CHAPTER 1

INTRODUCTION

Although natural waterbodies have been systematically used over the years to dump all kinds of rubbish, it is only in the last few decades that mankind has become aware of the danger brought by its attitude towards rivers, lakes, and coastal and ocean waters. The growing interest in environmental issues in general, and in water quality conservation in particular, has led to the establishment of a “prevention first” policy (in the long run, it is better to prevent than to lament), and to a rapid development of related sciences and engineering fields. The better understanding of physical phenomena involved in dispersion (both in waterbodies and in the atmosphere) has been immediately followed by advances in coastal and environmental engineering and, consequently, in the development of numerical models used to simulate real processes, which are now considered to be one of the first steps in the design and construction of any environmentally-friendly project.

The first chapter of this thesis intends to provide the reader with an overview of the main reasons leading to the development of the present numerical transport model, introduces the work of some researchers who approached the same problem in many different ways, and finally describes the methodology used in developing the model, and presents some of the results achieved and conclusions reached at the end of the process.

1.1 MOTIVATION AND SCOPE OF THE WORK

The Mediterranean Sea is a land-locked waterbody, with only the Straits of Gibraltar, the Bosphorus and the Suez Canal allowing the exchange of water with other neighbouring seas. Its total surface is about $2.5 \cdot 10^6$ km^2, and its volume is approximately $3.7 \cdot 10^6$ km^3, with an average depth of about 1,500 meters and a maximum depth of 5,121 meters (Kuwabara, 1984). Because the annual water mass input from rivers and rain (38,900 m^3/s; Mancy, 1986) is much smaller than the water mass loss due to evaporation (115,400 m^3/s), the Mediterranean can be classified as a concentration basin, in which relatively high values of salinity, between 36 PSU and 40 PSU, may be reached. The renewal rate of the Mediterranean Sea water is estimated to be of around 80 years, despite a freshwater input of 1,750,000 m^3/s from the Atlantic through the Gibraltar Strait; in comparison, the water exchange with the Black Sea and the Red Sea is negligible.

The total population of the countries bordering the Mediterranean was of about 400 million inhabitants in 1994, 44% of which lived in the coastal areas. The population is drastically increased during the tourist season (mainly in summer), when some 100 million tourists from around the world visit the region, representing one third of all tourist trips in the world (Tedeschi, 1986). Until recent years, the domestic wastewater generated at settlements and tourist resorts was mainly disposed of by direct discharge into the coastal sea, with no previous treatment. Although Kuwabara (1984) points out that the main responsible for pollution in the Mediterranean Sea are riverine discharges (which account for 60-65% of total organic matter, 75-80% of nutrients, and 92% of heavy metals), there is no doubt that domestic and industrial wastewater from settlements are the main source of pollution in the coastal waters, which are often used for recreation and food production.

Marine pollution has been defined as “the introduction by man, directly or indirectly, of substances or energy into the marine environment (including estuaries) resulting in such deleterious effects as harm to living resources, hazards to human health, hindrance to marine activities including fishing, impairment of quality for use of sea water and reduction of amenities” (Intergovernmental Oceanographic Commission -IOC-, cited in Albaigés, 1989).

According to Buceta (1995), the discharges of pollutant substances into marine environments can be classified as natural (or geochemical) and anthropogenic, depending on their origin. In the first case, a great number of substances that can be broadly classified as pollutants are released into the sea by natural phenomena, such as underwater volcanic eruptions -which heat up the water and discharge large amounts of heavy metals-, or river discharges, with the corresponding input of fresh and cold water. This contribution to marine pollution, however, can generally be assimilated by the system, and can be considered simply as an environment shaping factor.

On the other hand, pollution from human sources is discharged into the sea via three different paths (Buceta, 1995):

a) atmosphere, including the residues of engine combustion (aeroplanes, spaceships, etc), radioactive residues from nuclear experiments, or pesticides.

b) ocean, including derivatives from the use of the sea bottom and marine navigation, shipping operations, etc.

c) Earth, which is the main contributor to marine pollution, including the discharge of domestic and industrial wastewater, either from marine outfalls or from rivers.

Although during the last two or three decades the reconstruction of old sewerage systems and the construction of new systems has led to the use of marine outfalls and wastewater treatment plants in Mediterranean countries, thus reducing the direct impact of discharges on the overall pollution, it is still an important issue to know just how much the sea is able to absorb and recycle without suffering permanent ecological damage, specially in a nearly closed and highly populated sea as is the Mediterranean. Apart from the experience gained over the years by engineers with respect to the planning and construction of marine outfalls, it is also necessary to achieve a better understanding of the dispersion of harmful substances in coastal waters, in order to help to optimise the design of marine disposal systems (Zeidler, 1976).

The design and construction of marine outfalls require a great economic and human effort which cannot be misused because of errors in the outfall design process. It is therefore necessary to assure the perfect performance of the future outfall, either by constructing a physical model of the layout or by using numerical models. In the former, the region to be modelled is scaled down, both vertically and horizontally, and constructed within a large test basin. One of the disadvantages of this type of model is connected to a technical constraint in terms of scaling (Falconer, 1992); although the basin geometry, bathymetry and currents may be scaled down, other physical characteristics such as the level of turbulence (which is the governing mixing mechanism), and chemical and biological processes or decay rates may not, so the modelled case will not reproduce the real case correctly. Numerical modelling, on the other hand, allows an easy switching between a great number of different scenarios (the evolution of a discharged plume may be modelled assuming several discharge sites or depths –for the case of a marine outfall, different environmental setups, such as waterbody stratification, and various hydrodynamic conditions -typical current velocities and directions for different seasons-). The accuracy of the results, however, depends on how well the solution of the equations, and the equations themselves, reflect the true physical conditions in the coastal region (Falconer, 1992).

Predicting the mechanical transport of a substance in the ocean -as well as its concentration at a given point- is a difficult task, since it requires a knowledge of the regularities of a large number of factors influencing the process. Among them, there are biological (accumulation and transport of substances by living organisms), chemical (chemical decay of substances, their compounding with other substances resulting in transition to gaseous state or precipitation, etc.), physical (transition between states, coagulation, adsorption, nuclear decay) and, finally, mechanical (transport by the moving waters of the ocean) processes. For example, to calculate the advective transport, data on the vector field of mean current velocities for the region of interest are needed, as well as information on the variability of this field with time. These data can be obtained from maps, from field experiments, from numerical models, or through calculations using the water density fields or the wind fields and heat fluxes across the ocean surface. In addition, the setting or parameterisation of the turbulent components presents another problem, because the characteristics of the ocean turbulence depend on the dynamical state of the ocean (mean current velocity gradients, surface and internal waves, density stratification, etc.). For instance, under a stable stratification of the ocean waters, vertical turbulence and diffusion become considerably retarded.

In order to numerically simulate the fate of passive pollutants in a water body, two models are generally used (Dimou, 1992): a hydrodynamic model and a water quality model. The former simulates the movement of the water, whilst the latter simulates the movement, transformation and interactions of the pollutants within the water, as outlined in the previous paragraph. It is usual practice to let an intermediate (transport) model handle the physical displacement of the pollutant, so the water quality model can focus on pollutant transformations. Following Dimou (1992) the operating framework is then:

- a circulation or hydrodynamic model that solves the continuity and momentum equations, and the mass conservation equation for salinity and temperature,

- a transport model that accounts for the advective and dispersive motion of passive pollutants,

- a water quality model that accounts for the physical, chemical and biological transformation processes of all the water quality parameters. Examples of these processes include sedimentation of particles and the predator-prey relationship of zoo-phytoplankton.

Each one of these models differs from the others in the physical and mathematical character of the equations it solves, and also in the numerical techniques it uses for this purpose; in addition, because of the different time- and space-scales involved, the time and space discretisation in each model is different, and their coupling can become a difficult task. A detailed description of the plume evolution requires the solution of the full three-dimensional equations, which include the important buoyancy-induced vertical motion due to the initial density difference, and the possible trapping of the plume owing to the presence of a sharp picnocline; in some cases it is enough to use two-dimensional models (2DH or 2DV), since the net substance transport in one direction can be neglected in comparison to the transport existing in the other two, and the transport equation can be averaged along that direction.

The actual Spanish legal framework used when designing a marine outfall dates from 1993 (*Instrucción para el proyecto de conducción de vertidos desde tierra al mar*, O.M. 13-VII-1993). The calculation of dilution due to dispersion it proposes does not consider coastal dynamic features such as the existence of periodic tides, dependence of the current velocity on the cross-shore distance, wind effects on the upper layers of the sea, additional wave-induced dilution, or vertical dispersion which, even though is small compared to the horizontal dispersion, does play an important role in overall dilution. It certainly does not seem adequate, when designing an outfall, to rely on a theoretical dilution calculated ignoring all these factors: even if the calculated dilution falls within the required levels, reality may show areas of high pollutant concentration which can result in severe ecological damage. To avoid this, advanced model systems, capable of performing realistic predictions of concentration fields in selected areas, should be available and used by consultants, designers and administration itself.

The main goal of this thesis has been the development of one of such models, including many physical mechanisms of dispersion in order to allow as wide a range of applications as possible. The work done while developing the numerical model also included the attempt to achieve a satisfactory description of buoyant forces in the frame of discrete particle models, and the derivation of a formulation to allow a successful and easy uncoupling of the *nearfield* and *farfield* modelling, to reduce significantly the computation time usage.

1.2 BACKGROUND

During the last couple of decades, considerable research has been done in the mathematical modelling of pollutant dispersion and transport in coastal waters. The classical viewpoint adopted to solve this problem has been Eulerian, although Lagrangian models have also been developed by some researchers. The most popular amongst the Eulerian models are two-dimensional ones, in which the third dimension has been removed by integration (both depth-averaged and laterally-averaged approaches have been considered). As will be seen later in §5.1.1, both Eulerian and Lagrangian techniques present advantages and shortcomings, which are to be carefully evaluated before choosing one or another.

Examples of Lagrangian-type water quality models are those developed, for instance, by Hunter (1987), Al-Rabeh and Gunay (1992), or Spaulding and Pavish (1984). The former developed a particle-tracking model and applied it to the simulation of surface oil patch motion, and to the 2DH behaviour of thermal discharge plumes, computing the advective velocity with a hydrodynamic model, and obtaining the turbulent diffusive velocity by means of a random walk algorithm. He also compared the performance of a particle-tracking *vs*. a finite-difference model, and concluded that the Lagrangian technique was significantly more efficient than the Eulerian under certain conditions (§5.1.1).

Al-Rabeh and Gunay (1992), on the other hand, employed a three-dimensional Lagrangian discrete particle algorithm to simulate the dispersion of pollutants in the Safaniya Sea area, in the Arabian Gulf, and applied it to the particular case of a pollutant discharge from a projected offshore platform. Their model included the formulation for advective and diffusive transport, where the former was computed with velocity components supplied by a 3D hydrodynamic model of wind-induced and tidal circulation, and the latter was calculated with a homogeneous random walk algorithm. Although part of the effluent they modelled was expected to be oily water or crude oil, their model did not include evaporation effects at the water surface.

The 3D transport model developed by Spaulding and Pavish is somewhat different, since it obtained a diffusive velocity as the product of the particle concentration gradient across an Eulerian grid cell, multiplied by a local turbulent diffusion coefficient and divided by the local mean concentration. Mead and Cooper (1992) used also a random walk technique to simulate turbulent diffusion in their 3D dispersion model, considering a constant horizontal diffusivity and deriving the vertical diffusion coefficient from the vertical current shear and densities computed in a 3D hydrodynamic model.

Lagrangian models have also been used to study pollutant dispersal in the atmosphere. For instance, Hall (1975) used and compared two 2DV random walk models, differing in the treatment of turbulent motion, to obtain the concentration distribution resulting from a ground-level source, while Gaffen *et al*. (1987) simulated buoyancy dominated dispersal of passive contaminants in the atmosphere with a "quasi 3D" model (3D dispersion nurtured by 2DV -streamwise and vertical directions- flow predictor), solving the Reynolds averaged, incompressible Navier-Stokes equations, which also yields the eddy diffusivities. A drawback of this approach, and a common one in dispersion models, is that the equations for momentum and dispersion are uncoupled, thus neglecting the effects of density changes and mass forces due to the pollutant in the calculation of the velocity field and turbulent diffusion coefficients. Nonetheless, this model was applied successfully to the modelling of heavy gases and moist buoyant plumes from cooling towers.

The Eulerian approach has been followed, amongst others, by Hermosilla et al. (1996), and Glekas (1994). Hermosilla and co-workers developed a Q3D numerical model (i.e., solving first in the horizontal plane, and then going vertically downwards) to solve the transport equation in a finite element scheme. Owing to the predominantly advective nature of the problem, they used a two-step Taylor-Galerkin algorithm for time discretisation, and calculated the vertical profiles of the different variables with a spectral approximation in a finite series of even-order Legendre polynomials. The equation they solved included a source/decay term which accounted for sediment settling, chemical reactions between the pollutant constituents, or evaporation.

Glekas (1994) presented a fully three dimensional model, which numerically solved the time-averaged Navier-Stokes equations, written in their contravariant strong conservation form, in a non-orthogonal coordinate system. A coordinate transformation was used to map the physical domain onto a unit cube, where the transformed equations were solved *via* a finite volume technique. The model also simulated stratified flows and the buoyancy effects due to density differences between the effluent and the surrounding water, and simulated the turbulent character of the flow using a k-ε turbulence model. Although the numerical model was originally intended for atmospheric flows, it has been successfully applied to the dispersion of radioactive tracers in the sea off Cyprus's coast.

Another grid-based three-dimensional water quality model, but for surface discharges, was developed by Huang and Spaulding (1995), who opted for finite differences techniques to solve the conservation equations, and used a k-ε turbulent closure. They solved the conservation equations, referred to a coordinate system where the vertical coordinate z was transformed to a γ-coordinate ([0,-1]), by finite differences techniques, using a semi-implicit algorithm for the vertically averaged exterior flow, and a vertically implicit procedure for the interior flow, the pollutant constituents and the turbulent kinetic energy and dissipation. The procedure followed in their model allowed small vertical spacing without drastically reducing the time step, and had the advantage of coupling the circulation, the transport and the turbulence models, permitting the simulation of buoyancy effects on the general flow pattern.

Murthy and Kuehnel (1988) developed a 2DH model to predict the dilution contours of outfalls discharging into time-variant coastal currents. Their model was based on an analytical steady state Gaussian plume model, which generated successive realisations of the farfield plume for all the different speed and direction events of a shore-parallel current episode, and then weighted and averaged them according to the occurrence frequency of each event. The equation they solved was

$$\eta(x,y) = \frac{1}{2}\eta_{so} e^{-\lambda x/u} \left\{ \operatorname{erf}\left(\frac{(y+b)/2}{\sqrt{4KX/u}} \right) - \operatorname{erf}\left(\frac{(y-b)/2}{\sqrt{4KX/u}} \right) \right\} \tag{1.1}$$

where η is the farfield to source concentration ratio, η_{so} is the nearfield to source concentration ratio, λ is a decay or die-off constant, b is the line source length, u is the current velocity, x and y are directions parallel and perpendicular to the current, respectively, K is an eddy diffusivity, and X is related to x as follows:

$$\frac{4KX}{u} = \frac{b^2}{6}\left[\left\{ 1 + \frac{1}{n}\left(\frac{4Kx}{u} \right)\frac{6}{b^2} \right\}^n - 1 \right] \tag{1.2}$$

where $n = 1, 2, 3$ for Fickian, shear and inertial subrange diffusion models, respectively.

To derive equation (1.1) some simplifying assumptions were made, namely that the line source was perpendicular to a steady and uniform shore-parallel current, that longitudinal diffusion could be neglected in comparison to the advection, that the vertical diffusion coefficient was negligible compared to the lateral horizontal diffusivity, and that the latter was a function only of the distance from the source, x.

O'Connor and Nicholson (1988) developed a hybrid 3D model which solved the complete 3D diffusion-advection equation for suspended sediment concentration, based on a splitting technique and using a mixed characteristics and finite differences approach. The transport equation was broken into four parts, namely 3D advection, vertical diffusion and settling, diffusion in the longitudinal direction, and lateral diffusion, and each one was treated in a different manner. The advection was solved by a characteristics technique, whereas vertical diffusion and settling were simulated by an implicit finite differences method; an explicit finite differences approach was used to model the longitudinal and lateral diffusion. Their model could handle temporal water level changes, irregular bathymetry, irregular layouts and the wetting and drying of intertidal banks.

Another hybrid model is that developed by Dimou (1992), in which a particle-tracking approach was used to simulate the transport of passive pollutants near the source. When the standard deviation of the particle distribution reached a given lengthscale, the location of the particles was mapped onto node concentrations, and the calculations continued in a Eulerian-Lagrangian mode.

A splitting technique was also used by Bahia (1997) in his depth-averaged transport model, which solved the advection term of the convection-diffusion equation with a characteristics method, and obtained plume spreads by assuming Gaussian similarity profiles for the concentration distribution in the horizontal plane. The plume width depended on the turbulent mixing coefficients, that were taken to be a function of the water depth and the bottom shear velocity.

1.3 SUMMARY OF THE METHODOLOGY USED AND/OR DEVELOPED

With the intention of developing a self-contained fully three-dimensional transport model, which would have to be both accurate and computationally efficient in simulating coastal water mass dispersion, the numerical framework described below was adopted.

A Lagrangian discrete particle random walk approach to the 3D advection-diffusion equation (1.3) was chosen, after considering the cases to which the model was more likely to be applied (see §5.1.1). With this method, the substance to be dispersed is virtually broken up into discrete particles (Lagrangian elements) that are moved within the computational domain according to the actual hydrodynamic characteristics.

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + FD \qquad (1.3)$$

Because of the three-dimensionality of the problem to be solved, it is not sufficient to consider advection and turbulent diffusion only, as vertical motion due to density differences between the discharge and the receiving water may also appear. Therefore, particle-settling (in the case of sediment) or buoyancy-induced displacement (in the case of freshwater discharges) must also be included in the computations.

The procedure followed to solve (1.3) is as follows:

1) First, an alternative transport equation, equivalent to (1.3), has been obtained using a simplified version of the Langevin equation. This alternative expression, known as the Fokker-Plank equation -equation (5.8)-, describes the transport of particles in a random walk model, and is therefore suited to the purpose of this study.

2) Secondly, the effects on the particle distribution of all the relevant physical phenomena have to be computed, using different approaches:

   - advection is obtained from current fields and wave characteristics supplied by a hydrodynamic numerical model or, alternatively, by field measurements,

   - turbulent diffusion is calculated with a random walk algorithm, using diffusion coefficients given by different authors, depending on the case to be modelled,

   - particle settling and resuspension are modelled using empirical or semi-empirical equations for settling velocity and resuspension,

- buoyancy forces are simulated using a simple expression derived from dynamic considerations for stagnant environments, and a semi-empirical formulation for the case of non-zero currents,

- microbiological decay, when necessary, is computed based on empirical equations from several authors in different conditions.

3) The last step is to transform the set of particles into a continuous distribution of mass concentrations (or micro-organism concentrations). The mapping may be done using either a conventional box-counting method, or a more advanced smoothed-particle (SPH or kernel) method. The main difference between both lies in the fact that, in the latter, the mass of a particle at a given position ***x*** is spread out according to a defined distribution that somehow reflects the possible errors in position introduced by the random walk modelling. In other words, whereas a particle *is* at ***x*** when using the box-counting method, it *has a given probability of being* at ***x*** if the kernel method is used.

Because of the different timescales involved in the dispersion in the nearfield and in the farfield, the small computational timestep required to correctly reproduce the behaviour of the discharge near the source represents a burden once the plume enters the farfield phase; it is convenient then to uncouple the simulation of both phases. The methodology used in this study to allow for field uncoupling consists in considering two separate model runs, one for the nearfield, as defined by equations presented in Chapter 4, and with a small timestep, and one for the far field, for which buoyancy effects are not included in the computations and the timestep is larger. The sources and initial concentrations for the second run are given by the concentration distribution obtained from the first model run.

1.4 SUMMARY OF THE RESULTS

The main result of this thesis is the development and analysis of a fully three-dimensional numerical model, based on a Lagrangian approach to the advection-diffusion equation, to simulate the transport of passive substances in coastal waters.

This model has been developed in two separate parts, one devoted to simulate the physical transport of the substance, in the form of a set of particles, and the other used to map the final distribution of discrete particles onto the nodes of a computational grid in order to achieve a continuous concentration distribution.

The first (transport) module includes several submodules to account for the different physical mechanisms which govern the transport of common substances, together with a submodule corresponding to the particular case of wastewater discharges from a marine outfall, where pathological micro-organisms may be present. The main features of each submodule are described below:

a) Advection: Advection is treated by interpolating the current field obtained from a hydrodynamic model, or by using experimental velocity data. Wave-induced mass-transport is also considered, as is the initial discharge velocity.

b) Diffusion: Turbulent diffusion is treated using a random walk algorithm, and defining turbulent diffusivities according to different expressions found in the literature, for different situations. Molecular diffusivity, although negligible in most cases, is also included.

c) Buoyancy effects: Vertical transport due to the density differences between discharged effluents and the receiving waters is treated using semi-empirical formulations.

d) Sediment settling: Settling particles are modelled using experimental equations derived to obtain the fall velocity of sediment as a function of sediment density and diameter.

e) Sediment resuspension: Particle resuspension owing to bottom shear stresses is treated using a formulation based on the pick-up function concept, from which a vertical resuspension velocity is obtained.

f) Bacterial decay: Microbiological mortality is estimated using a statistical approach, after computing the decay rate using expressions found in the literature or constant values.

The second (mapping) part of the model includes three different algorithms to transform the cloud of particle positions resulting from the previous module into a “readable” concentration distribution, in order to obtain modelled concentration values. The algorithms implemented are:

a) BC: A simple and straightforward box-counting method, where the concentration is found by considering the mass of all particles found within a pre-defined volume (“box”).

b) kBC: An extension of the previous algorithm, in which part of the total mass in each one of the “boxes” is shared between neighbouring “boxes”, to smooth out sharp concentration gradients.

c) SPH: Based on the assumption that the mass of each particle is not located at the position given by the transport module, but follows a pre-defined mass distribution function centred at that position. The concentration is computed by considering the contribution of each particle to the total mass at a given point.

The application of the model to different validation tests has given the opportunity to estimate the accuracy of the different submodules, in some cases, and of the whole transport model in others. Some advantages and disadvantages of each have been made clear. The overall results of the transport model in these validation cases are good, closely matching the predicted behaviour and the analytical solutions to the proposed problems.

Finally, the simulation of several real cases, for which the modelled results could be compared to experimental data or observational evidence, has confirmed the ability of the developed code to reproduce the transport of substances to an acceptable degree of accuracy, for a wide range of situations. This model is currently able to simulate the two- and three-dimensional transport of a variety of substances, ranging from riverine freshwater to sediment particles and wastewater – including relevant features such as microbiological decay, buoyancy effects, and sediment settling and resuspension-, driven by 2DH, Q3D or fully 3D hydrodynamic fields, and considering the effects of waves both on the mass transport and on the local level turbulence. The model is applicable in general waterbodies, irrespective of their vertical density distribution, and allows the individual characterisation of boundary regions, to account for the presence of different base materials (such as sand, rock, etc.). LIMMIX also takes into account the different time- and lengthscales that exist in the transport process, allowing to uncouple the simulation of the nearfield from the farfield simulation, to maximise computational speed without loss of accuracy.

Coupled with a general circulation model, the transport model presented in this thesis illustrates the possibility of considering numerical hydrodynamic and transport models as useful engineering tools to deal with outfalls, river freshwater discharges, and other types of discharges into the sea. The model yields handy elements to evaluate the concentration levels of pollution generated by general discharges under different environmental conditions (such as waterbody stratification, intensity and direction of the wind, type of boundaries) or discharge characteristics (such as discharge position, orientation, buoyancy, concentration, number of constituents, number and type of nozzles for the case of marine outfalls, etc). Additionally, the model can be applied to a other situations of interest where it is important to foresee the behaviour and fate of water-transported substances, as can be the case of a river's freshwater plume or the settling of river-borne sediments in a semi-enclosed region. Accidental surface spills can also be simulated in an efficient manner.

1.5 STRUCTURE OF THE THESIS

This work is organised in seven chapters, including the introductory chapter, plus a list of references, and an appendix containing papers generated by the work undertaken in this study.

Chapter 2 presents the equations that govern the dynamics of fluids for laminar and turbulent flows, and gives the advection-diffusion equation which will be the basis for the development of the numerical transport model. The relevant hydrodynamic features of coastal waters are also presented, and a detailed description of wind-induced currents, oscillatory motion, nearshore currents, wave-currents interaction, turbulence and tidal currents and estuarine circulation is given. The third part of the chapter deals with the characteristics of mixing in coastal waters, and particular emphasis is given to turbulence and turbulent diffusion coefficients, including turbulent closure models; overall dispersion coefficients and the effects of oscillatory motion on mixing are also presented.

In Chapter 3 a summary of the different types of sources for coastal pollution is given, together with a classification of pollutant substances according to the World Health Organisation. Emphasis is placed on the contaminants more commonly found in coastal waters, and these are analysed in detail. Water quality degradation due to microbiological organisms resulting from outfall wastewater discharges, nutrients dragged into coastal waters by rivers, sediment loads related to river discharges or longshore transport, and heated water from cooling circuits is presented, and the related equations that will form the basis of the different numerical modules are given.

Chapter 4 deals with the particular characteristics of effluent discharges depending on the initial discharge parameters. The concepts of jet and plume are introduced, and the important issue of merging of plumes and jets is addressed, in order to better understand the dynamics of wastewater or heated water discharges. The influence of environmental factors, such as the density profile of the receiving waterbody or the presence of ambient currents, on the effluent dispersion is analysed and, finally, the different regions in which a wastefield is divided according to the relative importance of the initial discharge parameters are presented.

Chapter 5 focuses on the numerical aspects of the thesis. First, the most common numerical methods used to solve the transport equation are described and compared, highlighting the advantages and disadvantages of each type; the reasons why the Lagrangian approach is selected are given. In the second part of the chapter, the analogue equation –equivalent to the transport equation- on which the present numerical model is based is given, and the methodology followed to implement all the relevant transport mechanisms into the code is presented. The theory behind each one of the mapping algorithms, and their implementation in the model, is then given, and the last part of the chapter analyses the results of a series of validation cases designed to test different aspects of the numerical model, and draws conclusions.

Chapter 6 is devoted to the application of the transport model to different real cases. The model is used to simulate the transport of a substance in a situation where the numerical results can be checked against experimental data or observational evidence to estimate the accuracy of the simulation. Four different cases are presented: a marine outfall discharge near the city of Barcelona, a sediment settling problem inside the Tarragona harbour, the time evolution of a tracer cloud at the Barra del Trabucador (Ebre delta), and the freshwater plume of the river Ebre. Results are given, and conclusions are presented.

Finally, Chapter 7 closes the thesis summarising the major conclusions of this work, presenting its contributions to numerical transport modelling, and giving some indications on which aspects of the model could be improved, and future work to be done in order to implement these ideas.