CHAPTER 7

RESULTS, FUTURE WORK AND FINAL CONCLUSIONS

7.1 RESULTS

This thesis presents the development, testing and application to different situations of a fully three-dimensional numerical dispersion model. It is based on a Lagrangian approach to the advection-diffusion equation, and is therefore suitable for simulating the transport of passive substances in coastal waters.

7.1.1 General summary

The model has been developed in two separate parts, in order to simplify the acquisition of simulation results. The first part is devoted to simulate the physical transport of a substance, represented by a set of discrete particles, whereas the second part is used to map the final distribution of particles onto the nodes of a computational grid in order to achieve a continuous concentration distribution; this is done so because the results of the discrete-continuous transformation appear to depend on the value of different user-defined transformation parameters, and several transformations may be performed on the same set of particles.

The first (transport) module of the code contains all the submodules related to the different physical mechanisms that govern the transport of passive 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 a current field given by 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 from the literature, for different situations. Molecular diffusivity, although negligible in most cases, is also included.

c) Buoyancy effects: Vertical transport due to density differences between discharged effluents and 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 associated to bottom shear stresses is treated using a formulation based on the concept of sediment pick-up, from which a vertical resuspension velocity is obtained.

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

g) Physical boundaries: Realistic boundaries have been introduced, considering the variable degree of absorption as an additional model parameter.

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, in which 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, allowing a first approximation towards the performance envelope of the different mapping algorithms. 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.

7.1.2 Contributions to transport modelling

The transport model developed for this work contains several features that are not easily found in numerical models for dispersion in coastal waters:

a) It is a “complete” model that solves the transport equation in both the nearfield and the farfield. Because of the wide range of time and space scales over which the transport processes occur, in most cases the simulation of a real dispersion problem implied so far the use of two separate models, one for the nearfield and one for the farfield, ignoring any interaction between both. As an example, farfield models tend to ignore the existence of the nearfield, whereas nearfield models assume that substance mixing occurs with clean ambient water, ignoring any possible farfield pollution return. The advantage of the proposed approach is partly a consequence of the adopted Lagrangian formulation, which does not require the definition of a computational grid in order to estimate concentrations until after the transport processes have been modelled; in grid-based models, the fine grid resolution required to solve the nearfield burdens the computations of farfield dispersion, and the coarser grid resolution used for farfield calculations is unable to resolve nearfield characteristics.

b) The uncoupling of the nearfield calculations from those of the farfield improves the timewise performance of the model. Although this feature is optional and requires two consecutive model runs, it handles the disparity of timescales in both regions, and allows to achieve results similar to those obtained from a single complete model run, but with a more efficient CPU-time performance. Furthermore, it allows the model to simulate only the nearfield or the farfield region, depending on the user requirements.

c) Specific formulations for several transport mechanisms have been developed and implemented for the particular case of a Lagrangian particle numerical model. Advantage has been taken of the simplicity of the analogue equation solved by this type of models to introduce additional velocities accounting for wave-induced mass transport, buoyancy effects and initial jet velocity (only when the initial discharge velocity does not affect in a significant manner the ambient currents, as is the case of marine outfalls).

    c.1) Wave-induced transport is modelled using a a Lagrangian formulation based on equations provided by Davydov (1978). This transport mechanism is usually ignored, since it is assumed that the main substance transport is due to currents.

    c.2) The initial velocity of the particles due to the discharge flow rate, and its decrease as the jet mixes with the ambient water and becomes deflected by the ambient currents, has been taken into account, implementing a Lagrangian formulation based on experimental observations.

    c.3) A specific formulation for buoyancy effects (the treatment of which the author has been unable to find in the literature related to marine transport models), has been adapted to a marine environment from atmospheric dispersion models.

d) Realistic solid boundaries have been included, taking into account the specific absorbing properties of each computational cell by defining individual reflectivity coefficients.

e) A simple and straightforward procedure to include sediment resuspension has been proposed. The method takes advantage of the formulation introduced to treat the boundary conditions, which involves the definition of cell-specific variable reflectivity coefficients. Although yet to be rigorously tested, it has been used in a real case, and the results appear to be promising.

f) The application of the model to a set of different real cases show the ability of Lagrangian particle models to correctly reproduce a wide range of situations with different characteristic time- and lengthscales.

Contributions to specific transport processes have also been obtained from the application of LIMMIX to real cases. More details on these issues are given in §7.3:

g) Tracer patch: In the presence of a wave field, the time variation of the coefficient describing the horizontal dispersion parallel to the direction of wave propagation appears to be logarithmic, whereas the dispersion normal to this direction appears to be vary as a power of t.

h) River freshwater plume: The calibration of LIMMIX using field measurements of salinity have allowed an estimation of the coefficients which best describe the horizontal dispersion of the river Ebre freshwater plume.

i) Sediment settling in the Tarragona harbour: Modelling the settling of sediment transported by the Francolí river allows to estimate the conditions under which the circulation within the harbour is governed by the freshwater discharge, and when is the wind the main driving agent.

7.2 FUTURE WORK

Although the numerical model developed for this thesis is quite general and complete, it presents some aspects which could indeed be improved in the future. These involve both the conceptual part (i.e., the formulation of the different phenomena and transport mechanisms) and the numerical part of the model (i.e., the computational code itself). Some of the possible improvements which are to be done to increase the applicability and performance of this transport model are described below.

7.2.1 Model (conceptual) improvements

a) **Turbulent diffusion:** The actual use of a zero-order model to compute turbulent diffusion is a drawback of the formulation, due to its simplicity. In principle, a higher-order turbulence closure model should be used, implemented either in the present model or in the hydrodynamic model which supplies the velocity field. Turbulent diffusivities would then be cell-dependent within the computational domain, rendering a more realistic simulation of dispersion. If this is not possible, a thorough calibration of the turbulent diffusion formulations defined in the transport model is required.

b) **Sediment resuspension:** The formulation implemented for the resuspension of sediment particles from the bed could be improved, particularly in the computation of the number of particles picked up in each timestep. The inclusion of a suspension-maintaining mechanism would also increase the efficiency of the resuspension module. On the other hand, a more extensive analysis of the alternative resuspension approach outlined in §6.4, including calibration and comparison with field data, would be of interest to estimate the usefulness and capabilities of this approach.

c) **Buoyancy:** The module implemented to compute the effects of density differences, although checked, has not yet been calibrated against data from real cases. It would be desirable to do so in order to assess the performance of the chosen formulation in coastal waters.

d) **Wind-induced effects:** The transport of a substance by direct wind dragging might be important for surface pollutants; however, this effect is not included within the model. Wind-induced mixing at the waterbody surface should also be considered in detail and correspondingly implemented in the code.

e) **Non-physical interactions:** Chemical interactions between particles, and biological processes affecting them, are not currently considered, and are important issues in the transport of nutrient substances such as phosphorus and nitrogen. They could be directly included as part of the transport model, or coupled in the form of a water quality model. Complex biologic processes involving larvae or other organism populations could also be added in a biological module.

f) **Temperature:** An accurate module for temperature transport could be developed to account for heated water discharges, taking into account particular characteristics such as evaporation at the water-air interface.

g) **Oil simulation:** A module to simulate the dispersion of “two-dimensional” highly buoyant substances, such as oil, could be developed and implemented. This module should consider effects like biodegradation, sedimentation, aggregation and evaporation.

h) **Hydrodynamic field:** Coupling of the transport model to an efficient hydrodynamic model would simplify its use, and create a powerful integrated engineering tool for pollutant transport and fate.

7.2.2 Computational improvements

i) **Transport model programming:** The way the transport model is programmed may not be the optimum, taking into account the large number of particles that can be involved, and the number of calculations per particle and per timestep that must be done. A more efficient use of array variables would lead to a reduction of the computational memory requirements, and a more rational coding of the source program would reduce CPU-time necessities. Parallelisation of the code, taking advantage of the linear formulation used, would be a possibility when interactions between particles are not considered.

j) **SPH programming:** Possible improvements in the SPH algorithm implemented would include the accurate treatment of boundaries, and the development of an adequate and valid formulation to estimate the individual integration lengthscale. This would undoubtedly increase the accuracy of the method.

k) **Model interface:** The development of a user-friendly interface to simplify the input of initial parameters to define the case, and to check the consistency of the supplied data, would also make the model easier to use in real cases.

7.3 CONCLUSIONS

The main conclusions arising from the work developed in this thesis are:

a) Lagrangian models:

a.1) The use of a Lagrangian approach to solve the transport problem presents some advantages with respect to other formulations, particularly because it allows to identify different types of the transported substance, and/or single out individual “parts” of it. For instance, the discharge of a wastewater effluent containing different types of microbiological organisms, or the settling of sediment particles with different characteristics, is naturally modelled with this approach, and the treatment of the boundary conditions (both horizontal and vertical) is largely simplified when individual particles are considered.

a.2) However, the use of the Lagrangian formulation also introduces some disadvantages when compared to other (Eulerian) methods, mainly when volume forces –such as buoyancy- or processes which depend on concentration values –e.g., interactions between different constituents of the discharge- are to be included in the model. A further drawback in the Lagrangian approach is the need to define a mapping algorithm to obtain a continuous concentration distribution

b) Mapping methods:

b.1) The most simple and straightforward mapping algorithm, referred to in the thesis as the BC method, consists in counting particles inside a given “box”, and dividing the resulting mass by the volume of the “box”. The selection of the integration box, however, plays an important role in the accuracy of the obtained concentration field, since it can generate excessively jagged or excessively smoothed distributions.

b.2) The Smoothed-Particle Hydrodynamics (SPH) method, on the other hand, is based on probability functions, and depends on the specification of an integration length, which may depend on the local particle density. The results depend on the value of this characteristic length as they do on the integration volume in the case of the BC algorithm.

b.3) The comparison between both mapping functions reveals that the SPH method requires a smaller number of particles than the BC algorithm to obtain similar concentration distributions, although in general the CPU-time involved in the computations is larger. For both methods, the estimation of the integration parameter (volume or lengthscale) must be done with care, and effects such as the presence of solid boundaries, sharp concentration gradients (“edges” of the plume) and even the local particle density should ideally be taken into account.

c) LIMMIX:

c.1) The numerical dispersion model reproduces correctly the mechanisms of substance transport in coastal waters implemented into the code. In particular, the simulation of advection by currents and waves, turbulent dispersion, buoyancy, microbiological decay and sediment settling yields numerical data that acceptably agrees with expected results. In the coastal region, the three-dimensionality of its formulation becomes an important feature.

c.2) The numerical model is applicable to different situations, and is able to deal with discharges from marine outfalls, river mouths, and other type of substance discharges into the sea. Its versatility makes it useful for the evaluation of concentration levels of passive substances under a variety of design and environmental conditions.

c.3) The procedure introduced to uncouple the calculation of the dispersion in the nearfield from that in the farfield allows the numerical model to simulate only the relevant mixing zone (nearfield, when dispersion away from the source is not important; farfield, when the nearfield is negligible compared to the total mixing region). If the total mixing region is simulated, the computation time may be reduced by uncoupling the calculations in both fields, without a significant loss of accuracy.

c.4) Depending on the number of transport mechanisms included in the simulation, and the accuracy required in the results, the duration of a LIMMIX run may be large. This hampers its use as a real-time simulations model, and limits its application to forecasting situations.

d) **Model application:**

d.1) The results obtained from all the model applications agree with those expected using analytical solutions, experimental data, satellite images or video recordings.

d.2) The application of LIMMIX to the case of a tracer patch in a wave environment in the Ebro Delta suggests that the time dependence of the turbulent dispersion coefficient parallel to the direction of wave propagation is different from the coefficient normal to this direction. The former dispersion coefficient appears to vary logarithmically with time ($\propto \log(t)$), whereas the latter is proportional to some power of time ($\propto t^B$).

d.3) The application of the transport model to the case of the river Ebro freshwater plume, and the comparison of the numerical results with experimental salinity data, suggest that Elder's (1959) equations for the turbulent dispersion coefficients may be used, if it is assumed that the discharged freshwater remains in the upper (surface) layer of the sea. When the constant parameters in Elder's equations are taken to be in the range c_L = 500-1000 and $c_T \approx 700$, the salinity values and the overall shape of the river plume supplied by the numerical model show an acceptable agreement with observational evidence. The estimated values for these coefficients are several orders of magnitude larger than those proposed by in Elder's paper ($c_L = 5.91$ and $c_T = 0.23$). The simulations show that for "normal" river discharge rates (~ 300 m^3/s) the behaviour of the river plume is governed mainly by the wind-induced circulation, whereas for larger freshwater flows (~ 1400 m^3/s) the river momentum becomes the prevailing driving mechanism.

d.4) The application of LIMMIX to the freshwater discharge of the river Francolí in the Tarragona harbour shows that the hydrodynamic field within the harbour is determined mainly by the river momentum when the river outflow is large ($Q \geq 1000$ m^3/s, aprox.). whilst for smaller freshwater flows ($Q \cong 100$ m^3/s) the influence of the river discharge is limited to the region near the river mouth, and the circulation away from this zone is governed mainly by the wind. However, the simulations reveal that sediment transport is driven by the river, and it depends little on the characteristics of the wind.

The developed 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. It includes relevant features such as microbiological decay, buoyancy effects, and sediment settling and resuspension, driven by 2DH, Q3D or fully 3D hydrodynamic fields. It considers the effects of waves both on the mass transport and on the local level of 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 that of the farfield, 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.). Accidental surface spills can also be simulated in an efficient manner.