mechanisms change drastically from region to region, inside the estuary. A comprehensive discussion of the majority of characteristic processes occurring simultaneously, and their respective influence on the environment, is not feasible. However, it is possible to identify those mechanisms that, for specific forcing conditions, determine the behavior of the system. It was in this perspective that the following sections were elaborated, discussing with the detail considered adequate, the aggregation, transport and sedimentation of suspended and deposited particles in estuaries.
2.2—Characteristics of Sediments

Sedimentary particles are characterized by size, shape, fall velocity, composition, surface texture, orientation and cohesiveness. In natural environments, it is important to keep a statistical perspective throughout the analysis of those characteristics, so that diversity can be accounted in the establishment of the properties of the sediment load. These properties and their relationships are discussed below.

Fall velocity — Fall velocity is, by definition, the average terminal settling velocity of a solution of sediments, falling alone and considering a column of quiescent, distilled water of infinite extent \(^1\) (Table 1).

The concept of velocity of fall, or settling velocity in a fluid medium is integrated in almost all empirical and semi-empirical relationships used in studies of the dynamics of sedimentation. The intrinsic relationship between fall velocity and the characteristic diameters of sediments are available in large number (fig. 4.a,b).

Stokes' law (Appendix A) establishes the theoretical foundation for the computation of the settling velocity \(w\). It reads:

\[
  w = k \left( \rho_s - \rho_f \right) d^2 / \mu, \tag{2.1}
\]

where \(k\) is a constant dependent on the characteristics of the flow, heterogeneity of the distribution of particles, concentrations of material and chemical activity. The remainder variables are established as follows: \(\rho_s\) is the density of the particles, \(\rho_f\) is the density of the fluid, \(d\) is the normal diameter of the particles and \(\mu\) is the viscosity of water, assuming Newtonian fluid behavior.

While Stokes' law is frequently used in studies of sediment transport, its practical usefulness depends on the ability to empirically quantify the parameter \(k\), which depends
on changes in the fluid viscosity that may result by changes of temperature, changes in the dissolved ionic concentration, changes in the suspended particulate concentration or changes in the resistance to fall caused by varying the particles size or roughness. It may even happen that the fluid develops non—Newtonian viscosity, when very high concentrations of fine or colloidal particles are achieved\(^2\). Viscosity effects are generally neglected, because natural conditions of estuaries are far from inspiring concern in this context\(^{13,39,40}\).

Also, lift and drag forces altered by flow turbulence, agglomeration of particles by coagulation and flocculation, and the effect of heavy metal adsorption on the density of the materials, influence drastically the sinking rates of the particles. Table 2, from Bloesch and Burns(1980), presents vertical sinking rates of particles in presence of turbulence, and when compared with table 1, whose values were calculated for null flow velocities, gives qualitative indication of the impact of fluid flow on the settling velocities.

Hjulstrom, Sundborg, Smith and others have provided large amount of experimental work and related information, most of it contained in graphics, towards that end\(^{2,5,13,39,74}\).

**Size** — Several different standards have been used to measure the size of sediment particles. They include: normal diameter, sieve diameter, sedimentation diameter\(^1,4,5\). Normal diameter is defined as the diameter of a sphere having the same volume as the particle, and it is obtained by volumetric measurements; sieve diameter is the minimum sieve size through which a particle is able to pass; the sedimentation diameter is the diameter of a sphere that has a specific density of 2.65 (the typical average value for sediments), and also has the same volume as the particle in the same fluid, under the same conditions. Sieving, decantation, the hydrometer method and many other processes, when adequately applied to a consistent set of sediments samples, permit a thorough representation of size distribution by statistical parameters computed for the respective
frequency distribution curves. The formulation of the frequency distribution curves is based on the construction of histograms of particle concentrations or volumes versus size interval, for one or more samples of bulk sediments. Monomodal distributions are seldom found in natural waters. Indeed, most size frequency distribution curves of natural sedimentary environments are bimodal\(^{4,7,12,21,30}\). Statistically, a mode represents the most frequent size or size interval. Commonly found modes correspond to the interval 10–30 \(\mu m\) (clays, algae, bacteria and other micro-organisms), and 125–250 \(\mu m\) (flocculated clays, fine sand and organic debris) – Fig.6.

In general, statistical properties (mean and median values, variance, sorting skewness, kurtosis) may be defined in term of characteristic diameters \(D_x\). \(D_x\) corresponds to the diameter in the cumulative distribution function to which corresponds a probability of occurrence equal to \(X\). The heterogeneity of bulk samples is characterized by variance, sorting, skewness and kurtosis. The variance is a measure of the spreading around the mean; sorting gives the range of size distribution, reflecting the predominance of one mode of the size distribution over the others; skewness defines the degree of particles mixing —silt in sand gives a positive skew and silt in clay a negative skew\(^{32}\) — and kurtosis provides the relation between the magnitudes of higher and lower concentrations. It is possible to establish some semi-empirical expressions to evaluate the statistical variables previously referred\(^{32}\):

\[
\text{Mean} = (D_{16} + D_{50} + D_{84})/ 3
\]

\[
\text{Median value} = D_{50}
\]

\[
\text{Variance} = (D_{84} - D_{16}) / 4 + (D_{95} - D_{5})/16
\]

\[
\text{Sorting} = (D_{95} - D_{5})/ 2
\]

15
Skewness = D_{95} + D_{5} - 2 D_{50}

Kurtosis = (D_{95} - D_{5}) / 2.44 (D_{75} - D_{25})

The general sediment nourishment of estuarine systems varies according to local biological, geologic, geographic, climatologic and oceanographic regions. W. Stumm (1977) presents a size spectrum of waterborne particles. Fig. 6, and Table 3 provide a description of standard size classes of sediments, from Friedman and Sanders. Based on both classical references, the expected range of particle size to be found in solution goes from the colloidal clays up to the small cobbles — medium size gravel. The river and the ocean constitute basic sources of sediments in estuaries, with inputs that vary from clays to fine sands in the case of the river, and include coarse sand or other coarse marine debris from the oceanic contribution. Lateral runoff is characterized by diversified distributions of colloidal particles, coarse silt or even fine to coarse sand, whose relative concentrations depend on the type of soil occupation in the surrounding areas — urban, industrial or agricultural—, and respective characteristics. Other sources include wind-blown sediments, organic aggregates from waste disposals, and in situ production of biogenic sediments as plant detritus, fecal pellets and others, whose size range is similar to the one characteristic of runoff.

Sediments of interest for this work range from the colloidal clays (0.5 \mu m—50 \mu m) up to the coarse sands (>500\mu m)\textsuperscript{7,10,12,30}.
The table below, adapted from Castaing\textsuperscript{30}, summarizes relevant terminology:

<table>
<thead>
<tr>
<th>Size</th>
<th>Sediment</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 62.5 μm</td>
<td>very fine</td>
</tr>
<tr>
<td>62.5 – 125 μm</td>
<td>fine</td>
</tr>
<tr>
<td>125 – 200 μm</td>
<td>fine – medium</td>
</tr>
<tr>
<td>200 – 500 μm</td>
<td>medium – coarse</td>
</tr>
<tr>
<td>&gt; 500 μm</td>
<td>coarse – very coarse</td>
</tr>
</tbody>
</table>

The following table was elaborated from spread data collected in the literature\textsuperscript{2,74}. The actual conditions of sampling and criteria used to establish the mean values indicated are unknown, and consequently our capacity to make a consistent analysis is restricted to the qualitative appreciation that, the contribution of low-range very fine sediments to the overall concentrations found in estuaries is, indeed, remarkable. This conclusion justifies the relevance of the transport of very fine sediments in estuarine related studies.

<table>
<thead>
<tr>
<th>Estuary</th>
<th>Average particle size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cheasapeak Bay (USA)</td>
<td>1.3 μm</td>
</tr>
<tr>
<td>(Biggs, 1968)</td>
<td></td>
</tr>
<tr>
<td>James River (USA)</td>
<td>&lt; 40 μm</td>
</tr>
<tr>
<td>(Haven, 1968)</td>
<td></td>
</tr>
<tr>
<td>Delaware (USA)</td>
<td>1.5 – 2.5 μm</td>
</tr>
<tr>
<td>(Oostdam, 1971)</td>
<td></td>
</tr>
<tr>
<td>Wadden Sea (FGR)</td>
<td>5.5 – 19 μm</td>
</tr>
<tr>
<td>(Postma, 1954)</td>
<td></td>
</tr>
<tr>
<td>Essex (GBR) (Sheldon, 1968)</td>
<td>10 – 15 μm</td>
</tr>
</tbody>
</table>
Shape — Shape of particles plays a role in the aggregational processes of particles, and it is also related to the characteristics of porosity and permeability of soils.

One way to characterize the shape parameter of a particle is through its sphericity, which is defined as the ratio of the surface area of a sphere having the same volume as the particle, to the surface area of the particle\(^1\). If \(a\) is the longest dimension of the particle, \(b\) is the intermediate and \(c\) is the shortest one, Corey, Schulz, McNown and Inalaika\(^1\) established by experimental analysis, that the shape factor can be expressed as:

\[
S_p = \frac{c}{\sqrt{a \cdot b}}
\]

This shape factor is obtained for a series of bulk sediments, using sieving, filtering, and volumetric measurements to obtain the results that generate frequency curves, which can be described by the usual statistical parameters. In practical terms, and for the diversity of sediments found in estuaries, the evaluation of this parameter is impossible. However, visual observation of the shape of the sediments may help to identify the origin of the sediments: marine sands are usually almost spherical, whereas fluvial sands present much more irregular shapes.

Specific Weight — Specific weight is by definition the dry weight per unit volume of the sediment \textit{in situ}\(^1\). It depends on the size—frequency distribution of particles in the sediment, the nature of the particles and the degree of sorting of the material. In the case of submerged sediments, the specific weight also depends on the degree of the compaction of the sedimentary layers, as well as on the porosity or water contents (fig.7).

The surface weight is calculated proportionally to the percentages of the different essential fractions of sediments mixtures from field samples: sand, silt and clay (Table 4)\(^7\).
Cohesiveness — Cohesiveness is the property by which mixtures of very small size but large surface area, such as silts and clays, show predominance of physiochemical forces are over the weight, interlocking and particles mutual friction.

Cohesion is defined as the true shear strength of the saturated clays under zero confinement\(^{39}\). Although it is difficult to evaluate the magnitude of the internal deformations of the mass of soil, cohesion is an efficient measure of the surface net physiochemical forces.

The distribution of electrical charge in the surface of these particles is irregular and mostly negative, while the edges are positively charged. In the presence of small quantities of salt —2 ppt\(^{41}\) — the equilibrium of the physiochemical forces is governed by the Van der Waals forces and the electrostatic attraction between surfaces and edges, originating the agglomeration of the smallest particles in flocs. Therefore, due to the influence of salinity, the basic settling unit for cohesive sediments in estuaries is not the particle, but the floc.

The average size of the floc and its distribution in suspension depends also on the flow conditions: large velocity gradients enhance the efficiency of particles collision, increasing the rates of aggregation, but dispersion has the opposite effect. Particles sized in the range of 1 — 2 \(\mu\)m are below the scale of thermal motion (Brownian), and, apparently, they do not settle. This is one of the arguments used to justify the storage function of the region of maximum turbidity in the estuary, in consequence of the long residence times of particles in suspension.

The total resistance of clays to mechanical stresses is expressed as the shear strength \(S_h\). Coulomb's law\(^{39}\) gives:

\[
S_h = C_h + p_h \tan \phi.
\]

\(C_h\) is cohesion of the soil, \(p_h\) is the pressure normal to the plane of shear and \(\phi\) is the angle of internal friction, which accounts for interlocking and particles mutual friction.
Cohesion of deposited sediments is enhanced when salinity increases, in response to the
cationic exchange capacity (CEC) of the minerals present, Table 9. The CEC refers to the
property of clays, by which ions already present in the lattice structure of the minerals, or
on the surface, are exchanged with other ions existent in solution. The exchangeability of
these ions is permanent, but when high salinity concentrations are reached in solution, it
ceases to occur and the sediments reach stability.

Cohesive sediments and related sedimentary soils are much more complex to
understand than any other estuarial very fine sediment. The following table shows the
percentage distribution of the three major types of sediments found in estuaries classically
referred in the literature. Once more the relative importance of silts and clays over sands
and, or other coarse sediments in these natural systems, is clearly predominant

<table>
<thead>
<tr>
<th>Estuary</th>
<th>sand</th>
<th>silt</th>
<th>clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>Susquehanna</td>
<td>10%</td>
<td>50%</td>
<td>40%</td>
</tr>
<tr>
<td>(USA)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Delaware</td>
<td>5%</td>
<td>40%</td>
<td>55%</td>
</tr>
<tr>
<td>(USA)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mad River</td>
<td>23%</td>
<td>40%</td>
<td>27%</td>
</tr>
<tr>
<td>(USA)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rio Grande</td>
<td>3%</td>
<td>72%</td>
<td>25%</td>
</tr>
<tr>
<td>(USA)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In spite of the existence of some theoretical approaches generally accepted by the
scientific community —Einstein, Partheniades, Krone—, the establishment of the
properties of sediments, to be applied in the simulation of the transport of cohesive soils,
still relies basically on the evaluation of empirical or semi–empirical variables. New
projects to study the dynamics of sediment particles in different estuaries may use existing
data, which are very scarce, to define initial parameters for further extrapolation, or, otherwise, to proceed with collection of new sets of data for each case in study, which is expensive and often not feasible. Mehta$^4$, Krishnamurthy$^3$, Hayter$^8$ and Luettich$^3$ are very good references in the context of data collection and analysis.

2.3 — Dynamics of Sediments

The dynamics of sediments are governed by hydraulic transport of sediments, erosion and deposition developed at the solid boundaries of water-bodies, and the influence of biological and chemical activities in the global behavior of natural systems.

The following sections will discuss the hydraulic transport, erosion and deposition, and flocculation of sediments in estuaries. A qualitative description of biologically mediated processes is given in the last section.

2.3.1 — Hydraulic Transport

Sedimentary particles transported by bulk flow, may follow three distinct paths: rolling of coarse particles along the bottom (surface creep), jumping and bouncing (saltation), and suspension (fig. 24).

Particles moved by surface creep are not as abundant in estuaries as they are in rivers. Indeed, for the majority of studied estuaries, the contribution of those large-sized sediments is often neglected. Together with the particles transported by surface creep, saltation particles constitute the bed-load. Saltation particles are usually the largest ones in the typical size distribution of an estuary, and they refer to size ranges from
approximately 125 μm up to 660 μm\(^{30}\). Although their saltation heights are relatively small, particles in the range 125 – 250 μm have long jumping lengths, and flat bouncing trajectories\(^{44}\), which makes it controversial to classify the transport mode either as saltation or as suspension; some authors even call it: "degraded suspension"\(^{30}\).

In general, the three populations of particles of major interest are\(^{30}\):

<table>
<thead>
<tr>
<th>Diameter</th>
<th>Transport Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt;660 μm</td>
<td>surface creep</td>
</tr>
<tr>
<td>125 – 660 μm</td>
<td>saltation</td>
</tr>
<tr>
<td>&lt;125 μm</td>
<td>suspension</td>
</tr>
</tbody>
</table>

Figure 8 indicates the relative importance of these three populations in the Gironde estuary, France.

Suspended particles are also commonly referred as suspended–load. The use of terms as suspended–load, bed–load, wash–load and bed–material load, has also been an important point of controversy, since 1940. The discussion, initiated by Einstein, was continued by Partheniades, Krone and more recently Woo and van Rijn, among others.

Actually, the concepts of bed–load and wash–load are the basic reasoning for the establishment of most empirical and semi–empirical laws of sediment transport used during the past decades. Some of those laws have proved efficiency, as for example Einstein's or Schields' bed–load functions. The fate of suspended particles is more difficult to infer experimentally, which is testified by the absence of wash–load semi–empirical functions.

The approach sustained in this text follows the perspective of an unified view of the hydromechanical governing laws, in the sequence of the work of Partheniades\(^{18}\) (1977), Westrich\(^{13}\) (1985), and Woo\(^{16}\) (1987). However, since the distinction between wash–load,
bed-load and suspended-load was the conceptual basis for the physical interpretation of sediment transport in the past, and because the controversy about this subject is not yet closed in the literature, it is presented in the following paragraph a general review of the problem.

**Wash-load, Bed-load and Suspended-load**

Einstein \(^{37}\) defined wash-load as that part of the total sediment load, that was in suspension, and such that all particles were finer than the limiting size, which corresponded to the 10\% lower fraction of the material deposited on the bed. Bed-load was defined as the part of the total sediment load, composed of all particles greater than the limiting size, whether moving on the bed or in suspension, including all bed material in movement.

Basically, wash-load was associated to the concentrations of particles that would "never" deposit, or be submitted to surface creeping or saltation \(^{39}\).

In 1977, Partheniades \(^{18}\) verified constant interchange of particles between bed and water column, even for colloidal particles to whom that was not expected to happen. This fact induced the change of the concept of wash-load, to account for the variability of the behavior of sediments in function of circulation patterns: in estuaries, unsteady periodic flows result into alternate periods of deposition and resuspension.

However, as Woo \(^{16}\) points out, this problem is not clear: large concentrations of fines may behave as bed-load, likewise coarse sediments may be considered wash-load, in flows with transport capacity exceeding the sediments supply. Therefore, it is apparent that there is no final definition for wash-load, and it is useless to try to implement a concept not consistently defined. The terms suspended-load and bed-load will be frequently referred in this text, but it is important to realize that these concepts are intertwined, by a continuous, dynamic transfer between the bottom layer and the
water–column.

Although 90–95% of all sedimentary movements in estuaries are expected to occur in suspension, bed–load is important because: (a) — it shapes the bed, with direct implications on roughness; (b) — it determines the stability of the bed; and (c) — it constitutes a boundary condition of the water–column suspension, what is determinant in terms of modeling formulation.

**Transport Equation**

The advection and diffusion of sediment particles by the flow is mathematically expressed by:

$$\frac{\partial c}{\partial t} + \bar{v} \cdot \nabla c = \left( -\frac{\partial}{\partial x_j} \varepsilon_{ij} \frac{\partial c}{\partial x_j} \right) + Q \quad \text{(2.2)}$$

with:

- \(\bar{v}\) — flow velocity,
- \(Q\) — sources or sinks of sediments,
- \(\varepsilon_{ij}\) — diffusion coefficients.

The diffusion coefficients used in the advection–diffusion equation include Brownian diffusion and, turbulent diffusion due to the velocity fluctuations not included in the evaluation of the advective terms. In typical estuarine and coastal waters, the relative order of magnitude of these factors varies from \(10^{-9} \text{ m}^2/\text{s}\) for Brownian diffusion, to \(10^{-3} \text{ m}^2/\text{s}\) for turbulent diffusion, so that Brownian diffusion is naturally negligible. Since sedimentary particles have densities substantially different from the density of water — the
average density of sediments is about 2.65 gr./l, whereas water density is around one, and even salt–water just goes up to 1.025 gr./l—suspended concentrations of these particles affect the mode of dissipation of energy and the structure of turbulence\textsuperscript{45,84}. The turbulent diffusion coefficient can be corrected as follows\textsuperscript{45}:

\[
\varepsilon_S = \gamma \phi \varepsilon \tag{2.3}
\]

Experimental work and theoretical analysis of this subject has been done, almost exclusively, for turbulent diffusion in the vertical direction. Due to the homogeneous randomness of turbulence a similar correction should be introduced to the diffusion coefficients of the lateral and longitudinal directions. However, since density differences originate essentially buoyant forces, it is expected that the corrections can be neglected for the diffusion coefficients in the x, and y directions.

The semi–empirical factor \( \gamma \) accounts for the increase of the effective mixing length and diffusion rate, due to the fact that the sedimentary particles of higher density, submitted to intense centrifugal forces, are rejected to the outside of the eddies. Hence, \( \gamma \) is greater than one. Van Rijn\textsuperscript{45} introduced an equation to compute \( \gamma \) values, which is dependent on the settling velocity of the particles \( w \), and the characteristic velocity of the fluid in the bottom boundary layer \( u^* \).

\[
\gamma = 1 + 2 \left( \frac{w}{u^*} \right)^2, \quad \text{for } 0.1 < \left( \frac{w}{u^*} \right) < 1.0 \tag{2.4}
\]

Factor \( \phi \) expresses the damping effects, caused by sediments, on the turbulent structure of the fluid. It is impossible to obtain a general expression to calculate the values of \( \phi \), as it is impossible to make a full simulation of turbulence, with the presently available computational capabilities. However, there is experimental evidence indicating
that, only for concentrations larger than 2,500 ppm, the value of $\phi$ takes values less than one, about 0.9$^{45}$. This is corroborated by Partheniades, who establishes the concentration limits at 10,000 – 20,000 ppm. Typical values of the highest concentrations encountered in estuaries are much lower than the values referred above, and so it is reasonable to assume $\phi$ equal to unity.

The term Q, in the right-hand side of equation (2.2), describes sinks and sources of sediments. In the perspective of the water-column, and besides anthropogenic and, or natural point and diffusive sources, the settling of particles behaves as a sink, whereas entrainment acts as a source of material. Biological activity may play the role of sink or source, or both at the same time, in strict correlation with temperature, light penetration, nutrients supply, etc. Algae production is definitely a source, while selective feeding of zooplankton constitutes a sink.

2.3.2 – Mechanical Processes: Erosion and Deposition

Erosion

Erosion is the mechanism through which bottom layer particles, initially at rest, are forced to go into suspension, or eventually to move along the bed.

Particles on the bed-layer, or constituting the bed-layer are submitted to hydrodynamic and resisting forces, Table 10. The former ones develop as moments in function of the gradient of flow velocity, as well as lift and drag forces. Besides gravity, the resisting forces are due to interlocking between particles, and when relevant the effect of cohesion or adherence bonding$^{18,82}$. The results of both kinds of forces are usually
expressed in terms of shear stresses. The bottom shear stress, that evaluates the mechanical effect of hydrodynamic forcing, can be described as:

\[ \tau_b = C_D \rho \mathbf{U} |\mathbf{U}| \]  \hspace{1cm} (2.5),

where:

\( \mathbf{U} \) — mean flow velocity,
\( \rho \) — water density,
\( C_D \) — friction coefficient.

On the other hand, the resisting forces can also be evaluated in terms of a resultant stress, acting in the direction opposite to the applied bottom stress. The resistance stress is a function of particle size, density, particles interlocking, cohesive bonding, water contents, degree of consolidation, and fall velocity\(^{46,82}\).

In 1935, Hjulstrom (fig.9) presented a diagram that relates flow velocities, bottom sediments size, and bottom shear stress. Postma\(^\text{50}\) (1967), verified the relevance of water contents in the erosional process, and proposed the diagrams shown in Figure 10, 11, which gives the value of critical erosional flow velocity in function of the nature of the sediments, particles size, and water contents.

The use of these diagrams has been proved to be quite efficient in erosion studies, and it may be very helpful in the calibration of available bed–load equations, in the absence of field data. Nevertheless, these diagrams present remarkable weaknesses in the treatment of deposition, as it will be discussed later on.

Erosion begins when \( \tau_b \) exceeds a minimal value, which corresponds to the effective bed resistance stress: \( \tau_{e,cr} \). For values of \( \tau_b \) greater than \( \tau_{e,cr} \) there will be erosion. Indeed, erosion is a continuous process, and the actual relation between the amount of
particles eroded and net erosion stress, is such that:

\[
\frac{\partial c}{\partial t} = \beta (\tau_b - \tau_{e,cr})^n
\]  \hspace{1cm} (2.6)

where:

\( \beta \) – coefficient of erodibility,
\( \tau_b \) – bottom stress,
\( \tau_{e,cr} \) – bed resistance stress,
\( n \) – empiric coefficient.

Most bed–load equations are equations of this type. Table 6 presents a summary of equations elaborated by Larnsen\(^{39}\). Du Boys, Wes, Schields, Einstein, Kalinske, and Brown, introduced formulas, whose general format was similar to equation (2.6).

In most equations derived with basis on the erosion criteria, the value of \( n \) is approximately one. Exception to this rule is the Einstein's equation, where the power law is of the third order. This equation has been reported to be the most successfull of the above referred bed–load formulas.

Distinct values of \( n \) have been found in real–life situations, as reported by Luettich\(^{31}\), and consequently calibration and parametrization should be renewed for different estuaries. Lavelle\(^{7}\), for example, found values that were reasonably constant around 4, and exceptionally 3 and 5, in a sensitivity analysis made with field data collected in Puget Sound basin, Washington. \( \beta \) depends on the size distribution of the sedimentary particles. Lavelle suggests the value \( 1.7 \times 10^{-6} \), for the referred basin.

As the bed–layer is continuously submitted to erosional activity, hydraulic sorting develops, and the material on the bed surface becomes coarser and coarser, since finer material is removed first. This hydraulic sorting may also lead to the formation of an armor layer\(^{19}\).
The armor layer is constituted by sedimentary material, which is not removed by flow activity, and does not permit fine particles from lower layers to escape and reach the top surface layer. Hence, armoring originates the decrease of sediment supply to the water-column, and due to the fact that coarser particles have increased roughnesses, the friction factor of the bed, $C_D$, is also augmented. Although this process is more important in rivers, than in estuaries, its influence may be important in localized regions of deep tidal channels.

**Deposition**

Deposition refers to settling of initially suspended sediment, followed by eventual accumulation on the bed of the water-body. This process occurs in the so-called shoaling zones, where the sediment transport capacity of the flow is reduced, often because of the reduction of velocities. Deposition can be expressed as:

$$\frac{\partial c}{\partial t} = -\alpha (c - c_T) \quad (2.7)$$

The reference concentration $c_T$ corresponds to the limiting equilibrium concentration, that can be transported by the flow without deposition, and $\alpha$ is a coefficient that describes the influence of the particles size distribution, and concentration\textsuperscript{13,46}. According to Westrich\textsuperscript{13} $c_T$ is such that:

$$c_T = K \frac{\tau_b U}{(\rho_s - \rho) g h w} \quad (2.8)$$

For noncohesive particles in the size range 20 –200 $\mu$m, $K$ has the value 0.0018
(fig.12). This type of approach, also adopted by Luettich\textsuperscript{31} for cohesive sediments, is intrinsically mechanical and pretends to describe pure gravitational settling. In the case of cohesive sediments, it is used the steady state concentration $c_{ss}$ as reference value, since it is needed to account for flocculation.

For colloidal particles up to 62.5 $\mu$m—the limit between silt and fine sand—, deposition will be affected by flocculation, which is a chemically induced aggregational mechanism. Flocculation is introduced in the model of deposition with the term $\beta c^2$, discussed with detail in section 2.3.3. Hence, for cohesive sediments, the equation that describes deposition is:

$$\frac{\partial c}{\partial t} = -\beta c^2 - \alpha_s (c - c_{ss})$$  \hspace{1cm} (2.9)

In the past, Hjulstrom's criteria for deposition was broadly used. It was based on the assumption that the critical flow velocity for sedimentation is approximately equal to the fall velocity. However, turbulence contribution was neglected in that analysis. Because natural flows are turbulent, the use of Hjulstrom/Sundborg/Postma diagrams, often leads to underprediction of real deposition rates. In real systems, particles constantly settle for values of flow velocity much higher than the ones obtained consulting those diagrams. Deposition still occurs for particles of settling velocities $w$, when the time-averaged vertical component of the turbulent velocity is more or less of the same order of magnitude\textsuperscript{13}. The flow velocity is, in this case, at least two orders of magnitude larger than the settling velocity\textsuperscript{13}.

The value of critical stresses $\tau_{s,cr}$ below which sedimentation still develops, strongly depends on the sediment concentration\textsuperscript{30,31,82} (fig.13,fig.14). For very small concentrations of coarse sediments, the critical stress for erosion approaches the value of the critical stress for sedimentation. The reverse happens for high concentrations of those sediments, so that the critical stress of deposition is always larger than the critical stress
for erosion. This fact may be extrapolated for cohesive sediments, when flocculation is ineffective. The phenomena of hysteresis, verified in laboratory experiments, can also be justified by the eventual simultaneity of both processes. Mehta and Partheniades refer concentrations of (10–20 ppm) as a starting point for simultaneity to occur. The results presented by Luettich as evidence of hysteresis, (fig.16), show minimum concentrations of 40 ppm, which confirms what could be expected.

The fact that, at high concentrations, erosion and deposition may cohabit, is extremely important in terms of transport simulation. Figure 15 shows the hydromechanic interaction of transport, deposition and erosion, for some typical flow characteristics, and sediment concentrations. In estuaries, where concentrations of cohesive sediments are rather high, erosion and deposition are mutually exclusive at the very bottom of the interface bed/water—column, whereas the interchange of particles continuously proceeds at the top of the same interface. This fact justifies the physical evidence of a permanent minimum thickness of loosened material on the top of estuarine bed—layers.

**The interface water—column/ sedimentary bottom**

The transition zone between the water—column and the sedimentary bed is characterized by the highest concentrations of sediments in suspension, or in another way, it is characterized by the highest water contents of deposited layers. This is the region where bed—load is active, and in the case of estuaries, is called mud zone or fluffy zone, due to the extremely large values of silts and clays concentrations.

For coarse sediments, the height of the transition zone can be defined as the maximum saltation height reached by bed—load particles, when being transported by the fluid. Following van Rijn methodology to compute saltation heights, the maximum value is about tenfold the diameter. Since the influence of adjacent particles is not considered, the saltation height obtained by this method is always overpredicted.
Assuming that 250 μm is a representative size of the averaged largest particles, the depth of the transition zone would be equal to 2.5 mm. Even considering larger sizes, e.g. 500 μm, the values are still negligible.

However, in the shoaling zones of estuaries, the fluffy zone reaches depths of 2 m. This is for instance the case of the Gironde estuary\textsuperscript{24,30}, where concentrations vary from 200 ppm at the top of the fluffy zone, to 500 ppm at the bottom. Such large concentrations are typical of the maximum turbidity region. In the intertidal flats the fluffy zone is usually only a few centimeters height. The definition of fluffy zone is quite flexible, and it varies from author to author, reflecting different strategies to approach the dynamics of sediments. At the level of the consolidated bottom, there is either erosion or consolidation, whereas at the top of the fluffy zone, there is a continuous exchange of particles: settling and resuspension. Settling particles come from suspension into the fluffy zone. Some of these particles will deposit and adhere to the bottom, while others, although very near the bottom, or even in contact with it, will stay in suspension. Since the fluffy zone is highly permeable, turbulent fluid from the water-column penetrates the transition zone. Turbulent eddies pick the particles and carry them towards the water-column, outside the muddy layer. This process is called resuspension. At the bottom of the fluffy zone, the problem is not posed in terms of erosion and deposition, but otherwise in terms of erosion and consolidation, which are mutually exclusive\textsuperscript{18,31}.

**Consolidation**

The variability of bed resistance to erosion in time is very important in the case of cohesive sediments. These sediments are passive of fast consolidation, which is accelerated in the intertidal flats during the periods of contact with the atmosphere, by decrease of water contents.
The variation of the degree of consolidation with depth, and in time, is intrinsically related to the characteristics of the deposited sediments. As erosion proceeds, and reaches deeper layers, the bottom offers more and more resistance to desaggregation, and resuspension. On the other hand, as deposition increases, freshly deposited layers initiate consolidation. These aspects are determinant for the response of the bottom bed-layer to fluid forcing.

In general, the effects of consolidation, are expressed by exponential relationships of the form \(^{35,40,82}\):

\[
\tau = A e^{kz} \quad (2.10)
\]

or,

\[
\tau = D e^{kt} \quad (2.11).
\]

Hayter\(^{82}\) (1983) proposed the direct association of the effect of consolidation in the resistance stresses, with the temporal variation of sediments density with depth:

\[
\rho(z) = \bar{\rho} K_c T_{dc}^{n1} \left( \frac{H - z}{H} \right)^{n2} \quad (2.12),
\]

where \(T_{dc}\) is the minimum interval of time that allows consolidation to develop, and \(H\) is the total thickness of the unconsolidated or partially consolidated bottom layers. The resisting tensions are related to the density by a power law:

\[
\tau(z) = a \rho(z)^b \quad (2.13).
\]

The coefficients \(a, b, A, D, K_c\) can be obtained by experimental analysis of field core samples.
2.3.3 — Aggregational Processes of Very Fine Sediments in Suspension

The following discussion focuses on flocculation and coagulation, which are major aggregational processes in estuaries. Some secondary processes, such as bioturbation, are not considered, either by lack of reliable knowledge of their nature, or because their influence is not considered significant.

Coagulation and flocculation have often been used as synonyms. However, W. Stumm and J. Morgan\(^3\) define coagulation as the aggregational processes explained by the theory of surface chemistry, and flocculation as the aggregational processes described by solution chemistry processes. Further down, in this discussion, it will verify that for most estuaries, essentially those where the concentration of organic matter is relatively high, it is not possible to keep surface chemistry and solution chemistry in separated compartments\(^8,33\). Therefore, it will conclude in favor of the acceptability of the indistinct use of both terms.

Coagulation

The collision of suspended particles is consequence of three different mechanisms of transport\(^3,5,25,33\): Brownian motion, fluid shear, and differential settling. When particles approach one another by collision, attractive and repulsive forces interact, by means of surface chemistry processes, until equilibrium is reached. The equilibrium, if "suitable", may lead to the aggregation of particles and, hence, coagulation. Coagulation due to Brownian motion is called perikineti and is important in the range of very small colloids.
Orthokinetic coagulation is attributed to the collision of larger sized particles, induced by high fluid shear rates. Differential settling is predominant in the range of the largest particles. Coagulation does not result from every collision in suspension. Some particles stick together after colliding, but others remain separate. Whenever coagulation occurs, the collision is considered efficient.

According to Smoluchowski\(^3\), the variation of the concentrations \(c\) of a monodisperse particles distribution due to perikineti\-c motion, can be mathematically described as:

\[
\frac{\partial c}{\partial t} = -k_p c^2,
\]

(2.14)

with

\[
k_p = \alpha_p 4 D \pi d
\]

(2.15)

The efficiency of collisions is introduced by \(\alpha_p\). If the Brownian diffusion coefficient \(D\) is expressed in terms of the Boltzman constant \(K\), temperature \(T\), and \(\eta\) is the absolute viscosity, equation (2.14) becomes:

\[
\frac{\partial c}{\partial t} = -\alpha_p \left(4 K T/3 \eta\right) c^2
\]

(2.16)

In a similar way the orthokinetic agglomeration can be represented by:

\[
\frac{\partial c}{\partial t} = -4/3 \alpha_0 G d^3 c^2
\]

(2.17)

where \(G\) is the mean velocity gradient and \(\alpha_0\) stands for the collision efficiency, in the case of shear flow.

Accepting the fact that the kinetic agglomeration mechanisms are additive, and that
the size distribution of the suspended particles is plurimodal\textsuperscript{3,33,88}, then the differential equation that describes coagulation is:

\begin{equation}
\frac{\partial c}{\partial t} = -k_b c^2 - k_{sh} c^2 - k_{ds} c^2
\end{equation}

(2.18),

where:

- $k_x$ – constant or variable rate associated to each contribution: b – Brownian motion, sh – shear flow, ds – differential settling;
- $c$ – concentration of particles in solution;
- $k_b$ – constant function of the Boltzmann constant, temperature, absolute fluid viscosity, characteristic particles sizes and efficiency coefficient;
- $k_{sh}$ – parameter that depends on the characteristic sizes, shear and efficiency coefficients;
- $k_{ds}$ – parameter that varies with the kinematic viscosity of the fluid, density of suspended solids, gravity acceleration, characteristic size distribution, and obviously efficiency coefficient. For particles of diameter greater than 1 $\mu$m, the perikinetik contribution may be neglected\textsuperscript{4} (fig.17).

In 1982 Hunt\textsuperscript{25} presented a simplified expression to evaluate the influence of coagulation in the overall time variation of particles concentration, in natural suspensions:

\begin{equation}
\frac{\partial c}{\partial t} = -Bc^2
\end{equation}

(2.19),

where coefficient B treats simultaneously different agglomeration processes, and it is susceptible of being determined experimentally – Appendix B.

In 1986, Farley and Morel published numerical solutions for Smoluchowski and Friedlander theoretical approaches, complemented by laboratorial verifications. The main steps and conclusions of that analysis are discussed in Appendix B. The semi–empirical
relation obtained seems to be consistent with the conceptualization and laboratorial observations of these phenomena.

\[
\frac{\partial c}{\partial t} = -B_b c^{1.3} - B_{sh} c^{1.9} - B_{ds} c^{2.3} \tag{2.20}
\]

A critical review of equation (2.20) shows that, considering the approximation of shear flow and differential settling term by a second order power law, the equation proposed by Hunt is reformulated for natural waters — particles diameter > 1 \(\mu m\). This is a very convenient way to treat coagulation, in the perspective of modeling. Although all variables are perfectly identified, the complexity and alienation introduced by the use of large number of parameters is avoided through the consideration of a global coefficient, which may be calibrated for data collected in the natural system, or may rather be subject of a more theoretical analysis\textsuperscript{4,6}.

It is referred in Appendix B that, besides floc density and collision frequencies, the coefficient \(B\) also depends on the collision efficiency, hydrodynamic retardation and chemical activity. Collision efficiency is evaluated following VODL formulation, which is discussed in Appendix C, and summarized in Table 6\textsuperscript{3}. The application of this model has been successful for some situations, essentially those characterized by a very favorable interaction of particles — uniform electrochemical affinity—, with collision efficiencies equal or near unity. The results obtained for unfavorable interactions between particles are generally underpredicted, with differences that go up to several orders of magnitude\textsuperscript{33}. Why does this happen?

VODL is a two-dimensional model based on the assumption that: (a) — all relevant interactive processes between particles occur within the limits of the so-called characteristic distance between particles; (b) — the electrical charge distribution on the surface of the particles is uniform; (c) — those surfaces are regular. In fact, particles have irregular
surfaces, and the charge distribution on the surfaces is highly irregular. Clays, for example, have often their lateral surfaces charged negatively, whereas the edges are positively charged. Likewise, particles may interact with more than one other particle simultaneously. VODL lacks the three-dimensional character that would correspond to a substitution of the characteristic distance by the realistic characteristic volume, simulating the entire spatial area of influence of each particle.

On the other hand, the hydrodynamic retardation influences the chemistry within the electric double-layer as well as the collision efficiency of suspended particles, continuously transported by the fluid in motion. When particles approach one another, the streamlines are disturbed, and the collision becomes effective only if the hydrodynamic forces, associated to the drainage of the fluid between particles, are overcome by the Van der Waals forces. Until Van der Waals forces come into play, the interaction between particles is controlled by the slow drainage of the fluid\(^3\). The fluid drainage may carry solute, consequently altering the constitution of the interactive double-layers, and due to the increase of the collision time-scale, the ions present in the electric double-layer react chemically, reaching different states of equilibrium. The VODL model presumes that the constitution of the electric double-layers is constant during the interval of collision, as well as it assumes absence of chemical activity, and ignores the effect of ionic strength variability.

Coagulation happens, in natural environments, faster and with more impact than it can be predicted by the two-dimensional, steady approach of this model. However, we believe that the viability of equations (2.19) and (2.20) relies in the use of VODL theory supported by laboratorial work and experimentation in general, so that the heteromorphism and dynamic chemical equilibria may be accounted for.
Flocculation

Flocculation is an aggregational process associated to the accomplishment of chemical equilibrium, between the surface of sediments and polymers existent in solution. Polymer molecules are ions, or macro chemical structures, constituted by phenolic and carboxyl groups, that may be or may not be associated to other chemical groups (N, S, P). These groups can interact among themselves and the with surrounding environment. Cellulose, tannins and humic acids are examples of natural polymers. Polyvinyl and Polystyrene are synthetic polymers (fig.18).

Cationic adsorption can happen in the negatively charged surfaces and anionic adsorption is accomplished in the presence of cations that link together the surface of the particle and the active group in the polymer. Adsorption of this type is limited to the bonding of the functional group to a particular site in the particle surface. However, as polymers may contain several active groups, and the surface of the particles more than one suitable site for adsorption, the latter can happen repeatedly between a particle and a surface. The number of adjacent particles included in the same floc, and the stability of the floc are directly related to the length of the polymer. This kind of interactions is responsible for significative successful aggregation of particles in natural systems, and justifies the high degree of surface uniformity with respect to electrical properties found in estuaries, eventually baffling the influence of the mineral matrix of suspended particles in the geochemistry of the system.8,33,88

Synthesis

Most particles in natural waters are negatively charged.8,28,33 This is known to happen by adsorption of organic matter, essentially humic substances, onto the surfaces. Humic substances are anionic polymers of low to moderate weight, containing both aromatic and aliphatic components. Their life—time is of the order of centuries.33 The
adsorption of humic substances results from the interaction of hydroxyl groups on the surface of the particles and carboxyl groups on the humic substances. After adsorption, the humic coat on the particles surfaces acts as a stabilizing screen (fig.19.a,19.b).

In estuaries, the influx of sea-water increases the concentrations of divalent ions as Na$^{2+}$, Ca$^{2+}$ and Mn$^{2+}$. Flocculation is strongly favored in the presence of these cations, since they act as coordinating links, allowing the adsorption of anionic polymers on the negative surfaces of silts and clays. Laboratory experiments verified that the influence of Na$^{2+}$ in the stability of suspended particles is practically nil, whereas Mn$^{2+}$ and Ca$^{2+}$ definitely enhance instability$^{36}$.

In this context, "stability" refers to the maintenance of particles in suspension (a situation energetically unstable), and "unstability" refers to agglomeration and increased velocities of deposition.

The stability controlled by the humic coatings is due either to the uniformization of the electrical charge distribution, or to the presence of hydrophilic groups, which keep particles apart. When the activities of divalent cations are largely increased in solution, the bonds and links between cations and anionic polymers improve quantitative and qualitatively, generating all sorts of connections among adjacent particles. Interacting particles originate flocs, which process of formation include either surface or solution chemistry. In this text, the term flocculation is used referring to both mechanisms: flocculation, and coagulation.

Besides polymeric interaction, other chemical processes may play important role in the mechanisms of aggregation: metal complexation by coordination of multivalent cations with hydrophillic colloids, adsorption of hydrolyzed metal ions and bioflocculation. Bioflocculation results from agglomeration of bacteria or algae with hydrophillic surfaces, which enhances coordination chemistry, and the adsorption of polymers excreted by microorganisms (Table 7).
Predictive ability is the ultimate goal to be achieved by efficient research. However, some questions remain to be answered in the present state-of-the-art, in order to accomplish that objective: — how important is aggregation in the general context of sedimentation in estuaries?, — is it possible to simulate coagulation and or flocculation for real situations?, — should we make the effort to consider bioflocculation and turbulent sorting of suspended particles?, — how far can we get from complexity so that simple reliable conceptual schemes may be formulated?

There is factual evidence of the importance of flocculation in estuaries. It is expected that, the use of semi-empirical relationships, experimentally verified, together with a correct processing and management of field data, will allow a correct numerical simulation of that mechanism. Bioflocculation occurring in areas of intense biological activity, as tidal marshes and low intertidal flats, should be considered as well. However, the extreme complexity of biological processes, and the gap existent between abundant qualitative and almost null quantitative analysis of these mechanisms, limit any attempt of mathematical modeling. Finally, it is never too much stressed that the complexity in the mathematical simulation of natural phenomena is always a measure of the actual limits of our understanding.

2.3.4 — Biogenic mechanisms

Biodeposition

Biodeposition is responsible for hydrodynamic sorting and accumulation of very fine material in regions of intense turbulence, where otherwise that would not happen. The term biodeposition refers to settling and deposition of fecal pellets. Fecal pellets are
excretion products of suspension-feeders: oysters, copepods, etc; and detritus-feeders; and most mud-ingesting benthic population\textsuperscript{51}. Supension-feeders, and detritus-feeders remove, by ingestion, extremely fine sediments from solution (1 -2\mu m), which are afterwards processed and returned to the water with long cylindrical or ovoid form (50 - 3000 \mu m)\textsuperscript{51}.

Although the contribution of fecal pellets for the total suspended matter is generally smaller than 1\%, this value is often increased if the fecal pellets concentration is expressed in terms of retained percentage in filters of 125 \mu m or 50 \mu m. In this case, concentrations vary from 25\% to 50\%, but these are just averaged values, in the sense that there will be significant variation with the animal population of different regions of the same estuary, and from estuary to estuary.

Benthic organisms play an important role in the increase of organic contents in the sediments, as well as, in the texture of the sediments surfaces. Sorting is derived by suspension-feeders activity. Table 8, from Haven and Morales-Alamo, permits to compare settling velocities of pelleted and non-pelleted very fine particles. Settled pellets are later decomposed by microbial activity, and the particles are released into the sediment strata, as if they were submitted separately to gravitational settling. Pelletization of particles may be considered an aggregational process, working as a catalyst of settling, and so, it can be included in the deposition rate.

**Bioturbation**

Bioturbation refers to the turbulence and dispersion generated by aquatic biota in the water-column, or in the sediments.

Benthic invertebrates inhabit the upper layers of sedimentary regions, in estuaries. These organisms feed on organic material, benthic plants, and other microorganisms living in the sediments. Looking for protection, benthic invertebrates live often below the surface of the sediments, generating turbulence and particles entrainment. Polychaetes, olichaeetes,
and mud or fiddler crabs\textsuperscript{2,32} are the most important bioturbators, either because these worms, or crustaceans can penetrate as deep as 15–25 cm in the sediments, since they can tolerate low oxygen levels, or because their biomass is a major component of benthic fauna.

Therefore, bioturbation affects the diffusion coefficients, by increasing the rate of entrainment, and it also affects the critical erosion stress of the bottom surfaces. Although there is presently no way to quantitatively approach the simulation of these phenomena, it is important to be aware of their influence in the analysis of field data.

Most research dedicated to benthic invertebrates, and bacterial activity has taxonomic and descriptive characteristics. It is imperative to increase research, in the areas of the physical and chemical impact of aquatic forms of life in the environment.

**Productivity of organic sediments**

Algae, diatoms, plankton in general, and lower groups of zooplankton, continuously increase the concentration of organic sediments. This effect can be expressed in terms of decay rate—death and decomposition of organisms—, versus productivity rate—reproduction. The quantification of those two rates is an extremely difficult task, since they are directly related to light penetration, temperature, and nutrients availability. Nutrients, light, and temperature, are not included within the environmental sceneries that bound the objectives of this work. In this perspective, the formulation proposed by Farley\textsuperscript{73} will be accepted, as a starting point, to evaluate bioproduction of organic sediments:

\[
\frac{\partial c}{\partial t} = Pc
\]  \hspace{1cm} (2.21).

The coefficient \( P \) accounts for decay and productivity, and therefore can be designated by "effective productivity". Usually \( P \) is considered constant for regions of the estuary with similar biological activity, and is obtained from field data calibration.
2.4 – Implications on Water-Quality: The Fate of Trace Elements.

Trace elements are chemical elements whose natural concentrations are extremely small. The natural source of these elements is the geologic weathering of sediments, rocks and mineralized deposits. Weathered trace elements enter in lakes, rivers, estuaries and oceans by land drainage or atmospheric deposition. These natural inputs are responsible for the so-called base-line levels of trace element concentrations found in natural, unpolluted water-bodies.

Since the beginning of the Industrial Revolution, the use of trace elements in industries, agriculture and other human activities have been progressive and persistently accelerated. Therefore, industrial, agricultural and urban wastes are actually the main sources of trace elements into polluted natural waters. Because of the high indexes of industrial and urban occupation in adjacent areas, estuaries are particularly stressed water-bodies. Anthropogenic effluents are discharged into estuaries either by waste-disposal systems (point-sources), or by lateral run-off (non-point sources). Atmospheric deposition is the most important pathway of trace elements in the deep ocean and far continental shelf, but its contribution to the high concentrations of these elements in polluted estuaries is negligible\textsuperscript{76}.

Cromium (Cr), Cobalt (Co), Copper (Cu), Zinc (Zn), Cadmium (Cd), Mercury (Hg), Lead (Pb) and Tin (Sn) are the trace elements whose concentrations have been increased the most in the past decades\textsuperscript{60}. High concentrations of these elements are motive of big concern, because of: (a) – their almost null biodegradability at all levels of the food chain\textsuperscript{32}, and (b) – their affinity to adsorb on sediments surface, which results in increased residence times of those substances in estuaries.
Toxicity is the ability of specific substances to change the natural conditions of organisms to survive, or develop characteristic activities. Toxicity may be revealed at different processes in the living organisms: disturbance of enzymatic systems, complexation with metabolites and catalyze of metabolites breakdown, permeability of tissues and cell membranes, and substitution of other elements in cell metabolism leading to its inhibition. Frequently toxic effects are classified as sub-lethal, meaning that organisms present malformations, but do not die. Although exceptionally high concentrations are detected now and then, lethal effects are seldom verified, due to detoxifying interferences of other compounds. In general, the smaller the natural concentration of the element the more toxic it is: Hg, Ag, Cd, Sn, which natural base lines are of the order of a few ppb, are more toxic than As, Co, Cr, Cu, Zn, with natural base-lines expressed in ppm, which in turn are more toxic than Al, Ca, Fe, Na, Mn, usually present in quantities of mg/1\(^{32}\).

Bioavailability of heavy metals to aquatic biota is poorly understood; it is known, however, that either by ingestion or by skin penetration, these elements accumulate in zooplankton, benthic organisms and fish tissue, until highly toxic levels are reached\(^{28}\). The toxicity is more important for ionic species and complexes of higher oxidation number. The presence of very elevated salt concentrations, and relatively large amounts of organic matter, make estuaries to behave as big, extremely active chemical reactors. Microorganisms, essentially bacteria, present in the water-column or in the bed-layers, are also catalyst agents for chemical transformations: complexation and chelation\(^{67,77}\). The direct adsorption of trace metals by biota, from the water, was proved to be relevant by Fowler\(^{68}\) in the Mediterranum Sea, where the concentrations of mercury found in bioassays, exceeded the values predicted in function of concentrations found in the smaller prey groups of the food chain.

_Ecotoxicology of Trace Elements_
Mercury, lead, tin and cadmium are the most toxic of all trace elements. Trace metals react with either organic or inorganic anions, originating respectively organometals and inorganic compounds. Lead, mercury and tin are also passive of methylation, the formation of \((\text{CH}_3)\text{Me}\) compounds, in the water column or in the bottom sediments, due to microbi ally mediated redox chemistry.\(^{52,63,86}\) Although every trace metal compound is poisonous, organometals are particularly dangerous, since the rejection mechanism of the organisms for these compounds seems to be more relaxed and relatively inefficient.

Methylmercury is the most common of all organomercury compounds, and it has been identified as the most toxic, as well. Besides direct intoxication, methyl compounds pass from pregnant women to their fetus; this was how Minamata disease, a congenital intoxication, developed.

Tin was historically considered as an inoffensive chemical element. Suddenly, in the past five to ten years, and specifically under the form of tributyltin (TBT), the toxicological effects of this element became more and more apparent, in such a way that presently, organotin concentration is considered a very important water—quality indicator. The speciation of tin in estuaries is distributed by butyl, methyl and mixed butylmethyl forms.\(^{78}\) Butyltin is originated from a diverse range of anthropogenic activities, but it seems to be the use of tributyltin, incorporated in the paints of the ships as a biocide for fouling organisms, that has the greatest short—term toxicological influence in harbors and coastal waters adjacent to harbors.\(^{63,78}\) TBT is also highly toxic to mysid shrimps, shore and mud crabs, mussel and lobster larvae, copepods, and in general all small elements of the food chain.\(^{63,78}\) Inorganic tin is non—toxic, and toxicity increases with the number of butyl groups up to 3, decreasing for tetrabutylin.\(^{78}\)

Lead methylation is still poorly understood, although some experimental work has been done very recently.\(^{86,87}\) However, transmethylation between organometallic species in the case of lead and TBT appears to be very important. Indeed, the formation of methylbutyltin compounds by release of lead methyl groups was reported by Chau.\(^{87}\)
estuarial waters, as an important pathway in the process of TBT breakdown.

Due to its extended half-time in human or other organisms, cadmium is special motive of concern in the domain of heavy metals toxicology\textsuperscript{69}. One of the past recent epidemic manifestations also occurred in Japan, where cadmium contaminated waters were used for drinking and for irrigation. The large amounts of cadmium incorporated in the human organism (up to 15000 µg/l) lead to chronic poisoning of bones and consequent decalcification at extremely drastic levels (Itai–Itai disease).

Trace metals are not ingested alone. As a matter of fact, most heavy metals are persistently present in natural waters. This fact leads the very important subject of metal interference and detoxification. Detoxifying activities are mainly conducted by proteins, or by kinetic and metabolic interference of different metals in the organism\textsuperscript{69}. S, Co and Se, for example, play a detoxifying role in relation to cadmium, molibdenum and mercury respectively\textsuperscript{83}. Environmental water—quality analysis in terms of a specific metal species are legitimate, but extrapolations about its real potential for toxicological impact are strictly dependent on the nature of metabolic interactions with other elements\textsuperscript{83}.

\textbf{Chemistry of Trace Elements}

Trace metals transported to estuaries can be present in the water column in dissolved (20\%) or particulate form (80\%)\textsuperscript{88}. When they are present in particulate form, heavy metals can be adsorbed on surfaces, in solid organic particles, in organic or oxide (Fe/ Mn) coatings, in lattice positions of silts and clays or others, and precipitated as pure phases on detrital particles\textsuperscript{66}.

Elements located in lattice positions of crystals or precipitated in pure phases are usually rapidly taken out from solution, and deposited on the bottom, since they are
integrated in particles that are in the range of the fine sediments and up. Whether deposited or in solution, these trace metals are not available for chemical reactions or biologic activity. Higher concentrations of elements with these characteristics are found in the anoxic sedimentary layers.

Suspended metals, either dissolved or adsorbed to particles are submitted to chelation, complexation, adsorption and desorption to sedimentary suspended particles. Adsorption of metal on the surfaces of suspended particles is a stable process in estuaries, and it has been proposed as the only geochemical parameter determining the metal speciation in natural waters, Morel$^{88}$ (1983). The most common expression to describe adsorption is the so-called Langmuir isotherm:

$$\Gamma = \Gamma_{\text{max}} \frac{K_{\text{ads}}(C)}{1 + K_{\text{ads}}(C)}$$ \hspace{1cm} (2.22)

$\Gamma$ is the adsorption density parameter —mass of C adsorbed per unit mass of solid sorbent X—, and $K_{\text{ads}}$ is the rate at which the process occurs.

Dilution, pe, pH, ionic strength/ salinity, and organic matter present in solution are all variables that influence the fate of heavy metals in estuaries (fig.20). As it was referred previously, in section 2.2.2, humic substances usually exist in relatively large amount in estuaries, dissolved, in particulate form or coating sedimentary particles. Trace metal ions have strong affinity with humic substances, and so stable complexes can be generated.$^{28,32,78}$ The adsorption of metals can result from direct complexation with humic coatings, or $a$ $\textit{posteriori}$ adsorption on sedimentary particles surface of humic—metal complexes in solution. However, due to conditions related to pH and ionic strength in estuaries, iron and manganese oxides and hydroxides form very fast and in large amounts.$^{52,65,66}$ These newly formed solids precipitate very often on the surfaces of organic or mineral particles, and they may often compete with humic material for the scavenging of trace metals.$^{52,65}$ Lion $et$ $al.$$^{65}$ found that binding of Pb is controlled by
Fe/ Mn oxide coatings, whereas Cd adsorption for example was strongly correlated to the presence of organic coatings. It is also possible to verify from the results presented by these authors that, for the range of alkaline pHs in natural waters, adsorption governed by humic substances was almost 100% (fig. 21). Note that these experiments were made in ideal conditions, and besides problems related to the chemical techniques used, the competing effect of chloride and sulfate was not considered, since those ions were absent in solution. Dilution influence may also be relevant, as it can be inferred from the analysis of figures 27.a and 27.b\textsuperscript{61,88}.

There are three main pathways to remove heavy metals in particulate phase from the water column: by deposition of particles, by biological uptake, or by transport and discharge into the sea. Particles exported to the coastal shelf may return during flood tides or penetration of maritime currents in the estuary.

Bacterial and algal population in the water column have also been reported to have influence on the uptake of trace elements, although conclusive information is scarce. Methylation mechanisms, referred with relative persistence, are mostly unknown. Hart\textsuperscript{77} suggests that the rapid uptake of trace metals by the bacterial population associated to the sediments, and subsequent incorporation of bacterial biomass into the sediments, together with algal mineralization, can be an important pathway of trace metals in the water column. Many other pathways of this type have been proposed, yet they generally lack a reliable quantitative analytical formulation.

Nevertheless, Wangersky\textsuperscript{52} refers that most literature agrees that the majority of heavy metals are indeed scavenged essentially by organic matter, being the concentration of those metals and particulate organic matter very well correlated.

On the other hand, the fate of deposited or sedimentated particles is rather more complex. Some deposited heavy metals in zones of intense shoaling, become rapidly unavailable for any kind of interchange with the water column. Indeed, the accumulation of sedimentary layers limits drastically the circulation of interstitial water, such that
anoxic conditions develop, which may inhibit microbial activity. However, during dredging operations those materials become readily available, and trace elements are introduced in the water column by resuspension. Particles that stay in the top layers are constantly submitted to chemical and biological activity. Metals associated to organic matter are separated due to microbial decomposition, and segregated in the sedimentary layer.

Chemical interchange between sediments and the water column can happen by dissolution or chemical interaction with oxides and humic substances present in the water column, by release of organometals into solution after bacterial methylation in reducing conditions, or finally due to the effects of bioturbation, and eventually methane production\textsuperscript{32,52,59,61,63,65,66}. The formation of methylmercury, dimethylmercury, dimethyltin and trimethyltin is very important in terms of ecotoxicological consequences in the food chain. TBT degradation apparently follows a stepwise oxidation of the butyl groups\textsuperscript{77}, although it can also interact with methylated species, as discussed before. The tracking of these pathways is extremely difficult, and most research efforts in this area are still dedicated to the identification of different compounds present in natural waters, rather than in the evaluation of the chemistry involved.

Higher concentrations of Pb, Cd, Hg, and Sn are detected in the shoaling zones of estuaries, corresponding to the deposition of very fine material\textsuperscript{59}. Figure 22 is particularly elucidative of this aspect, although it refers to a specific case: the estuary of Ems River.

\textbf{Assessing Trace Elements as Water–Quality Indicators}

In the next paragraphs, two different strategies to approach this problem are suggested. Method A is based on the classic methodologies used to simulate the chemistry of a specific element, while Method B relies on the use of real field data analysis, collected in the literature, as support for non–conventional assumptions in the formulation of a simplified mathematical model.
Method A — The lack of quantitative tools to describe biogeochemical processes in natural waters, and in particular in estuaries, limits the formulation of a detailed speciation model to evaluate the impact of different compounds in the environment. However, a simpler approach may be attempted. Trace elements are present in natural waters essentially in three forms: dissolved, as suspended particulate matter or incorporated in deposited sediments. Instead of making a detailed identification of different compounds eventually present in the environment, the distribution of trace metals will be assumed to be restricted to the three general forms referred above.

Because of erosion and deposition, there is a constant interchange between the bed-layers and the water column. This continuous interchange is treated as a flux bottom boundary condition \( \eta \), in the case of dissolved phase:

\[
\eta = k_b (c^d - c_b) + \mu_t c_b \tag{2.23}
\]

Osmose due to concentration gradients and tidal pumping—effect on the interstitial water circulation are included in the coefficient \( k_b \); \( \mu_t \) is a methylation rate; \( c^d \) is the concentration of dissolved trace metal in the water column and \( c_b \) is the total concentration in the sedimentary layers. In intertidal flats, submitted to intermittent aeration, and scenery of big amplitude changes in the reducing conditions, the coefficient \( \mu_t \) must be considered in a flexible way, so that for different conditions of aeration different oxidizing conditions may be accounted for.

In the case of sorbed trace metals, the bottom boundary condition is similar to the bottom boundary condition already proposed for sediments, in section 2.3.2.

The coexistence of dissolved and particulate phases in the water column is established through the definition of a partitioning coefficient, \( k_w \):
\[ c^p = k_w c \]  \hspace{1cm} (2.24),

\[ c^d = (1-k_w) c \]  \hspace{1cm} (2.25);

leading to

\[ c^d = \frac{(1-k_w)}{k_w} c^p \]  \hspace{1cm} (2.26),

where \( c^p \) is the concentration of the particulate phase, and \( c \) is the total concentration in the water column. The partitioning coefficient, which is variable in time, must depend on \( p_H \), ionic strength (salinity), and available adsorption sites (very fine sediments concentration), and can be inferred from the Langmuir adsorption rate (fig. 23). As the concentrations of very fine sediments are always large in most estuaries, and consequently the total surface area available for adsorption, it is legitimate to presume that the availability of adsorption sites does not constitute a limiting factor in the this process.

Analysis of Figures 22.(a) and 22.(b) indicates that linear variation is also expected to develop in the longitudinal direction of the estuary\(^{66,68} \), although in two different patterns: dissolved and adsorbed particles concentration suffer a very strong variation in the maximum turbidity zone, due to flocculation\(^{39,40} \), and then behave almost conservatively in the lower end of the estuary. Mercury, tin and lead are not shown in the figures, but they have been reported to behave in the same fashion\(^{59,80} \) Tables 9,10,11. This dependence on the values of salinity can assume great importance either in the modeling process itself, because it constitutes a clear indicator of salinity influence on the aggregational processes of particles, or as a verification of the results obtained.

The transport equation can be applied to both, dissolved and particulate phase, in
the water column, and finally total concentrations can be evaluated.

**Method B** — Experimental results collected in the literature give strong support to the linear correlation between heavy metals concentrations in solution, and organic contents of the sediments. As humic acids are presumed to coat almost entirely very fine sediments present in solution$^8,28,33,77$, the statement presented in the previous paragraph can be extrapolated for very fine sediments with confidence, although additional work of verification must be done. The theoretical argumentation for this defense of linearity is given by Bernard Patten$^70$ in his discussion about necessary conditions for realism in ecological models. Hence, as a first conclusion:

$$[\text{Me}]_s = M_s [\text{VF}]_s \tag{2.27},$$

where $[\text{Me}]_s$ is the concentration of trace metal in solution, $[\text{VF}]_s$ is the concentration of very fine sediments in suspension and $M_s$ is the correlation coefficient, for a specific region of the estuary. Dissolved and particulate phase are related by a partitioning coefficient, although it is expected that the percentage of particulate form is overwhelming$^{52}$.

According to the state-of-art associated to the quantification of microbial activity, it is difficult to try to delineate a mathematical approach for the problem. The biotic production of methyl compounds is strongly dependent on the amount of organic carbon present in the sediments, as well as on the nature of the redox conditions. Assuming that a parameter $M_t$ can be found, relating total methylmetal to the initial metal concentration in the sediments, then:

$$[\text{Me}]_o = M_t [\text{Me}]_b \tag{2.28},$$

with $[\text{Me}]_o$ being the methylated concentration of trace element released from the bottom,
and $[\text{Me}]_b$ is the concentration of the trace metal at the bottom. $[\text{Me}]_b$ can also be related to the concentration of very fine sediments in the bottom, using another correlation coefficient. The total concentration in solution will be:

$$[\text{Me}]_t = [\text{Me}]_s + [\text{Me}]_o \quad (2.29).$$

There are two ways of considering eventual formation of heavy metals compounds with Cl and S, both based on the assumption that those compounds will have a minimum contribution to the overall concentrations balance: either it is accepted that the coefficient $M_s$ or $M_b$ accounts for their presence, which is valid if the correlation is established in terms of global concentrations, or it may be included as noise, at the time of model calibration.

The decision of choosing one of the methods proposed, instead of the other, is strongly dependent on the conditions existent to establish the different coefficients. It is perceived that, the effective implementation of Method B will lead to the use of sophisticated techniques of signal processing, but it seems to be the way to obtain the ability of making quantitative prediction of environmental quality indicators. The results obtained by that initial attempt may be used, afterwards, as background information to implement Method A.
3. MODELS OF SEDIMENT TRANSPORT: SELECTED REVIEW.

3.1 Introduction

The scheme presented below will be the basic guideline used for the review of the available models of sediment transport, whose formulation accounts for the processes considered, in this analysis, as the most relevant in the dynamics of estuarial sedimentation and, or implications on water-quality. The guideline was established to specify and identify the main phenomena associated to the role of sediments as a major carrier of contaminants in natural waters, as well as the details of the approaches of different authors to the understanding of the mechanisms associated to it.

The processes associated to the dynamics of sedimentation, generally identified as (A), are distributed according to the following pattern: dimensionality of the model and solution of the transport equation; type of sediments and characteristics of sources and sinks; flocculation and settling; dispersion and advection; deposition/sedimentation; erosion/resuspension; bottom evolution and consolidation.

Likewise, the processes associated to the fate of contaminants, and respective interaction with sediments (B) are differentiated as follows: partitioning; adsorption/desorption; chemical activity; microbial activity; removal rate, burial and decomposition. The analysis of each model concludes with the reference of a relevant field application (C). Table 14 identifies the models included in this review by author, date and field of application.
3.2 - "A Simplified Deposition Calculation For Organic Accumulation Near Marine Outfalls". 73

A - The model accounts for advection, particle transport, organic carbon cycles, and includes the effects of coagulation and settling of effluent particles and natural organic material. The applicability of the model is limited to deep waters, since sediment redistribution caused by complex circulation, which is characteristic of shallow waters is not considered. The model also attempts to quantify the fate of toxic chemicals, with particular relevance for heavy metals.

Although being bi-dimensionable, the model considers two different layers in the vertical direction: the surface layer above the pycnocline and the lower layer, below the pycnocline. Both layers are considered vertically well-mixed. The transport equation is provided with analytical solution.

Particles of anthropogenic origin are considered by the introduction of a constant term in the convection-diffusion equation: S; however, the concentrations of natural particles are expressed in terms of productivity rates. As a matter of fact, natural particles considered are exclusively organic particles, whose concentrations are assumed to be correctly expressed by the phytoplankton productivity P, quantified experimentally:

\[
\frac{\partial c}{\partial t} = \frac{P}{h}
\]

A second order relation, similar to the one presented in section 2.3.3, is used for the evaluation of the effects of flocculation in the deposition process. Its mathematical and physicochemical support comes from Farley and Morel work for colloidal sized particles, explained with detail in Appendix B.

\[
\frac{\partial c}{\partial t} = -Bc^2
\]
The transport of natural particles is ignored, since phytoplankton productivity is considered spatially uniform. Advection of non-natural particles is assumed to be caused by two different mechanisms: tidal forcing, which distributes the discharges over an extended area, and non-tidal components of flow (wind-driven currents and large-scale circulation), which advect the plume outside the discharge area.

As the model does not have a module to simulate circulation, the velocity distributions are defined in terms of significative time-scales, and then averaged. Brownian diffusion and turbulent diffusion are neglected.

The net sedimentation is expressed as an accumulation concentration, and established in terms of deposition flux, and removal rate, which includes burial effects and in the case of contaminants, decomposition and metabolism rates. The burial effect may be associated to the consolidation effect, in the sense that is intrinsically related to the inaccessibility of a specific material, due to its position in the sedimentary layers.

\[
\frac{\partial c_s}{\partial t} = -K_s c_s
\]

Erosion or resuspension are considered in terms of turnover rates in the surface sediments, and also included in the same coefficients described before.

B — Organic particles decomposition is described by a first order decay law, which coefficient is \(K_d\).

The general form of the PDEs that give form to DECAL is:

\[
\frac{\partial c}{\partial t} + \vec{v} \frac{\partial c}{\partial l} = S - kc - \frac{Bc^2}{h} + \frac{P}{h}
\]

\(-1\) is distance from reference point—
\[ P = 0 \quad \text{(inorganic particles)} \]
\[ S = 0 \quad \text{(lower layer)} \]
\[
\begin{cases} 
  k = k_d \quad \text{(surface layer)} \\
  k = k_s \quad \text{(lower layer)} 
\end{cases}
\]

In the case of heavy metals, a partitioning coefficient \( k_p \) between dissolved and particulate phase is defined, such that if \( C_{\text{dis}} \) is the concentration of dissolved material, the particulate phase concentration is expressed as:

\[ C_p = K_p C_{\text{dis}} M \]

\(- M \) is the mass concentration of suspended particles–

The advection–diffusion equations have the following form:

\[
\frac{\partial c}{\partial t} + \nabla \cdot (\vec{v} c) = S - B k_p C_{\text{dis}} M^2
\]

and

\[
\frac{\partial c_s}{\partial t} = B k_p C_{\text{dis}} M^2 - k_r c_s.
\]

The concentration, \( c \), in the transport equation, is total concentration.

\[ c = C_p + C_{\text{dis}}. \]

The coefficient \( k_r \) is of the same type as \( k_d \) and is defined as an "apparent interfacial removal rate, including chemical reactions, macrobial activity, adsorption/desorption and burial effects."
C - The model was applied in the study of marine sewage outfalls environmental impact along the Californian coast.

3.3 - "Resuspension Model"\textsuperscript{31}.

The model is formulated for cohesive sediments, and is applied to a shallow lake, hence with circulation patterns completely different from the ones of the estuarial domains discussed in this text. Although that fact inhibits the use of the analytical solution proposed by Luettich as solution of the advection-dispersion equation, the way deposition/sedimentation and erosion/resuspension are handled, is relevant in the context of the transport of sediments. The model does not provide any insights in terms of the simulation of water-quality indicators, and flocculation is ignored.

A - The model is initially presented as a two-dimensional depth averaged model, but according to the specific circulation characteristics of wind-induced waves, an analytical equation is presented: zero-dimensional model.

Deposition/sedimentation and erosion/resuspension are described together, expressed in terms of a bottom boundary condition:

\[ \phi = -\beta \bar{c} + \beta k (\tau_b - \tau_c)^n, \]

where \( \phi \) is the net sedimentary flux at the bottom, \( \tau_b \) is the shear stress at the bottom water/sediment interface, \( \tau_c \) is the critical bottom shear stress; \( k \) and \( n \) are functions of the
consolidation degree, armoring and sorting conditions, texture and in general all sediments characteristics. The coefficient $\beta$ depends on the settling velocity, bottom and depth averaged concentrations, respectively $c_o$ and $\bar{c}$:

$$\beta = w_s \frac{c_o}{\bar{c}}$$

In areas of reduced turbulence and for fine cohesive sediments $c_o \approx \bar{c}$, and so $\beta = w_s$.

The suspended sediment transport equation as established by Luettich is:

$$\frac{\partial \bar{c}}{\partial t} = \frac{\phi}{h} - \frac{\partial}{\partial x} \left( \bar{u} \epsilon_x \frac{\partial \bar{c}}{\partial x} \right) - \frac{\partial}{\partial y} \left( \bar{v} \epsilon_y \frac{\partial \bar{c}}{\partial y} \right)$$

The quantification of deposition and erosion rates at the bottom of the water-column, in terms of a bottom boundary condition, is referred previously in the literature by Somlyody$^{14}$, Aalderink$^9$ and, Lavelle$^7$.

C — The model was applied to the Balaton Lake, in Hungary.

3.4 — "Suspended Sediment Transport Model in Non–Uniform Flows".$^{17,44,45}$

The model is exclusively dedicated to sediment transport, relying on the availability of an extensive field data basis, and it is particularly adequate for sand type material.

A — This is a two–dimensional vertical model, width averaged, that utilizes the classical convection–dispersion equation. A finite–element technique is used to solve the differential equation.
Flocculation is not considered, and the settling velocity is introduced as a deposition term in the distribution of vertical flow velocities.

Since the model is width averaged, the velocity field is reduced to the longitudinal and vertical directions of flow. In the absence of a circulation module, the model utilizes empirical and semi-empirical vertical velocity profiles, which must be calibrated for each application. Dispersion is represented by a sediment mixing coefficient $\epsilon_s$, variable in the vertical direction and that has the following distribution function:

$$\epsilon(z) = 0.25 \kappa u^* h \left[ 1 - \left( 1 - \frac{2z}{h} \right)^2 \right], \quad \frac{z}{h} < 0.5$$

$$\epsilon(z) = 0.25 \kappa u^* h, \quad \frac{z}{h} \geq 0.5$$

$u^*$ — shear velocity

$\kappa$ — Von Karman coefficient

$h$ — water column depth.

To account for the effect on turbulence of the presence of sedimentary particles:

$$\epsilon_s(z) = \epsilon(z) \beta \phi, \quad \phi = 1 \text{ and } \beta \epsilon [1,3]$$

This aspect was previously discussed in Section 2.3.2. The transport equation that summarizes what has been described until now is:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x} (uc) - \frac{\partial}{\partial x} (\epsilon_s \frac{\partial c}{\partial x}) + \frac{\partial}{\partial z} [(w - w_s) c] - \frac{\partial}{\partial z} (\epsilon_s \frac{\partial c}{\partial z}) = 0$$

The concepts of deposition and erosion are substituted by the imposition of a
bottom boundary condition at depth (h−a), which includes the consequences of the occurrence of flow separation and flow reversal. The boundary condition may be imposed in terms of concentrations or upward sediment fluxes:

\[ c = c_a \quad \text{at} \quad z = a, \]

or

\[ E_a = -\left( e_s \frac{\partial c}{\partial z} \right)_a = w_s c_a \quad \text{at} \quad z = a. \]

Although very complex, the expression of \( c_a \), provided by the author\textsuperscript{17,45}, is only valid for sand particles in the range 100 – 500 μm.

The height \( a \) corresponds to the height above the mean bed level, that separates the region of the flow where sediments behave as suspended matter, from the region of the flow where the movement of sedimentary particles is represented by a bed-load transport formula.

Accepting that the suspended load transport \( S_s \) is:

\[ S_s = b \int_{z_b + a}^{z_b + h} c \, dz, \]

and that \( S_b \) is obtained using a bed-load transport equation\textsuperscript{17}, the variation of the bed level \( z_b \) with respect to a horizontal reference can be described by:

\[
\frac{\partial}{\partial t} (b \, z_b) + \frac{1}{\rho_s (1-p)} \frac{\partial}{\partial S_s} (S_s + S_b) = 0
\]

\(- p \) is the porosity of bed material—

C – The model was applied to the study of sedimentation in the navigation channel
of Asan Bay, Korea.

3.5 - "Modeling Bottom Boundary Layer and Cohesive Sediment Dynamics in Estuarine and Coastal Waters"\textsuperscript{84}.

This model is applied to cohesive sediments, and its principal characteristic relies on the very detailed theoretical approach used in the simulation of the three dimensional turbulent dispersion of sedimentary particles. Erosion, deposition and floculation are modeled as separate processes.

A - The model is three-dimensional. However the treatment of deposition presumes the existence of resistance layers, whose distribution is similar to the equivalent of a stratified water-column. The resistance layers include hydraulic boundary layers, as well as bottom flora interference.

The model simulates cohesive sediments dynamics. Floculation is approached as a separate mechanism, although its effects on the deposition rates are accounted for. Smoluchowski formulation to describe the collision of suspended particles is used, and the variation of particles density, as well as the velocity of deposition are evaluated with Friedlander theory. The evolution of particles size distribution is described as:

\[
\frac{Dm}{Dt} + \frac{\partial m}{\partial x_i} \frac{U_{ci}}{\partial x_i} = 0,
\]

\[
\frac{Dn_f}{Dt} = -N_{ff} - N_{fc} - N_{cf}\]

65
\[
\frac{Dm_c}{Dt} + \frac{\partial m_c}{\partial x_i} \cdot U_{ci} = M_{fc} + M_{cf},
\]

\[
\frac{Dn_c}{Dt} + \frac{\partial n_c}{\partial x_i} \cdot U_{ci} = N_{fc} - N_{cc},
\]

where:

- \( m \) = mixing ratio,
- \( n \) = number density,
- \( N_{ff} + N_{fc} \) = loss of fine particles due to collision between fine particles,
- \( N_{fc} \) = production of coarse number density,
- \( M_{fc} \) = mixing ratio due to self-collisions among fine particles,
- \( N_{cf} \) = rate of loss of fine particles density,
- \( M_{cf} \) = rate of production of coarse mixing ratio by collisions between coarse and fine particles,
- \( N_{cc} \) = rate of loss of coarse number density by self-collision of coarse particles.

A second-order closure model of turbulent transport is used in connection with a non-newtonian fluid flow model, so that the damping effect of high sediments concentrations near the bottom can be simulated. A second order closure model of turbulent transport consists on the successive application of the continuity and Navier Stokes hydrodynamic equations considering the mean velocities of the flow, velocity fluctuations, fluctuating temperatures, and turbulent macroscales.

Erosion and deposition are included in the transport equation as boundary conditions. Erosion is represented by the classical expression:
\[ E = M \left( \tau_b - \tau_{e,cr} \right). \]

The simulation of deposition is carried on by the evaluation of a 'deposition' velocity \( V_d \), different from the settling velocity \( w_s \), and that includes the resisting effects of: hydrodynamic factors, sublayer resistance and bottom morphology\(^8\).

The general transport equation has the form:

\[
\frac{\partial c}{\partial t} + U_j \frac{\partial c}{\partial x_j} = -w_s \frac{\partial c}{\partial z} - \frac{\partial u_j c}{\partial x_j} + D_B \frac{\partial^2 c}{\partial x_j^2} + S.
\]

The boundary conditions are described as follows:

\[-w_s - \bar{wc} = 0 \quad \text{at} \quad z = \eta (x, y, z),\]

and

\[-w_s c - \bar{wc} = V_d c_+ - E \quad \text{at} \quad z = -h(x, y);\]

where \( c_+ \) is the concentration at some distance above the bottom, \( \eta (x, y, z) \) is the free surface elevation, and the term \( \bar{wc} \) reflects the influence of the vertical fluctuations of the turbulent velocity. Consolidation and bottom evolution are not simulated by the model.

C - The model was applied in sedimentation studies of the Mississippi Sound estuary, among others.
3.6 "Prediction of Cohesive Sediment Movement in Estuarial Waters"

The model, which is exclusively applied to cohesive sediments, relies strongly on the analysis and statistical treatment of a large data base, that includes results obtained by the author, as well as data collected in the literature. It was specifically developed for estuaries.

A - The model is a 2-D depth averaged finite-element model. Only cohesive sediments are considered: silts and clays.

Flocculation enhanced by salinity is not treated as an independent process, but otherwise associated to the settling velocity and other empirical parameters considered in the formulation of deposition. These variables are obtained from laboratory experiments.

The model has access to a sub-model, that describes circulation based on the numerical solution of the 2-D depth averaged Navier-Stokes equations for shallow waters. A classical 2-D depth averaged advection is afterwards solved, where erosion and deposition are included as source and sink, respectively.

Deposition is essentially evaluated through the use of complex semi-empirical relationships, that typically depend on salinity, steady state concentration of sediments and time. Due to the intrinsic empirical nature of the expressions used, only the general form of the deposition rate is introduced:

\[ D = A e^B, \]

where A and B are obtained experimentally.
The erosion rate is described by the following expression:

$$\epsilon = M \left( \frac{\tau_b - \tau_{e, cr}}{\tau_{e, cr}} \right),$$

where $M$ is the erodibility constant of the eroded layer, empirically established.

The sub-model designated to simulate the effects of consolidation and bottom evolution during time is very detailed, and it is also supported by large experimental observation.

The bed sedimentary thickness is conceptually divided in three regions of different characteristics: the top zone or stationary suspension, the middle zone in process of consolidation, and the settled bed. Each of these regions is then sub-divided into sub-layers of individual thicknesses $T_i$. Consolidation is intimately related to the variability of density in time and with depth:

$$\rho(z_b) = \bar{\rho} K T_{dc}^{n_1} \left( \frac{H - z_b}{H} \right)^{n_2}.$$

The values $K$, $n_1$, $n_2$ are empirical coefficients, $T_{dc}$ is the time of consolidation, and $z_b$ is the depth. The thicknesses $T_i$ of each discrete layer are chosen so that, the profile $\rho(z_b)$ may be linearly approximated within the layer. For the stationary suspension, an additional profile $\rho(z_b)$ must be found experimentally, with data collected in the region where the model is going to be applied. The stationary suspension is established for a concentration of 480 g/l, near the bottom. The resistance of the bed is calculated from the values of $\rho(z_b)$, according to the next relationship:
\[ \tau(z_b) = a \rho(z_b)^b. \]

Eroded or deposited thicknesses are proportionally distributed through the entire bottom sedimentary system, in function of the initial thicknesses of the discrete layers. The discretization of the bottom leads to the necessity of using iterative algorithms, in order to guarantee relative accuracy in the representation of bottom resistance.

C — The model was applied to the study of sedimentation of Marina Bay, Florida.

3.7 — "2D — Model of Mud Transport"\textsuperscript{12}.

The model provides mathematical formulation to simulate advection and deposition of well—mixed cohesive sediments (clays and silts) in suspension. Its aim is not water—quality quantification, but rather the evaluation of siltation rates. According to the authors, in spite of the difficulty to predict accurate rates of siltation, the qualitative information obtained is very good in the perspective of management and engineering projects.

A — The model is two—dimensional vertically averaged, and the transport equation is solved by an implicit finite—difference scheme.

The settling velocity is considered proportional to the concentration, and along with a coefficient related to the efficiency of deposition is utilized to evaluate the deposition rate:

\[ \frac{\partial c}{\partial t} = w_s c P. \]
P is the probability that settling particles stick to the bed. As defined by Krone:

\[ P = 1 - \frac{\tau_b}{\tau_d}, \quad \text{for } \tau_b < \tau_d, \]

where \( \tau_b \) is the local bed stress and \( \tau_d \) is the critical deposition stress, calculated in laboratory tests. Flocculation is not contemplated.

Longitudinal dispersion \( D_s \) and lateral dispersion \( D_n \) are defined in terms of critical shear velocity and water depth:

\[ D_n = 0.2 \, h \, u^* \quad \text{and} \quad D_s = 6 \, h \, u^*. \]

The authors consider that, owing to "a lack of knowledge about the physics involved", it was decided not to include erosion explicitly in the model. Hence, as the model is essentially a qualitative tool, inferences on the characteristics of erosion are made in connection with field data and for particular applications. Resuspension effects may be considered, in the definition of the probability \( P \).

The global mass conservation equation is described as follows:

\[
\frac{\partial}{\partial t} (hc) + \frac{\partial}{\partial x} (uhc) + \frac{\partial}{\partial y} (vhc) = \frac{\partial}{\partial s} \left( h \, D_s \frac{\partial c}{\partial s} \right) + \frac{\partial}{\partial n} \left( h \, D_n \frac{\partial c}{\partial n} \right) -
\]

\[ -w_s c \left( 1 - \frac{\tau_b}{\tau_d} \right) H(1 - \frac{\tau_b}{\tau_d}). \]

where \( H \) is the Heaviside operator, which is equal to one when the argument is greater or
equal than zero, and null otherwise.

C – The model was applied to sedimentation studies of the Peel Harvey estuary, Australia.

3.8 – "Sediment Contaminant Transport Model".¹¹,⁷¹

The model was elaborated to assess the interaction sediments/contaminants, and the fact that contaminants use sediments transport as a major migration process.

A – FETRA is a two-dimensional vertically averaged model, that uses a Galerkin finite element method, to solve the transport equation. It is subdivided in three modules: sediment transport, dissolved contaminant transport and particulate contaminant transport.

The sediments are fractioned twice: first according to rheologic characteristics, and afterwards as a function of size. Three different categories are initially considered: cohesive and non-cohesive sediments, and organic matter. It is assumed that the mechanisms governing the erosion and deposition of organic matter are similar to those of cohesive sediments, but the coefficients should reflect characteristics of density, size, cohesiveness and consolidation of the sediments involved.

Sediment erosion and deposition rates are calculated using different schemes for cohesive and non-cohesive sediments.

– non-cohesive sediments:
\[ S_r = \frac{\psi \left( \tau_b - \tau_c \right)}{1} - qc \]

\[ S_d = -S_r, \]

where \( \psi \) is Du Boy's coefficient for sediment size, \( c \) is sand concentration, \( q \) is the flow rate, \( l \) the characteristic length of calculus, and \( S_r \) and \( S_d \) respectively erosion and deposition rates;

- cohesive sediments:

\[ S_r = M \left( \frac{\tau_b}{\tau_{c,e}} - 1 \right) \]

\[ S_d = w_s c \left( 1 - \frac{\tau_b}{\tau_{c,d}} \right) \]

where \( \tau_{c,e} \) and \( \tau_{c,d} \) are critical shear stresses for erosion and deposition, \( M \) is an erodibility coefficient, \( c \) is the cohesive sediments concentration and \( w_s \) the fall velocity, which is calculated as:

\[ w_s = K c^{-4/3}, \text{ for each sediment type.} \]

Armoring, consolidation and the evolution of bottom morphology are simulated representing the riverbed by a layered structure of standard thicknesses, with the exception of the top layer. Each layer contains contaminants and sediments of different types expressed in percentages. While the model is running, erosion and deposition occur.
continuously changing the thickness of the top layers, until the carrying capacity of the flow is saturated or the available amount of sediment in the bed is completely eroded, whichever occurs first. On the other hand, the model is established in such a way that for finer sized sediments, the number of eroded layers can not be larger than the number of layers eroded for sediments of upper size range, what is intended to model the protective function of armoring.

The advection–dispersion equation for sedimentary particles has the form:

\[
\frac{\partial c_j}{\partial t} + \left( u - \frac{E_x}{h} \frac{\partial h}{\partial x} \right) \frac{\partial c_j}{\partial x} + \left( v - \frac{E_y}{h} \frac{\partial h}{\partial y} \right) \frac{\partial c_j}{\partial y} = \frac{\partial}{\partial x} \left( E_x \frac{\partial c_j}{\partial x} \right) + \\
+ \frac{\partial}{\partial y} \left( E_y \frac{\partial c_j}{\partial x} \right) + \frac{S_{r,j}}{h} - \frac{S_{d,j}}{h} + Q_j.
\]

The subscript \( j \) refers to the sediment fraction and \( Q_j \) is a source or sink.

**B –** Contaminants are considered in two phases: dissolved, and particulate. The dynamic equilibrium between the two phases is expressed by the establishment of a partitioning coefficient, as well as, the establishment of a rate of adsorption/desorption for sediments of different characteristics, either in solution or deposited.

For Dissolved Contaminant Transport:

\[
\frac{\partial G_i}{\partial t} + \left( u - \frac{E_x}{h} \frac{\partial h}{\partial x} \right) \frac{\partial G_i}{\partial x} + \left( v - \frac{E_y}{h} \frac{\partial h}{\partial y} \right) \frac{\partial G_i}{\partial y} = \frac{\partial}{\partial x} \left( E_x \frac{\partial G_i}{\partial x} \right) + \\
+ \frac{\partial}{\partial y} \left( E_y \frac{\partial G_i}{\partial y} \right) - \left[ \lambda + \Sigma_j K_{ij} K_{dj} c_j + \Sigma_j K_{Bj} \gamma_j (1-p) \frac{D_j}{h} K_{dj} \right] G_i + \]

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\[ + \sum_j K_j G_{ij} + \sum_j K_{Bj} \gamma_j (1-p) \frac{D_j}{h} G_{iBj} + Q_{ij}, \]

with:
- \( G_i \) — dissolved concentration the contaminant i,
- \( \lambda \) — chemical and biochemical first order degradation rate,
- \( K_j \) — rate of adsorption/desorption to sediment type j in motion,
- \( K_{Bj} \) — \( K_j \) for the riverbed sediment,
- \( \gamma_j \) — density of the sediment,
- \( p \) — porosity of the riverbed,
- \( D_j \) — diameter of sediment j in the riverbed,
- \( K_{dj} \) — partition coefficient associated to sediment j,
- \( G_{ij} \) — particulate contaminant associated to sediment j,
- \( G_{iBj} \) — \( G_{ij} \) in the riverbed sediment.

The transport equation presented above accounts for convection—dispersion, adsorption/desorption, chemical and biological degradation. Water—quality parameters as pH, temperature, salinity and sediment characteristics should be included in the evaluation of the partitioning coefficients.

For Particulate Contaminant Transport:

\[
\frac{\partial G_{ij}}{\partial t} + \left( u - \frac{Ex}{h} \right) \frac{\partial G_{ij}}{\partial x} + \left( v - \frac{Ey}{h} \right) \frac{\partial G_{ij}}{\partial y} = \frac{\partial}{\partial x} \left( Ex \frac{\partial G_{ij}}{\partial x} \right) + \\
+ \frac{\partial}{\partial y} \left( Ey \frac{\partial G_{ij}}{\partial y} \right) - \left[ \lambda + K_j \right] G_{ij} - \frac{S_{dj}}{h} G_{ij} + K_{dj} K_j c_j G_i + \frac{S_{ij}}{h} G_{iBj} + Q_{ij},
\]

C — The model was applied to the transport of Kapone, an industrial contaminant, in the James River estuary.
CHAPTER 4
4. – ELASED: A MODEL FOR SEDIMENT TRANSPORT IN ESTUARIES

4.1 – Formulation

ELASED is a 2-D depth averaged model that solves the transport equation in the water-column, and includes a simplified model of bottom evolution to simulate consolidation and morphologic changes.

4.2.1 – Governing Equations

Part A – The water column.

The system of equations, presented below in final form, have already been partially derived in section 2.3.1, and consequently further discussion is excused. Three types of sediments are identified:

\[ c_1 \] - concentration of very fine sediments (silts and clays),
\[ c_2 \] - concentration of organic sediments,
\[ c_3 \] - concentration of fine sands.

The transport equation has the form:

\[
\frac{Dc_k}{Dt} = \frac{1}{h} \left( \frac{\partial}{\partial x_i} \epsilon_{ij} \frac{\partial c_k}{\partial x_j} \right) + \phi_{e,k} - \phi_{d,k} + \phi_{p,k} + Q \tag{4.1}
\]

This is the equation already presented in section 2.3.1, averaged in respect to depth. The turbulent–diffusion coefficients are now substituted by the correspondent dispersion
coefficients, in order to account for the negligence of the vertical component of the flow.

The term $\phi_{p,k}$ represents the internal productivity of organic sediments in the estuary:

$$\phi_{p,k} = 0, \quad \text{for } k=1,3$$  \hspace{1cm} (4.2)  

and,

$$\phi_{p,k} = P_c^2, \quad \text{for } k=2$$  \hspace{1cm} (4.3).

The term $\phi_{d,k}$ accounts for deposition:

$$\phi_{d,k} = Bc_k^2 + \alpha_{s,k} (c_k - c_{ss,k}), \quad \text{for } k=1,2$$  \hspace{1cm} (4.4)  

and,

$$\phi_{d,k} = \alpha_c (c - c_T), \quad \text{for } k=3$$  \hspace{1cm} (4.5).

Finally, the term $\phi_{e,k}$ represents the contribution of erosion:

$$\phi_{e,k} = \beta (r_b - r_{e,cr})^n, \quad \text{for } k=1,2,3$$  \hspace{1cm} (4.6).

The external sources and sinks are included in the factor $Q$.

**Part B** – Bottom evolution: morphology and consolidation – Figure 25.

For the partially consolidated strata, the bottom resistance stress, at a specific instant, can be obtained through the use of the following exponential law:

$$\tau(z_x,t) = A e^{k_1 z_x}$$  \hspace{1cm} (4.7)

$$z_x = |Zt - z|$$
On the other hand, at a specific depth \( z \), the expression above becomes:

\[
\tau(z_x,t) = D e^{k_2t}
\]

Finally, for specific depth and time, and assuming that the time scales, and net balance between erosion and deposition, have equivalent effects in the process of consolidation:

\[
A e^{k_1z_x} = D e^{k_2t}
\]

and,

\[
t = \frac{1}{k_2} \ln \left( \frac{A}{D} + \frac{k_1}{k_2} z_x \right)
\]

Substituting in equation (8),

\[
\tau(z_x,t) = D e^{(\ln \frac{A}{D} + k_1 z_x)}
\]

The parameters \( A, B, \) and \( K_1 \) must be determined for each case study, by means of field data analysis.

The fluffy zone is characterized by two distinct layers: the top layer, of thickness \( h_1 \), variable for different zones of the estuary, but always present, and a second layer of maximum thickness \( H-h_1 \). Recently deposited sediments are stored in the fluffy zone, but when the maximum thickness \( H \) is reached the correspondent lower layer of the fluffy zone initiates its process of consolidation. Although the dependence of \( \tau(z_x,t) \) with time
and depth, of partially consolidated sediments, has been extensively studied in the past, the behavior of the fluffy zone is not yet fully understood. Hayter advises the establishment of a special $\tau(z_x,t)$ profile for this zone, using field samples. Since it is not perceived how undisturbed samples of typical fluffy zones in the estuary can be obtained for later experimentation, and, on the other hand, the thickness of the fluffy zone will generally be very small, a few centimeters the most, it is assumed that the value of $\tau(z_x,t)$ is constant, and equal to the minimum value prescribed by equation (11), $\tau_m$.

In the maximum turbidity zone of the estuary, the fluffy zone is very much enlarged, and, in those circumstances, the resistance of the bottom should be evaluated as follows:

$$\tau(z_x,t) = \theta \tau_m \quad (4.12).$$

The coefficient $\theta$ must be obtained by model calibration, or field data analysis.

It is important to note that the magnitudes of the resisting bottom stresses are presumed to reflect the presence of fine sand in the sedimentary layers, and in suspension. Because of the predominance of very fine sediments over sands, or eventually other coarse particles, the effects of sorting and armoring, whose importance is recognized in riverine systems, may be neglected in estuaries. This argument, and the absence of a solid process of quantification, support the fact that, at this stage, armoring effects will not be introduced in the model. Due to the unlikelihood of the establishment of a reasonable process of quantification, bioturbation is also not considered.

The change of bottom thickness, correspondent to a time step in the numerical model, is computed by the application of the mass balance principle to the interface bottom/water column. If $M$ is the net mass value of erosion and deposition, the variation of the depth of the bottom top layer with time, can be equated as:
\[
\frac{dz}{dt} = \frac{\partial z}{\partial t} + k_x \frac{\partial z}{\partial x} + k_y \frac{\partial z}{\partial y} = \frac{1}{\rho_s} \frac{\partial M}{\partial t}
\] (4.13).

Assuming that the distribution of deposited or eroded mass is spatially homogeneous, then:

\[
\frac{dz}{dt} = \frac{\partial z}{\partial t}
\] (4.14),

\[
\Delta z = \frac{M}{\rho_s}
\] (4.15),

and ultimately,

\[
Z_{t_{i+1}} = Z_{t_i} + \Delta z
\] (4.16),

where \( \rho_s \) is the sediments density, considered in an averaged sense, and \( i \) is an instant of reference. For erosion situations, the value of \( Z_t \), used in the calculus of the actual stresses of bottom resistance, is the value of \( Z_t \) in the beginning of the erosive process: \( Z_{t_0} \). This way, the effect of strata of higher level of consolidation on the decrease of the flow erosive efficiency in time, can be simulated. When deposition is happening, the value of \( Z_t \) used is the actual value of the depth of the top of the bed–layer. Erosion is limited by the depth at which the bed–rock is located.

### 4.1.2 – Numerical solution

ELA\textsuperscript{89}, a 2-D depth averaged finite element model, that solves the transport equation by means of an Eulerian–Lagrangian method, is the numerical basis used to generate the transport model for sediments, conveniently adapted to the formulation proposed here. The flow field is computed by a second finite element method that solves the 2D Navier–Stokes equations for shallow waters, considering tidal forcing –TEA.
Associated to the applicability of ELASED is the permanent interaction between flow field and bottom morphology. The evolution of the topography of the bottom in time domain definitely influences the characteristics of the flow field, and so it is extremely important the elaboration of an adaptive structure that may jump from TEA to ELASED, and backwards, in order to simulate always the most circulation.

The numerical strategy adopted by ELA consists in the splitting of the transport equation into two independent equations: the advection equation, and the diffusion equation. The advection equation is solved by means of a backwards method of characteristics: Lagrangian approach. The diffusion equation is solved using a classic Galerkin formulation: Eulerian approach. The diffusion equation adapted for sediment transport is referred as diffusion–transformation.

The development of equation (4.1) gives:

\[
\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = \frac{\partial \xi_i}{\partial x_i} \frac{\partial c_i}{\partial x_i} + \frac{\xi_i}{h} \frac{\partial h}{\partial x_i} + \frac{\xi_i}{h} \frac{\partial c}{\partial x_i} + \xi_i \frac{\partial^2 c}{\partial x_i^2} + \frac{\phi_e - \phi_d + \phi_p}{Q}.
\]

i, j = 1, 2

This equation can be separated into the advection equation,

\[
\frac{\partial c}{\partial t} + (u_i - \frac{\partial \xi_i}{\partial x_i} - \frac{\xi_i}{h} \frac{\partial h}{\partial x_i}) \frac{\partial c}{\partial x_i} = 0,
\]

and the diffusion–transformation equation,

\[
\frac{\partial c}{\partial t} = \xi_i \frac{\partial^2 c}{\partial x_i^2} + \frac{\phi_e}{Q} - \phi_d + \phi_p + Q
\]

As it is discussed with more detail by Baptista\textsuperscript{85,90} the traditional Eulerian
perspective of transport, commonly utilized in finite-difference schemes or conventional finite-element methods, has extreme difficulty in dealing with large time steps, presenting very poor resolution of the energy transfers between the low and the high frequencies of the transport components. The most direct consequence of such a problem is the oscillatory behavior of numerical solutions of the transport equation, which increases drastically, and out of control, for increasing timesteps — Courant numbers greater than 1—. In estuaries, and coastal waters in general, the interest of numerical modeling relies on the possibility of simulation of natural phenomena in large periods of time. With the computational power presently available, the feasibility of that objective implies the use of large timesteps, and as it can be readily observed from figure 26, ELA, an Eulerian–Lagrangian model, shows best results for larger Courant numbers, although limited by an optimum value.

**Advection equation**

The advection equation (4.17) can be simplified, such that

\[ u_i \frac{\partial c_i}{\partial x_i} - \frac{\varepsilon_i}{h} \frac{\partial h}{\partial x_i} = u_i^* \]

and replacing in (4.17), the final equation is:

\[ \frac{\partial c}{\partial t} + u_i^* \frac{\partial c}{\partial x_i} = 0 \]  (4.19).

The application of the backwards method of characteristics consists in solving the differential equation of first order:

\[ \frac{dx_i}{dt} = u_i^* (x, y, t) \]  (4.20).

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At each timestep, the characteristic line associated to a specific node is tracked backwards, until its position at the previous timestep is determined. The concentration at this point is calculated using functions of spatial interpolation. The interpolated concentration is assumed to be transported conservatively during the time interval, by the advective flow.

**Diffusion–Transformation equation**

The diffusion–transformation equation (4.18) is solved approaching the time derivative domain using an Euler backwards scheme:

\[ \frac{\partial c}{\partial t} = \frac{c_j - c_{j-1}}{\Delta t} \]  \hspace{1cm} (4.21),

where \( c_j \) and \( c_{j-1} \) are respectively the concentrations at the present timestep \( j \), and at the previous timestep \( (j-1) \).

The right hand side is submitted to the Galerkin – FE technique for minimizing discretization errors (Appendix D), which will give, following a hybrid implicit scheme:

\[ \frac{c_j - c_{j-1}}{\Delta t} I = -Dc_j + S \]  \hspace{1cm} (4.22),

where:

- \( c \) are concentration vectors at all nodes,
- \( D \) is the diffusion matrix,
- \( S \) is the vector resultant from erosion and deposition,
- \( P \) is the productivity,
- \( I \) is the identity matrix.

The equation that is solved numerically can be described as:
\[(\Delta t \, D + I) \, c_j = I \, c_{j-1} + P \, \Delta t + S \, \Delta t \]  

(4.23).

In summary, the transport equation is solved as if mass was initially conservatively transported by the flow, and at the new position the effects of diffusion, erosion and deposition were linearly added.

The coagulation step is evaluated separately, after the diffusion step, and it is based in the analytical solution of the equation:

\[
\frac{\partial c}{\partial t} = -B \, c^2
\]  

(4.24),

already discussed in section 2.3.3. The final value of the concentration at time \( j \) is:

\[
c_j^* = \frac{c_j}{1 + c_j \, B \, \Delta t}
\]  

(4.25),

and \( c_j^* \) is the concentration obtained at the end of the diffusion step.

At each element, the variables that it will be necessary to determine for input of the model, are the following: consolidation \(-A, D, k_1, h_1, H\); productivity \(-P\); flocculation \(-B\); deposition \(-\alpha_{s,i}, \alpha_c, c_{ss,i}, \rho_i, w_i\); erosion \(-\beta_i\) and \( n_i \), and eventually some secondary parameters. In real-life applications these variables will be attributed to characteristic regions, according to the criteria defined in section 2.1, rather than to individual elements, and defined with base on field data analysis in situ, and in the laboratory. When field campaigns are prohibitive, either economically, or by any other reason, the values of the parameters necessary to implement the transport model must be inferred from the literature, according of the physical characteristics of the system. Detailed information on this matter can be found in Hayter\(^{82}\).
4.2 — Preliminary testing

The preliminary testing of ELASED was designed so that two objectives could be accomplished: the verification of the simulation of the mechanisms of sediments dynamics, and the evaluation of the model efficiency.

4.2.1 — Recirculating plume experiment \(^\text{82}\).

The first set of problems developed to test ELASED includes runs 1, 2, and 3, considering exclusively the occurrence of erosion. Run 4 tests deposition alone, whereas run 5 allows the competing interaction of erosion and deposition. The problems were elaborated based on the results reported by Hayter \(^\text{82}\) of a recirculating plume experiment. The objective of this verification was the qualitative analysis of the performance of ELASED in critical situations of sediments dynamics.

The recirculating plume experiment was simulated for a laboratory-scale channel of 0.6 x 18 m\(^2\), and 0.91 m of water-column height. Only cohesive sediments were considered. The parameters \(A\), \(D\), \(k_1\) used to simulate bottom consolidation are respectively 0.2, 11.27 and 1.2. The coefficients \(\beta\) and \(n\) to compute the erosion flux are 17000.0 and 3, whereas the coefficient \(\alpha\) used in the evaluation of the deposition flux was taken equal to 0.8 for the deposition experiment, and 0.08 for the erosion—deposition experiment. The value of the settling velocity was 0.004 m/s. In the deposition experiment the coefficient \(D\) was taken equal to 11.27E+08. The thickness of the fluffy zone was made equal to 4 cm, the initial bottom slope null and the bed—rock was located at 5 m depth. The effects of salinity were not accounted for. These parameters are summarized in Table 15.

The different sets of bottom stresses were obtained by means of the imposition of stepwise time—distributions for the velocity. The variation of the bottom stresses allowed
the verification of the model ability to respond to different forcings. The imposition of the boundary conditions was limited to the specification of constant concentrations at the upstream boundary conditions. The value specified was 0.4 in the erosion experiments and 0.8 in the experiments involving deposition. The concentration at steady state was also made equal to 0.4.

**Erosion test** — Figures 27, 28, 29 present the results obtained for the erosion test. For each figure, part (a) shows the variation of concentrations with time at a point in the middle of the channel, part (b) shows the relative bottom evolution for the same period, and part (c) presents the flow velocity variation in time. Figures 27 and 29 show very clearly the response of the bottom resistance for different flow velocity forcings: the increase in the concentrations for increased velocities is almost instantaneous, decreasing slowly in time for increased bottom resisting stresses. In Figure 28, correspondent to Run 2, the evolution of the bottom topography and water-column concentrations can be followed with more detail, for a constant velocity equal to 0.08 m/s. Indeed, the initial increase of the erodibility leading to an equilibrium situation, which is finally altered due to the increase of the bottom resisting ability, are shown with much evidence.

**Deposition test** — The deposition test described in Figure 30 agrees with the physics of deposition early described in this work, section 2.3.2. In particular it is possible to observe the progressive decrease in the concentrations of the water column, while the bottom depth is decreasing at similar rate.

**Erosion—Deposition test** — The simultaneous occurrence of erosion and deposition, run 5, is presented in Figure 31. In this case erosion predominates over deposition. However, the effects of deposition are clearly exposed during the first step of the velocity law, or in the steeper decrease of concentrations in the water-column due to the attenuation of bottom degradation in time. Nevertheless, we are aware that additional work has to be implemented to optimize the numerical scheme used, as well as the quantification and internal correlation of parameters.
4.3.4 — Illustrative case study

The test generated by Run 6 is also an erosion–deposition test, but it was intended
the verification of ELASED in an estuary–like system — Figure 32. The heigt of the
water–column was imposed equal to 10.0 m, and the permanent flow field is shown in
Figure 33. The coefficient β was changed to 1.7E–05, whereas the parameter α was taken
equal to 0.0008. The other parameters remained equal to the ones used in the previous set
of problems. This was a "blind" choice of parameters, and its effect can be inferred from
the results obtained for bottom evolution. These results are not presented because the
effective variation of depths was of the order of 1.0E–09, which may involve problems of
computational precision. However, a closer look at the depth evolution showed that
erosion is more rapid at points located in the corners of the expansion (3,5) than at the
remaining sampling points, what confirms our expectations for regions of lower velocity.
As it happened with run 5, erosion is again predominant in this situation, although it is
possible to verify the occurrence of deposition at all sampling points in the beginning of the
experiment. In the points located in the main channel (1,2) we can observe the existence of
an initial perturbated zone, which it is likely to be generated by an adaptive process of the
system to the upstream boundary, and the relatively high velocities of the flow field. The
effect of the downstream open boundary is also clear in the concentrations obtained for
point 4, which are consistently lower than the concentrations in the corner nodes. In
general, the results follow the behavior previously observed for run 5.

It is recognized that the sampling procedure was not fast, or long enough,
considering the scale of the problem: only five data sets were collected in time, and the
experiment runned for seven and a half hours. Further testing of ELASED must also
involve long–time simulations of real–like systems, so that the effective performance of the
model may be evaluated.
5. — CONCLUSIONS AND RECOMMENDATIONS

The concepts integrated in the formulation of ELASED are not new, but they reflect the results of the past fifty years of research on: hydraulic transport, erosion, deposition, flocculation, bottom consolidation, and internal production of organic sediments. Several models of similar purpose have been developed since the seventies, some of which reviewed in Chapter 3. The difference between ELASED and those models consists essentially on two distinct facets: the first inherent to the approach used to formulate the dynamics of sediments, and the second associated to the numerical technique used to solve the transport equation.

In the context of the numerical strategy, ELASED is the only model of sediment transport that uses an Eulerian–Lagrangian solution for the transport equation. Although models in the past have considered one or more of the mechanisms of the sediments dynamics referred above, ELASED is the most complete considering the following aspects: (a) the applicability to both cohesive and non-cohesive sediments; (b) the inclusion of the possible simultaneity of erosion and deposition; (c) the treatment of flocculation; (d) the introduction of internal sources of organic sediments; (e) the treatment of the mechanism of bottom–consolidation.

The reliability of ELASED, as any other model of sediment transport, depends strongly on the access to a consistent set of field data. Because so many empirical values are incorporated in the governing equations, problems originated by inconvenient handling of the boundary conditions and interface bottom/water–column, and ignorance of the intrinsic balance among the mechanisms that play role in the fate of sediments are
commonly found. Sediment transport is not suitable for the use of "most likely", or "averaged" parameters that work so well in other simulations of real-life phenomena, and consequently, a great effort must be directed to the calibration of the model. Calibration consists of the iterative verification of the model performance for adaptive values of the empirical parameters, using as guideline values collected in the literature either from laboratory or from field experiments. The development of our skills on the technology of field data surveys, as well as on the techniques of data analysis for modeling purposes are the next steps of this research to proceed with.

ELASED also requires further development: (a) optimization of the algorithm efficiency; (b) improvement of the formulation of the transfer mechanisms at the interface bottom/water-column. The interface bottom/water-column is one of the critical points in the formulation of the model. The response of this interface strongly depends on the flow patterns and on the parameters used to quantify erosion and deposition. This is particularly important because this region is a governing buffer of the chemistry of the natural system, allowing chemical transfers between buried contaminants and the water-column.

ELASED is integrated in a more complex structure aimed at the simulation of water-quality problems. However, further work is needed in tying sediments dynamics to the scavenging of pollutants from dissolved phase by adsorption onto sediments, in the spatial and time scales that govern the fate of contaminants in estuaries.

We expect that an effective contribution for the long-term prediction of water-quality standards in estuarine environments might become a reality.
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Fig.1. – Maps of some typical estuaries: Coos Bay – USA, Mondego – Portugal, Peel Harvey – Australia, and Tejo – Portugal.
Fig. 2. — Estuary: a characteristic transversal profile.

Fig. 3. — Bioactivity at the water–column — bottom surface interface and bed top layers.
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**Figure 14**: The graph illustrates the relationship between suspension concentration, denoted by $c_{ss}$ (g/m$^3$), and applied shear stress (N/m$^2$) with varying levels of $T_d$ (N/m$^2$), measured in hours (hrs). The data points are as follows:

- $0.050$ N/m$^2$ for $24$ hrs
- $0.015$ N/m$^2$ for $40$ hrs
- $0.0$ N/m$^2$ for $135$ hrs
<table>
<thead>
<tr>
<th>HYDRAULIC CRITERIA</th>
<th>INTERACTION</th>
<th>REMARKS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{crit,s} &lt; \tau_0 &lt; \tau_{crit,E}$</td>
<td>$\dot{M} = \text{const.}$</td>
<td>No sedimentation, no erosion, no interaction</td>
</tr>
</tbody>
</table>
| $c < c_T$ | | - coarse bed material  
  - consolidated bed material |
| $\tau_{crit,s} > \tau_0 > \tau_{crit,E}$ | $\dot{M} = \text{const.}$ | Sedimentation  
  - erosion, strong interaction with sediment exchange  
  - rivers (and estuaries) with erodible fine bottom sediment |
| $c = c_{eq} > c_T$ | | |
| $\tau_0 < \tau_{crit,E} \ll \tau_{crit,s}$ | $\frac{d\dot{M}}{dx} = 0$ | Sedimentation, net sediment flux from water to bed  
  - river section as "settling tank" (harbours, flood plains)  
  - disposal of dredged sediment |
| $c > c_T$ | | |
| $\tau_{crit,s} > \tau_0 > \tau_{crit,E}$ | $\frac{d\dot{M}}{dx} < 0$ | Sedimentation and erosion, interaction with sediment exchange  
  - mean flow discharge  
  - disposal of dredged sediment |
| $c \gg c_{eq}$ | | |
| $\tau_0 > \tau_{crit,E}$ | $\frac{d\dot{M}}{dx} > 0$ | Resuspension, net sediment flux into the water body  
  - tailwater bed erosion  
  - flood situation |
| $c_{eq} < c_0$ | | |

Fig. 15 — Hydromechanic interaction.
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Fig. 23 — Relationship between the trace element composition and the grain size distribution.
- □ — surface creep,
- ^ — saltation,
- * — suspension.

Fig. 24 — Paths of hydraulic transport of sediments.
MSL — mean sea level

\( z \) — depth referred to MSL

\( h_1 \) — minimum thickness of the fluffy zone

\( H \) — maximum thickness of the fluffy zone

\( Z_t \) — top of the fluffy zone depth

Fig. 25 — Schematization of bottom and water-column profiles used as reference in the algorithm of ELASED.
Fig. 26 — Accuracy of an Eulerian–Lagrangian technique as a function of the timestep.
Fig. 27a - ELASED: erosion test (run 1)

$\text{concentration (g/l)}$

$x = 9.0 \text{ m}, y = 0.3 \text{ m}$

$time (s)$
Fig. 27.b - ELASED: erosion test (run 1)

x=9.0 m, y=0.3 m

Bottom evolution (m)

Time (s)
Fig. 27.c – ELASED: erosion test (run 1)
Fig. 28a – ELASED: erosion test (run 2)

\[ x=9.0 \text{ m}, \ y=0.3 \text{ m} \]
Fig. 28.b - ELASED: erosion test (run 2)

$x = 9.0 \text{ m}, \ y = 0.3 \text{ m}$
Fig. 29.b – ELASED: erosion test (run 3)

$x=9.0\ m, y=0.3\ m$
Fig. 29.c – ELASED: erosion test (run 3)
Fig. 30.a - ELASED: deposition test (run 4)

x = 0.0 m, y = 0.3 m
Fig. 30.b - ELASED: deposition test (run 4)

$x = 9.0 \text{ m}, \ y = 0.3 \text{ m}$
Fig.30.c – ELASED: deposition test (run 4)
Fig. 31.a – ELASED: erosion–deposition test (run 5)

concentrations (g/l)

x=9.0 m, y=0.3 m

time (s)

0.0 100.0 200.0 300.0 400.0 500.0

0.0 10.0 20.0 30.0 40.0 50.0 60.0
Fig. 31.b - ELASED: erosion-deposition test (run 5)

\( x = 9.0 \text{ m}, \ y = 0.3 \text{ m} \)
Fig. 3.1.c - ELASED: erosion-deposition test (run 5)
Fig. 32 – Finite element grid (run 6)

520 Elements
1131 Nodes

0  1  2 km
Fig. 34.a – ELASED (run 6)
sampling points: 3

concentrations (gr/l)

0.00  0.15  0.30  0.45  0.60  0.75  0.90

0.0  5000.0  10000.0  15000.0  20000.0  25000.0  30000.0
time (s)
Fig. 34.c – ELASED (run 6)
sampling points: 4
Fig. a1 — Drag coefficient versus Reynolds number.

Fig. a2 — Relationship between drag coefficient of falling particles and Reynolds number.
Fig. b1 - Variation of the concentration of particles with time for constant ionic strengths (A, B, C)^4.
Fig. cl - Physical model for colloid stability.$^4$
<table>
<thead>
<tr>
<th>Size (μm)</th>
<th>Approximate distance (cm) traveled prior to reaching terminal velocity</th>
<th>Approximate terminal velocity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000</td>
<td>1.2 × 10^7</td>
<td>240</td>
</tr>
<tr>
<td>200</td>
<td>1.2 × 10^2</td>
<td>2.4</td>
</tr>
<tr>
<td>20</td>
<td>1.2 × 10^-6</td>
<td>2.4 × 10^-2</td>
</tr>
<tr>
<td>2</td>
<td>1.2 × 10^-10</td>
<td>2.4 × 10^-4</td>
</tr>
<tr>
<td>0.2</td>
<td>1.2 × 10^-14</td>
<td>2.4 × 10^-6</td>
</tr>
<tr>
<td>0.02</td>
<td>1.2 × 10^-14</td>
<td>2.4 × 10^-8</td>
</tr>
</tbody>
</table>

Table 1 — Fall rate of particles having a specific gravity of 2, in water (25°C).74

<table>
<thead>
<tr>
<th>Particle</th>
<th>Diameter</th>
<th>Sinking velocity</th>
<th>Wind speed or horizontal current velocity</th>
<th>Proportional difference in velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rain drops</td>
<td>0.05-5 mm</td>
<td>2.3-9.3 m s^-1</td>
<td>&lt; 10 m s^-1</td>
<td>&lt; 10</td>
</tr>
<tr>
<td>Snow flakes</td>
<td>-</td>
<td>0.5 m s^-1</td>
<td>&lt; 100 cm s^-1</td>
<td>10-10^4</td>
</tr>
<tr>
<td>Sedimenting particles</td>
<td>1 μm</td>
<td>10^-4 cm s^-1</td>
<td>&lt; 200 cm s^-1</td>
<td>10^-4</td>
</tr>
<tr>
<td>Sedimenting particles</td>
<td>10 μm</td>
<td>10^-1 cm s^-1</td>
<td>&lt; 20 cm s^-1</td>
<td>10^-4</td>
</tr>
<tr>
<td>Fecal pellets</td>
<td>-</td>
<td>0.04-1.0 cm s^-1</td>
<td>&lt; 30 cm s^-1</td>
<td>5 cm s^-1</td>
</tr>
</tbody>
</table>

Table 2 — Virtual sinking rates of particles in relation to horizontal movements.32

<table>
<thead>
<tr>
<th>Density, g/cm^3</th>
<th>Diameter, μm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>&lt; 38</td>
</tr>
<tr>
<td>1.0-1.16</td>
<td>~0</td>
</tr>
<tr>
<td>1.16-1.58</td>
<td>~0</td>
</tr>
<tr>
<td>&gt; 1.58</td>
<td>58.3</td>
</tr>
<tr>
<td>Total</td>
<td>58.3</td>
</tr>
</tbody>
</table>

Table 3 — Size-density matrix for surficial sediments in Puget Sound Estuary.7
Table 4 - Standard size classes of sediments.
<table>
<thead>
<tr>
<th>Location</th>
<th>Concentration (mg/liter)</th>
<th>Modal size (μm)</th>
<th>Organics (%)</th>
<th>Recognizable mineral grains (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Roanoke River near Plymouth, N.C.</td>
<td>29.1</td>
<td>8–16</td>
<td>33</td>
<td>3.0</td>
</tr>
<tr>
<td>Albermarle Sound (center)</td>
<td>5.1</td>
<td>4–8</td>
<td>24</td>
<td>1.9</td>
</tr>
<tr>
<td>Pamlico Sound south of Swanquarter</td>
<td>5.1</td>
<td>4–8</td>
<td>28</td>
<td>2.1</td>
</tr>
<tr>
<td>Charleston Harbor Offshore shelf SE of Charleston</td>
<td>5.5</td>
<td>4–8</td>
<td>31</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>0.4</td>
<td>8–16</td>
<td>58</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 5 — Suspended sediment data for Southeastern United States Coastal surface waters.
Additive interactions of repulsive interaction energy $V_r$ and attraction energy $V_a$:

$$V_r = V_a + V_a$$

Repulsive interaction per unit area between flat plates:

$$V_r = \frac{64n_k T}{\kappa} \left[ \frac{Z e^4 \Psi_x}{4 k T} \right]^2 e^{-\kappa d}$$

for spherical particles:

$$V_r = \frac{64n_k T (a + \delta)^2}{\kappa} \left[ \frac{Z e^4 \Psi_x}{4 k T} \right]^2 e^{-\kappa (a + \delta)}$$

Van der Waals attraction per unit area:

for flat plates:

$$V_a = -\frac{A_{1112}}{12\pi (d + 2\delta)^2}$$

for spherical particles:

$$V_a = -\frac{A_{1112}}{6} \left( \frac{2}{s^3 - 4} \ln \frac{s - 4}{s^2} \right)$$

where:

$$s = \frac{R}{a}$$

For very short particle distances $(3b)$ may be replaced by:

$$V_a = -\frac{A_{1112} a}{12H}$$

Electrolyte concentration required to just coagulate the colloids (25°C):

$$c_i = 8 \times 10^{-3} \frac{[\tanh(Z e^4 \Psi_x / 4 k T)]^2}{A_{1112} a^2}$$

Valence effect on stability for small $4d$:

$$\epsilon_s = \frac{3.125 \times 10^{-34}}{A_{1112}^2 \left( \frac{e^4 \Psi_x}{k T} \right)^2}$$

Stability Ratio:

$$W = 2n \int_{2a}^{\infty} \exp \left( \frac{V_r}{k T} \right) R^{-2} dR$$

Table 6 — VODL mathematical description.
<table>
<thead>
<tr>
<th>Phenomena</th>
<th>Aggregation by “inert” Electrolytes Coagulation</th>
<th>Aggregation by Adsorbable Species Adsorption Coagulation</th>
<th>Chemical Bridging Model Flocculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrostatic interaction</td>
<td>Predominant</td>
<td>Important</td>
<td>Subordinate</td>
</tr>
<tr>
<td>Chemical interactions and adsorption</td>
<td>Mostly absent</td>
<td>Important</td>
<td>Predominant</td>
</tr>
<tr>
<td>Zeta potential for optimum aggregation</td>
<td>Near zero</td>
<td>Not necessarily zero</td>
<td>Usually not zero</td>
</tr>
<tr>
<td>Addition of an excess of destabilizing species</td>
<td>No effect</td>
<td>Restabilization usually accompanied, by charge reversal</td>
<td>Restabilization due to complete surface coverage</td>
</tr>
<tr>
<td>Relationship between optimum dosage of destabilizing species and the concentration of colloid (or the concentration of colloidal surface)</td>
<td>Very virtually independent of colloid concentration Dense, great shear strength, but poor filtrability in cake filtration</td>
<td>Stoichiometry usual Flocs of widely varying shear strength and density</td>
<td>Stoichiometry, a linear relationship between flocculant dose and surface area</td>
</tr>
<tr>
<td>Physical properties of the aggregates produced</td>
<td>way more independent of colloid concentration Dense, great shear strength, but poor filtrability in cake filtration</td>
<td>Stoichiometry usual Flocs of widely varying shear strength and density</td>
<td>Flocs of three-dimensional structure; low shear strength but excellent filtrability in cake filtration</td>
</tr>
</tbody>
</table>

Table 7 — Modes of particle desestabilization and their characteristics.
<table>
<thead>
<tr>
<th>Material</th>
<th>Size ²</th>
<th>Settling velocity (cm/sec)</th>
<th>Diameter of quartz sphere with same settling velocity (μ)</th>
<th>Time for quartz sphere to settle 1 m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component particles of oyster and barnacle faeces (as spheres)</td>
<td>2 μ</td>
<td>0.00006³</td>
<td>2</td>
<td>18 days</td>
</tr>
<tr>
<td></td>
<td>3 μ</td>
<td>0.0006³</td>
<td>3</td>
<td>50 h</td>
</tr>
<tr>
<td>Faecal pellets collected on 44 μ sieve during study (mean size)</td>
<td>76 μ × 49 μ</td>
<td>0.013⁴</td>
<td>15</td>
<td>2 h</td>
</tr>
<tr>
<td>Barnacle pellets collected in laboratory aquaria</td>
<td>330 μ × 132 μ</td>
<td>0.35⁵</td>
<td>75</td>
<td>5 min</td>
</tr>
<tr>
<td></td>
<td>2.1 mm × 0.6 mm</td>
<td>0.95⁵</td>
<td>123</td>
<td>2 min</td>
</tr>
<tr>
<td></td>
<td>3.6 mm × 0.9 mm⁶</td>
<td>2.22⁵</td>
<td>189</td>
<td>45 sec</td>
</tr>
</tbody>
</table>

In quiescent water, t = 10°C, salinity = 15⁰/₀₀.

² Diameter or length × width.
³ From Stokes’ Law; assumed density of 2.6 g/cm³.
⁴ From Stokes’ Law; assumed density of 1.09 g/cm³.
⁵ Empirical data.
⁶ Mean size

Table 8 – Settling velocities of fecal pellets and their component particles.
<table>
<thead>
<tr>
<th>Structure</th>
<th>Remarks</th>
<th>Names</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>A. Two-Layer Clays</strong></td>
<td>Little isomorphous substitution</td>
<td>Kaolinite</td>
</tr>
<tr>
<td></td>
<td>Small cation exchange capacities</td>
<td>Dickite</td>
</tr>
<tr>
<td></td>
<td>(CEC)</td>
<td>Nacrite</td>
</tr>
<tr>
<td></td>
<td>Nonexpanding</td>
<td>Halloysite (Interlayer water)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>B. Three-Layer Clays</strong></td>
<td>Substitution of a small amount of Al for Si in T-sheet and of Mg, Fe, Cr, Zn, Li for Al or Mg in O-sheet</td>
<td>Montmorillonite</td>
</tr>
<tr>
<td></td>
<td>Large CEC ($M^{m+} = Na^+, K^+$, Li$^+$, Ca$^{2+}$, ...)</td>
<td>Nontronite</td>
</tr>
<tr>
<td></td>
<td>Swell in water or polar organic</td>
<td>Volkhonskyite</td>
</tr>
<tr>
<td></td>
<td>compounds</td>
<td>Hectorite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Saponite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sauconite</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Vermiculite</td>
</tr>
<tr>
<td><strong>C. Chlorites</strong></td>
<td>About $\frac{1}{4}$ of Si in T-sheet replaced by Al, similar O-sheet substitutions</td>
<td>Poorly crystallized</td>
</tr>
<tr>
<td></td>
<td>Small CEC</td>
<td>Micas (muscovite, biotite, phlogopite)</td>
</tr>
<tr>
<td></td>
<td>$M^{m+} = K^+$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>D. Fibrous Clays</strong></td>
<td>Three-layer alternating with brucite</td>
<td>Attapulgite</td>
</tr>
<tr>
<td></td>
<td>Brucite layer positively charged</td>
<td>Polygorskite</td>
</tr>
<tr>
<td></td>
<td>(some Al(III) replacing M(II)), partially balances negative charge on T-O-T (mica) layer</td>
<td>Sepiolite</td>
</tr>
<tr>
<td></td>
<td>Low CEC, nonswelling</td>
<td></td>
</tr>
</tbody>
</table>

Table 9 - Types and characteristics of clay.
HYDRODYNAMIC FACTORS (Erosive Force)

BED SHEAR STRESS
- Flow Characteristics
- Bed - Fluid Interface

BED AND FLUID PROPERTIES (Resistive Force)

SEDIMENT COMPOSITION
- Clay Mineral Type
- Ion Exchange Capacity
- Clay Percentage by Weight
- Organic Matter

PORE FLUID COMPOSITION
- Mono- and Divalent Cations Concentrations
- Relative Abundance of Mono- and Divalent Cations
- SAR (Na⁺, Ca²⁺, Mg²⁺)
- Conductivity
- Temperature
- pH

ERODING FLUID COMPOSITION
- Salinity (NaCl, CaCl₂, MgCl₂)
- Temperature
- pH
- Cementing Agents (Iron Oxide, etc)

BED STRUCTURE
- Stress History
  - Placed Bed
  - Deposited Bed

Table 10 — Principle factors controlling erosion of saturated cohesive sediment beds.
Summary of Aquatic Fate of Cadmium

<table>
<thead>
<tr>
<th>Environmental Process</th>
<th>Summary Statement</th>
<th>Confidence of Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photolysis</td>
<td>Not an important process.</td>
<td>High</td>
</tr>
<tr>
<td>Chemical Speciation</td>
<td>In most unpolluted waters the majority of the cadmium will exist as the hydrated divalent cation. In polluted waters, complexation with organic material will be most important. Affinity of ligands for cadmium follows the order of humic acids $&gt;\text{CO}_3^{2-}\text{OH}^-\text{Cl}^-\text{SO}_4^{2-}$.</td>
<td>Medium</td>
</tr>
<tr>
<td>Volatilization</td>
<td>Not an important process.</td>
<td>High</td>
</tr>
<tr>
<td>Sorption$^a$</td>
<td>Various sorption processes reduce the mobility of cadmium and result in the enrichment of suspended and bed sediments relative to the water column. In unpolluted waters, sorption onto clay minerals, and hydrous iron and manganese oxides are controlling factors. In polluted waters, sorption onto organic materials is the controlling factor.</td>
<td>High</td>
</tr>
<tr>
<td>Bioaccumulation</td>
<td>Biota strongly accumulate Cd with concentration factors ranging from $10^2$ to $10^4$ or more. Bioaccumulation is greater in soft than hard water.</td>
<td>High</td>
</tr>
<tr>
<td>Biotransformation</td>
<td>No biomethylation in evidence. Organic ligands of biological origin may affect solubility and adsorption.</td>
<td>Medium</td>
</tr>
</tbody>
</table>

Table 11 – Water chemistry of Cadmium$^{80}$
<table>
<thead>
<tr>
<th>Environmental Process</th>
<th>Summary Statement</th>
<th>Confidence of Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photolysis</td>
<td>Important in determining the form of lead entering the aquatic environment. Importance within natural waters is undeterminable.</td>
<td>Medium</td>
</tr>
<tr>
<td>Chemical Speciation</td>
<td>Determines which solid species controls solubility in unpolluted waters. Over most of the normal pH range, PbCO₃ and PbSO₄ control solubility in aerobic conditions. PbS and Pb control solubility in anaerobic conditions. In polluted waters, organic complexation is most important.</td>
<td>Medium</td>
</tr>
<tr>
<td>Volatilization</td>
<td>Probably not important in most aquatic environments.</td>
<td>Medium</td>
</tr>
<tr>
<td>Sorption</td>
<td>Adsorption to inorganic solids, organic materials, and hydrous iron and manganese oxides usually controls the mobility of lead.</td>
<td>High</td>
</tr>
<tr>
<td>Bioaccumulation</td>
<td>Lead is bioaccumulated by aquatic organisms. Bioconcentration factors are within the range of 10² - 10³.</td>
<td>High</td>
</tr>
<tr>
<td>Biotransformation</td>
<td>Biomethylation in sediments can re-mobilize lead.</td>
<td>Medium</td>
</tr>
</tbody>
</table>

Table 12 – Water chemistry of Lead[^80]
### Summary of Aquatic Fate of Mercury

<table>
<thead>
<tr>
<th>Environmental Process</th>
<th>Summary Statement</th>
<th>Confidence of Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photolysis</td>
<td>Important in the breakdown of airborne mercurials, might be important in some aquatic environments.</td>
<td>Medium</td>
</tr>
<tr>
<td>Chemical Speciation</td>
<td>Controls volatility of metallic mercury by conversion to complexed species. In reducing sediments HgS will precipitate and may constitute a major chemical sink.</td>
<td>High</td>
</tr>
<tr>
<td>Volatilization</td>
<td>Important to the movement of mercury compounds in and out of the aquatic environment.</td>
<td>High</td>
</tr>
<tr>
<td>Sorption</td>
<td>Sorption processes result in the strong partitioning of mercury into suspended and bed sediments. Sorption is strongest into organic materials.</td>
<td>High</td>
</tr>
<tr>
<td>Bioaccumulation</td>
<td>Bioaccumulation has been proven to occur via numerous mechanisms. Most are connected to methylated forms of mercury.</td>
<td>High</td>
</tr>
<tr>
<td>Biotransformation</td>
<td>Mercury can be metabolized by bacteria to methyl and dimethyl forms which are quite mobile in the environment.</td>
<td>High</td>
</tr>
</tbody>
</table>

Table 13 — Water chemistry of Mercury
<table>
<thead>
<tr>
<th>Model (author, date)</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-K.J. Farley (1987)</td>
<td>1D model; organic sediments and/or heavy metals from marine outfalls; coastal circulation averaged.</td>
</tr>
<tr>
<td>2-R. Luettich Jr. (1987)</td>
<td>Analytical solution; erosion and deposition considered simultaneously, as bottom boundary condition; strong experimental support; cohesive sediments.</td>
</tr>
<tr>
<td>3-L.C. van Rijn (1986)</td>
<td>2D laterally averaged model; detailed analysis of mechanisms involved; extensive use of empirical and semi-empirical relationships; strong experimental support.</td>
</tr>
<tr>
<td>4-Y. Peter Sheng (1984)</td>
<td>3D model; detailed analysis of bottom boundary layer; erosion, deposition, and flocculation processes approached separately; cohesive sediments.</td>
</tr>
<tr>
<td>5-E.J. Hayter (1983)</td>
<td>2D depth averaged model; very detailed model of bottom consolidation and evolution; strong experimental support; cohesive sediments.</td>
</tr>
<tr>
<td>6-P. Cole, G. Miles (1983)</td>
<td>2D depth averaged model; erosion not considered; qualitative tool; Cohesive sediments.</td>
</tr>
<tr>
<td>7-Y. Onishi (1981)</td>
<td>2D depth averaged model; bottom armoring and evolution considered; the model is also formulated for contaminants.</td>
</tr>
</tbody>
</table>

Table 14 – Review of selected sediment transport models.
<table>
<thead>
<tr>
<th>Bottom Parameters (SI units)</th>
<th>Erosion</th>
<th>Deposition</th>
<th>Erosion Deposition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.20</td>
<td>2.0E+08</td>
<td>0.20</td>
</tr>
<tr>
<td>$k_1$</td>
<td>1.2</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>D</td>
<td>11.27</td>
<td>11.27E+08</td>
<td>11.27</td>
</tr>
<tr>
<td>$h_1$</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>H</td>
<td>0.04</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.0</td>
<td>0.8</td>
<td>0.08,0.8</td>
</tr>
<tr>
<td>$c_{ss}$</td>
<td>0.</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1.7E+04</td>
<td>1.7E+04</td>
<td>1.7E+04</td>
</tr>
<tr>
<td>n</td>
<td>3</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>w</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>CD</td>
<td>5.0</td>
<td>5.0</td>
<td>5.0</td>
</tr>
<tr>
<td>$\rho$</td>
<td>2.7</td>
<td>2.7</td>
<td>2.7</td>
</tr>
<tr>
<td>$\theta$</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Zt</td>
<td>0.91</td>
<td>0.91</td>
<td>0.91</td>
</tr>
<tr>
<td>Zb</td>
<td>5.0</td>
<td>5.0</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Table 15 - Sediments Parameters used to test ELASED. (Zb - "bed-rock" location)
POWER LAW RELATIONSHIP FOR COAGULATION/SETTLING KINETICS
FROM FARLEY AND MOREL (1986)

\[
\frac{dC}{dt} = -b_{ds} C^{2.3} - b_{sh} C^{1.9} - b_{b} C^{1.3}
\]

\[
b_{ds} = 3.12 (S/b)^{-0.32} \rho_e \alpha_b^0.1 \tau_d^{1.15} \tau_{ds}
\]

\[
b_{sh} = 10.0 (S/b)^{0.15} \rho_e \alpha_b^0.1 \tau_d^{0.75} \tau_{sh}
\]

\[
b_{b} = 1.33 (S/b)^{0.6} \rho_e \alpha_b^0.4 \tau_{bs}
\]

where \(C\) is the mass concentration of particles, expressed in terms of wet weight; \(b_{ds}, b_{sh}, b_{b}\) are the sedimentation rate coefficients corresponding to coagulation by differential settling, shear, and brownian motion; \(\alpha_{ds}, \alpha_{sh}, \alpha_{b}\) are the efficiencies of particle collision; \(\tau_{ds}, \tau_{sh}, \tau_{bs}\) are dimensional parameters for the collision frequency functions.

\[
K_b = \frac{2kT}{3\mu} \text{[cm}^3\text{sec}^{-1}]; \quad K_{sh} = \frac{G}{\pi} \text{[sec}^{-1}]; \quad K_{ds} = \left(\frac{6}{\pi}\right)^{1/3} \frac{g}{12\nu} \left(\frac{\rho_e - \rho_f}{\rho_f}\right) \text{[cm}^{-1}\text{sec}^{-1}}
\]

\(S/b\) is the dimensional parameter for Stokes settling in a vertically homogeneous water column of depth, \(b\)

\[
S/b = \left[ \frac{1}{6\pi^2} \frac{g}{\mu} \frac{\rho_e - \rho_f}{\rho_f} \right]^{1/3} \text{[cm}^2\text{sec}^{-1}]
\]

\(k\) is the Boltzmann constant; \(T\) is the absolute temperature; \(\mu\) and \(\nu\) are the dynamic and kinematic viscosities of the fluid; \(G\) is the shearing rate of the fluid; \(g\) is the gravitational acceleration; \(\rho_e\) is the floc density

\[
\rho_e = (1-e) \rho_p + e \rho_f
\]

\(e\) is the floc porosity; \(\rho_p\) and \(\rho_f\) are the particle and fluid density.

Table b1 – Power law relationship for coagulation/settling kinetics.
APPELLIX A

Fall velocity and Stokes' Law.

A particle is kept in suspension as long as the equilibrium between the force of
gravity acting on the particle and the lift and the drag forces of the liquid persists.

Stokes Law sustains that the drag force due to the viscous resistance to the fall of a
particle in a fluid is equal to the buoyant weight of the particle falling at settling velocity.

Considering spherical particles,

\[ F_d = C_d \ A \ \rho_t w^2 / 2 \]

\[ F = g \ d^3 (\rho_s - \rho_t) / 6 \]

where,

- \( F_d \) - drag force
- \( F \) - buoyant weight
- \( C_d \) - drag coefficient
- \( A \) - projected area of the particle in the direction of fall (\( \pi d^2 / 4 \))
- \( w \) - terminal fall velocity of the particle
- \( \rho_s \) - sediment particle density
- \( \rho_t \) - fluid density
- \( d \) - diameter of the particle

\[ C_d = \phi \left( Re, S_p, \frac{f d}{w}, \frac{\rho_s}{\rho_f} \right) \]
with \( R_e \) as the Reynolds number, \( S_p \) as the shape factor of the particle and \( f \) is the frequency of oscillation and tumbling.

Figure(a1) presents a graphical representation that permits to obtain \( C_d \) for different \( R_e \) and some discrete values of the shape factor: 0.3, 0.7 and 0.9.

The equilibrium equation is stated by the following expression

\[
F = F_d
\]

Substituting \( F \) and \( F_d \) by their respective expressions, and considering that for spheric particles and low \( R_e \) numbers

\[
C_d = \frac{24}{R_e},
\]

then, if \( \mu \) is water viscosity

\[
w = g (\rho_f - \rho_g) d^2 / (18 \mu)
\]

The **Stokes Law** for settling velocity is applicable only under the following conditions:

- the particles size is large enough, so that Brownian motions can be neglected, and small enough to allow laminar settling (0.5 \( \mu m < d < 62.5 \mu m \));
- the particles are smooth, rigid and pratically spherical.

For non—spherical particles, considering \( d_s \) the diameter of a sphere having the same volume as the irregular shaped particle, and \( \phi \) is a coefficient of form resistance, the settling velocity can be calculated using the expression
\[ w = g \left( \rho_s - \rho_f \right) d_s^2 / (18 \mu \phi). \]

Smith (1975) studied the relationship between settling velocity, diameter and shape. Figure (a2) summarizes his results.

Particles smaller than 62.5 μm are usually classified as silts and clay. The equations established above show that the fall velocity of these particles is proportional to the square diameter. It can also be shown that for coarser particles, \( d > 62.5 \mu m \), the settling velocity is proportional to the square root of the diameter. Different proportionalities have been found in experimental analysis, but the main point is that exists an intrinsic relationship among fluid turbulence, settling velocity and particle size.
APPENDIX B

A semi-empirical law for coagulation—Farley and Morel\textsuperscript{5}.

Trying to find an analytical equation for coagulation, some theoretical work based in similarity analysis and laboratorial experiments were implemented. The correlations between the results of both approaches were analysed using numerical simulations.

The theoretical background was provided by previous results obtained by Friedlander in the area of the atmospheric sciences, but also valid for water suspensions in the range of colloidal particles size. Assuming a vertically homogeneous quiescent water column of depth $h$, the variation of the suspended particles volume distribution with time corresponds to

$$\frac{dn(v)}{dt} = \frac{1}{2} \int_0^v \beta(v-v') n(v') n(v-v) d\bar{v} - n(v) \int_0^v \beta(v-v') n(v) d\bar{v} - \frac{w(v)}{h} n(v),$$

where: $v$ — particles volume

$\bar{v}$ — mean particles volume

$n(v)$ — particles volume distribution

$\beta(v-v')$ — collision frequency function

$w(v)$ — settling velocity given by Stokes law.

The same differential equation expressed in terms of concentrations, assuming the floc density $\rho_e$ constant, is expressed as follows:

$$\frac{dc}{dt} = -\rho_e \int_0^v \frac{w(v)}{h} n(v) dv.$$
The assumptions that support the validity of these equations are such that:

- the shape of the particles after and before each aggregation is spherical;
- particles approach one another on rectilinear paths, without interaction;
- no force acts on the particles until they come into physical contact, after which adherence occurs.

To provide a definition of the distribution function for practical applications, Farley introduced a new expression for the distribution

\[ n(v, t) = b(t) \psi\left(\frac{v}{a(t)}\right), \]

with \( a(t) \) — faster depletion of larger sized particles,

\( b(t) \) — uniform reduction of particles over the entire distribution,

\( \psi\left(\frac{v}{a(t)}\right) \) — self preserving function.

In order to define a version of the second equation more suitable for practical purposes, additional assumptions were made before further mathematical work:

- since Brownian motion is expected to be important in the range of the very small particles, they are considered to have zero settling velocity,
- the volume flux of particles through the size distribution (coagulation rate) takes place continuously and is constant at any instant,
- for particle sizes greater than the one determined as critical, the particles are assumed to fall infinitely fast,
- vertical mixing is fast relative to sedimentation.

The solutions found are characteristic solutions, expected to be asymptotically approached in time and susceptible of being expressed in power terms of the concentration, with exponents dependent on the mode of coagulation. Since different mechanisms of coagulation are relevant for distinct and limited size ranges, it is acceptable the assumption
that they are additive and so

\[
\frac{Dc}{Dt} = -B_c c^{1.4} - B_{sh} c^2 - B_{ds} c^3
\]  \hspace{1cm} (1).

Laboratorial experiments verified the general expression (4), but numerical simulations using the results as data base lead to the computation of slightly different exponents:

\[
\frac{Dc}{Dt} = -B_c c^{1.3} - B_{sh} c^{1.9} - B_{ds} c^{2.3}
\]  \hspace{1cm} (2)

This is the final semi-empirical formula associated to the coagulation process of a hydrosol, corresponding to initial conditions of a fully developed characteristic size distribution in suspension. Table 1 explains the computation of the B coefficients. The most outstanding difference between equations (1) and (2) is the exponent related to the differential settling mode. The reason why this happens is associated to the fact that there is no physical evidence of a determined critical particle size for settling to occur, as well as the frequency of collision is not constant. Other conclusions of fundamental interest are related to the variability in time of the shape of size distribution and rate of coagulation. It was also concluded that not only the particle size is indicator of the predominance of the coagulation mode but also does the concentration. At low concentration the process is controlled by Brownian motion and at large concentrations differential is determinant.

For practical applications in real field situations, where turbulence is intense and concentrations are rather high, the term dependent on Brownian motion may be neglected. This analysis leads to the final simplified analytical expression, previously used by Hunt

\[
\frac{Dc}{Dt} = -Bc^2
\]
The coagulation factor B is a function of the settling velocity, floc density, collision efficiencies and hydrodynametic retardation. The effect of salinity intrusion in estuaries, and its reflex on the activities of the electrolytes in solution, and on the adsorption of polymers onto particles surface, generating flocs of diversified density, was not considered in the presented work. However, there is strong evidence (Edzwald, fig.b1) to make us believe that as soon as equilibrium positions are reached, and for a constant ionic strength, the rates of coagulation are constant in time. There will always be a random factor dependent on the speciation of the natural water in study, but that will be evaluated in function of adequate field measurements of the variables of interest.

Lavelle (1984) presents a consistent method to process field data based in Fourier analysis and in the formulation of a response function for the system in study as it is currently done with digital signal processing theory.
APPENDIX C

The electric double-layer theory—Verwey, Overbeek, Derjaguin and Landau.

**VODL** is a theoretical model that permits to evaluate quantitatively the efficiency of kinetic collisions. It is a reductive approach in the sense that neglects all factors besides Van der Waals attraction forces and electrostatic double layer repulsion.

The majority of particles suspended in water are electrically charged. As a consequence, a cloud of ions and particles with charge of opposite sign, will develop around each particle, generating an electrical field. When two particles equally charged are forced to get near or even in contact with each other, repulsive electrostatic repulsive forces are produced. The van der Waals forces are electrochemical valence forces, due to the mutual interference of electrons during their motion in the area of influence of the respective atoms. These forces are always attractive and independent of the solution chemistry. Van der Waals forces reach maximum magnitudes for the short–length scales, and decay rapidly with distance. The model consists in the calculus of the total Gibb's free energy as an additive result of attractive and repulsive actions. When the total energy is positive the collision is not effective. If negative, the collision is efficient with a degree that depends on the magnitude of the net energy, (fig.c1).

There are two different ways for particles to interact: at constant charge and at constant potential. When the surface potential is determined by adsorption of ions, according to chemical affinity, the proximity between two particles will provoke desorption of the potential–determining ion, keeping the surface potential constant while surface charge is reduced, and the two electric double–layers equilibrate. If the surface charge of the particles remains constant, consequently the surface potential has to increase, and steady equilibrium is never accomplished. "In general, the type of electric double–layer interaction will depend on the kinetics of ions and particles transport."
(O'Melia, 1987). Constant-charge interactions are more repulsive than constant-potential interactions.

Whenever the electrolyte activity increases, as a result of saline intrusion for example, the reciprocal thickness of the double layer diminishes and so the amplitude of the region of predominance of the electrostatic repulsive forces, together with the magnitude of the interaction energy, (fig.c1). The impact of salinity depends on the respective change of ionic strength, to which corresponds a certain efficiency. Maximum efficiency would be achieved when the net energy in solution is such that all particles are reduced to only one. This situation never happens in real natural systems because such high levels of energy are never reached, because the largest particles could settle first and finally because there are plenty of competing chemical processes happening simultaneously.
APPENDIX D

Finite-element formulation of the Diffusion equation.

The primary step of a finite element method is the establishment of a grid, corresponding to spatial discretization. The grid is constituted by elements of area, and in each element it is chosen the position of characteristic points, the nodes, that will generate the shape functions $N$, used for the spatial interpolation. The shape functions are defined for each element, and they will be as many as the number of nodes previously established, although this value might be increased for higher interpolation schemes. The interpolation scheme is established such that:

$$c(x,y) = \Sigma_j \Sigma_i N_i(x,y) c_j \quad (1),$$

where $N_i$ is the shape function attributed to node $i$, and $c_j$ is the value of the variable $c(x,y)$ at node $j$. The shape functions are defined as:

$$N_i(x_i, y_i) = 1.0, \text{ and } N_i(x_j, y_j) = 0 \text{ with } j \neq i.$$  

The diffusion equation has the form:

$$\frac{\partial c}{\partial t} = \epsilon_i \frac{\partial^2 c}{\partial x_i^2} + \phi_e - \phi_d + \phi_p + Q.$$

Since the time derivative is solved by means of an Euler backwards scheme, the weighted averaged residual error (WARE) due to discretization will be calculated for the
right-hand side of the diffusion equation. The weight functions in each element coincide with the shape functions of the same element — Galerkin formulation. The expression for the weighted averaged residual error over the domain $\Omega$ can be expressed as:

$$\text{WARE} = \int \int_{\Omega} N \left( \epsilon_i \frac{\partial^2 c}{\partial t^2} + \phi_e - \phi_d + \phi_p + Q \right) d\Omega.$$ 

Considering the discretized domain:

$$\text{WARE} = \sum_e \int \int_{\Omega_e} N \left( \epsilon_i \frac{\partial^2 c}{\partial t^2} \right) d\Omega_e + \sum_e \int \int_{\Omega_e} N (\phi_e - \phi_d + \phi_p + Q) d\Omega_e.$$ 

Integrating by parts the first term, of the right-hand side of the equation above:

$$\sum_e \int \int_{\Omega_e} N \left( \epsilon_i \frac{\partial^2 c}{\partial t^2} \right) d\Omega_e = -\sum_e \int \int_{\Omega_e} \epsilon_i \frac{\partial N}{\partial x_i} \frac{\partial c}{\partial t} d\Omega_e +$$

$$+ \sum_e \int \int_{\Gamma_e} N \epsilon_i \frac{\partial c}{\partial x_i} n_i ds,$$

where $\Gamma_e$ is the boundary of the element, and $s$ is a length coordinate. The boundary conditions imposed to the transport equation are such that, at the solid boundaries the fluxes specified are null, whereas concentration values are imposed at the liquid boundaries. Consequently:

$$\sum_e \int \int_{\Omega_e} N \left( \epsilon_i \frac{\partial^2 c}{\partial t^2} \right) d\Omega_e = -\sum_e \int \int_{\Omega_e} \epsilon_i \frac{\partial N}{\partial x_j} \frac{\partial c}{\partial x_i} d\Omega_e = [D_{ij}].$$
The matrix $D$ is the diffusion matrix. The additional terms have the form:

$$S = \sum_e \int_{\Omega_e} N (\phi_e + Q) \, d\Omega_e + \{ \sum_e \int_{\Omega_e} N (P - \alpha) \, d\Omega_e \} \, c.$$ 

Substituting back in the diffusion equation, and considering already the inclusion of the time discretization scheme – time interval $\delta t$ –:

$$\frac{c_k - c_{k-1}}{\delta t} = -Dc_k + S_{k-1}$$

and,

$$(\delta t \, D + I) \, c_k = c_{k-1} \, \delta t + S_{k-1} \, \delta t,$$

where $c_k$ and $c_{k-1}$ refer to the concentrations vector at times $k$ and $(k-1)$.

Note that the implicit scheme does not include the terms associated to the dynamics of sediments simulation, which was considered adequate in terms of efficiency of the computational algorithm. The problem now is reduced to the solution of the system of linear equations:

$$[GD] \, c_k = \text{RHS},$$

with:

$$[GD] = \delta t \, D + I,$$

$$\text{RHS} = c_{k-1} \, \delta t + S \, \delta t.$$