A Lagrangian 3D Numerical Model of Pollutant Dispersion in Coastal Waters

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Abstract

Two-dimensional numerical models have been extensively used in the far field to solve hydrodynamics and the associated pollutant transport. However the results obtained from these models may not be suitable when used in the near field or in areas where the hydrodynamics has three-dimensional features, such as wind-induced currents in the nearshore region or wave-induced currents in the surf zone. A 3D Lagrangian numerical model has been developed to solve the three-dimensional convection-diffusion equation in order to simulate pollutant transport in non-uniform and stratified hydrodynamic flows. In this paper the model characteristics and its calibration process are described and posteriorly it is applied to the case of the Besòs marine outfall, near Barcelona (Spanish Mediterranean coast) and to simulate tracer clouds dispersion in the surf-zone.

1 Introduction

The simulation of marine outfall discharges must take into account the existence of two differentiated regions in which the pollutant evolution is governed by different physical mechanisms. Nearest the source, in the near-field, transport is driven by the discharge characteristics, such as initial momentum or density differences, as well as the nozzle geometry and orientation. On the other hand, in the far-field, dispersion is due exclusively to the hydrodynamic velocity field and environmental turbulence.

In this latter region, the net substance transport in one spatial direction can often be neglected in comparison to the existing transport in the other two. The problem can then be solved by averaging the transport equation along that direction. This is the basis for 2DH models which generally solve the vertically-averaged form of the transport equation.

Nevertheless, this averaging procedure can not be carried out in the near-field, since pollutant transport is equally important in each direction. The application of two-dimensional models in this region may lead to unreliable results, and as a consequence the use of fully 3D algorithms becomes necessary. Moreover, when the hydrodynamics (circulation and turbulence) changes significantly in the vertical direction, as in the case of nearshore wind-induced currents or wave-induced currents inside the surf-zone, it is suitable to use 3D dispersion models even in the far-field.

This paper presents a recently developed 3D Lagrangian numerical model for the transport of pollutant substances (Sánchez-Arcilla et al. [6]). Several reasons exist to justify the use of a Lagrangian approach, such as the concentration of computational effort in the region where pollutant accumulates, the capability to simulate dispersion of different constituents and the simplicity arising in the formulation and implementation of the various physical processes.

2 Model formulation

The model solves the three-dimensional equation for mass transport due to diffusion and advection, averaged over the time-scale of turbulence (Reynolds average):

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} =$$

$$\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right) + \left(D_y\frac{\partial C}{\partial y}\right) + \left(D_z\frac{\partial C}{\partial z}\right) + DS \tag{1}$$

where C is the concentration, u, v and w the components of the velocity field, D_x, D_y, D_z the diffusion coefficients in the x, y, z directions respectively and DS is a source/decay term.

2.1 Transport mechanisms

The Lagrangian approach herein followed assumes that the pollutant mass is divided into small particles (Lagrangian elements) which are moved inside a water body according to the different physical mechanisms involved in the transport. Eventually, these particles may disappear if microbiological decay exists, or if they become trapped at physical boundaries (bottom or dry edges).

Under this hypothesis, each particle is displaced a certain distance (Δx, Δy, Δz) during a timestep Δt, with a velocity which depends on the different processes involved in the overall dispersion. The individual contribution to the total velocity arising from each mechanism is calculated in the following way:

$$\begin{aligned} x^{n+1} &= x^n + (u_C + u_w + u_o + u_{D_L}\cos\theta - u_{D_T}\sin\theta + u_{D_M})\Delta t \\ y^{n+1} &= y^n + (v_C + v_w + v_o + u_{D_L}\sin\theta - u_{D_T}\cos\theta + u_{D_M})\Delta t \\ z^{n+1} &= z^n + (w_C + w_w + w_o + w_{D_V} + u_{D_M} + w_S + \frac{1}{2}w_B)\Delta t \qquad (2) \end{aligned}$$

where u_C, v_C, w_C are the velocity components from the hydrodynamic model; u_w, v_w, w_w the wind induced velocity components; u_o, v_o, w_o the wave-induced transport velocity components; u_{D_L}, u_{D_T}, w_{D_V} the turbulent diffusion velocity components in the longitudinal, transversal and vertical direction respectively; u_{D_M} the molecular diffusion velocity; w_B, w_S the buoyant and settling velocity components and θ the angle between the x-axis and the current lines.

The components of the 3D velocity field are computed with the help of a 2DH hydrodynamic model (Sánchez-Arcilla et al. [5]) which solves the vertically integrated mass and momentum conservation equations, including wave and wind effects, but without considering the circulation due to density gradients. Once the 2DH mean velocities are determinated, they are vertically modified assuming a logarithmic profile in the bottom boundary layer and a parabolic profile elsewhere. Then the vertical velocity component can be calculated by solving the mass conservation equation.

The oscillatory flow effects must be taken into account because the surface waves affect the pollutants transport in two different ways: generating a net advective transport and enhancing the local turbulence level which stimulate the vertical turbulence mixing. The transport by oscillatory flow is included in the model distinguishing between outside and inside the surf zone.

Outside the surf zone the effects are modelled using a formulation proposed by Davydov [2] in which the wave field is described by a linear theory. The pollutant flow in the horizontal directions is

$$q_j = \delta_j \frac{\partial C}{\partial z} \tag{3}$$

and in the vertical direction is

$$q_z = \delta_j \frac{\partial C}{\partial x_j} \tag{4}$$

where the subscript j indicates the components in the x and y directions and δ_j is

$$\delta_j = \frac{H^2 \pi \sinh(2kz) k_j}{8T \sinh(kh) |\vec{k}|} \tag{5}$$

where $\vec{k}$ is the wave number vector, with components k_j, T the characteristic wave period and H the wave height. If it is assumed that q_i (with $i = 1, 2, 3$) represents the pollutant flux per unit area and unit time in the x_i direction, then

$$q_i(l, m, n) = u_{oi}(l, m, n) C(l, m, n) \tag{6}$$

and a "psuudo-velocity" generated by the oscillatory flow can be deduced for each particle contained inside a certain cell (l, m, n) with concentration $C(l, m, n)$.

In order to model diffusive processes, a diffusive velocity can be defined as

$$u_D = (2R_{01} - 1)\sqrt{\frac{6D}{\Delta t}} \tag{7}$$

where D is the diffusion coefficient and R_{01} is a random number $(0 < R_{01} < 1)$.

Outside the surf zone, the turbulent dispersion is splitted into vertical and horizontal components. The latter component is further decomposed into a diffusion paralel to the horizontal current lines and a lateral diffusion. Following Holly [3], the corresponding diffusivities are given by

$$\begin{aligned} D_L &= c_L u_* h \\ D_T &= c_T u_* h \end{aligned} \tag{8}$$

where u_* is the shear velocity ($u_* = (\tau/\rho)^{1/2}$, τ is the bottom shear stress), h is the local depth and c_L, c_T are empirical coefficients with typical values of $c_L = 5.93$ and c_T between 0.07 and 0.23.

On the other hand, an accepted estimation for the vertical diffusivity outside the surf zone is

$$D_z = c_V u_* h \tag{9}$$

with c_V ranging from 0.16 to 0.23.

Inside the surf zone, additional mixing due to wave breaking has to be considered. The horizontal diffusivity, assumed isotropic, can be estimated with a number of expressions, like the one proposed by Battjes [1],

$$D_H = c_H \left(\frac{D_b}{\rho} \right)^{1/3} h \tag{10}$$

where c_H is an experimental coefficient, usually taken as 4.5 and D_b is the wave breaking dissipation, obtained from the wave propagation module in the hydrodynamic model.

The vertical diffusion coefficient is computed following Nadaoka and Hirose [4]:

$$D_z = 0.18 \left(\frac{H}{h} \right)^{7/3} L^{1/3} h^{2/3} (gh)^{1/2} i^{1/3} \tag{11}$$

where i is the bottom slope and L the wave length.

Even though its effects are small compared to turbulent diffusion, molecular diffusion is also included in the computations for model completitude. In this case, the diffusivity is assumed isotropic and constant and depends on the discharged substance. Other effect taken into account into the model is the particle settling when dealing with suspended sediment.

For the treatment of discharges whose density ρ is different from that of the receiving water body ρ_0 (due either to salinity or temperature), or in situations where environment stratification exists, buoyancy effects are included by means of a buoyancy velocity

$$w_B = \frac{\rho_0 - \rho}{\rho_0} g \Delta t \tag{12}$$

Endly, the effect of microbiological decay on dispersion is also included in the transport calculations when urban sewage is discharged directly, or by marine outfalls, into the waterbody. The concentration $C(t)$ at time t is

$$C(t) = C(t_0) e^{-K_d (t - t_0)} \tag{13}$$

where $C(t_0)$ is the concentration at time t_0 and K_d is a decay coefficient which depends on a number of factors (organism type, temperature, solar radiation, etc.). This coefficient can be evaluated from several expressions with different accuracy.

2.2 Discrete-continuous transformation

A transformation scheme is required to obtain the concentration field from the modelled cloud of Lagrangian particles. The model allows to perform this transformation with three different methods:

- The classical particle-in-cell (PIC) method which consists in dividing the volume affected by the pollutant in "concentration cells" and counting the number of particles in each one. The concentration in an individual cell is obtained dividing the total mass in the cell by its volume.
- The smoothed-particle hydrodynamics (SPH) method, based in the hypothesis that each particle can be replaced by a smoothed-out density distribution W. The mass concentration at a point is found by adding all the contributions from individual particles.
- The hybrid (kPIC) method is conceptually similar to the first one, but in this case, the mass of a particle is spread out amongst the cell which contains the particle and its 26 neighbours, according to a predefined mass distribution.

3 Model validation

The model has been validated with a number of simplified analytical cases, two of which are shown in the present paper.

The first validation test is an instantaneous release of conservative pollutant in a stagnant environment, in which mass transport is driven exclusively by diffusion. The analytical solution in a three-dimensional space is

$$C(x,y,z,t) = \frac{C_0}{(4\pi D_x D_y D_z t)^{3/2}} e^{-\frac{(x-x_0)^2}{4D_x t} - \frac{(y-y_0)^2}{4D_y t} - \frac{(z-z_0)^2}{4D_z t}} \qquad (14)$$

The concentration distribution resulting from a 15 s diffusion process has been computed using the PIC and kPIC methods, with a cloud of 100,000 particles. The obtained distributions are plotted in figure 1, showing a relative error of about 2%.

The second validation test shown here corresponds to a continuous release of infinite duration, whose 1D analytical solution for a conservative substance is

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x-ut}{2\sqrt{Dt}}\right) + erfc\left(\frac{x+ut}{2\sqrt{Dt}}\right)\exp\left(\frac{ux}{D}\right)\right] \qquad (15)$$

where $erfc$ is the complementary error function. For this test, 17 particles were discharged every 0.05 seconds during a period of 30 seconds. The results obtained with the PIC method are shown in figure 2, where it can be seen a good agreement between the analytical function and the numerical results.

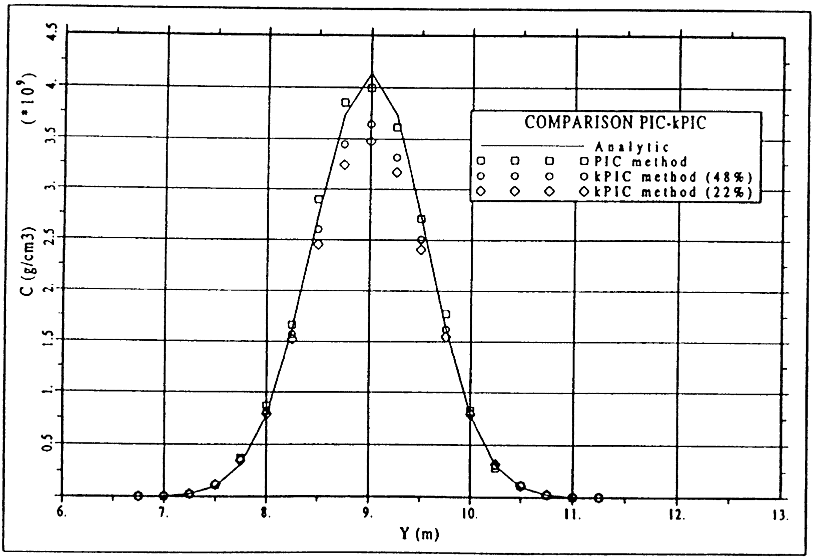

Figure 1. Model validation. Instantaneous release.

4 Model application

The model was firstly applied to simulate the sewage discharges from the Besòs marine outfall (Barcelona, Spanish Mediterranean Coast). In figure 3, the results of the discharge from 10 diffusers are shown. In this case, a stratified environment was assumed, which is a typical summer condition in this area. The plume has been computed by releasing 36,060 particles for a period of 30 minutes, with a 3 seconds computational timestep and an effluent density of $\rho = 1.026$ g/cm^3.

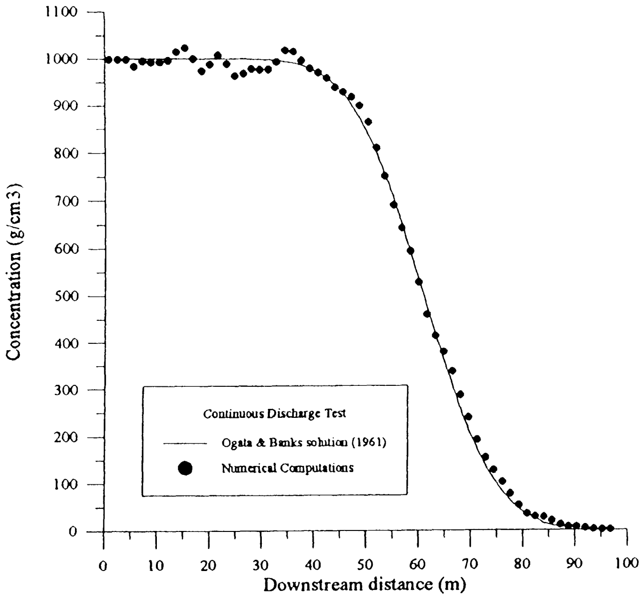

Figure 2. Model validation. Continuous release

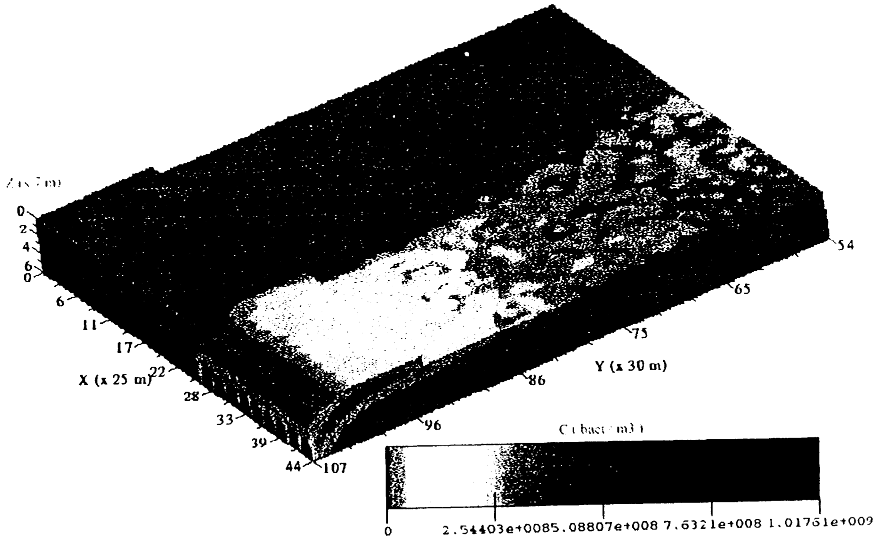

Figure 3. Simulation of Besòs marine outfall discharge

In the second case of model application, the horizontal length scales of a tracer cloud released in the surf-zone (in the Ebro Delta area) have been modelled as a first step towards reproducing the tracer overall behaviour. Approximate longitudinal and transverse dispersion coefficients have been calculated using the random-walk step equation

$$r_{max} = \sqrt{6K\Delta t} \tag{16}$$

where r_{max} is the maximum step a particle can jump in a timestep. The patch diameters were obtained from a series of digitised video images. These coefficients have then been used to model the time evolution of the released trazer and to estimate the size of the resulting patch. Figure 4 compares the modelled longitudinal patch diameters for different dispersion coefficients with that obtained from video images.

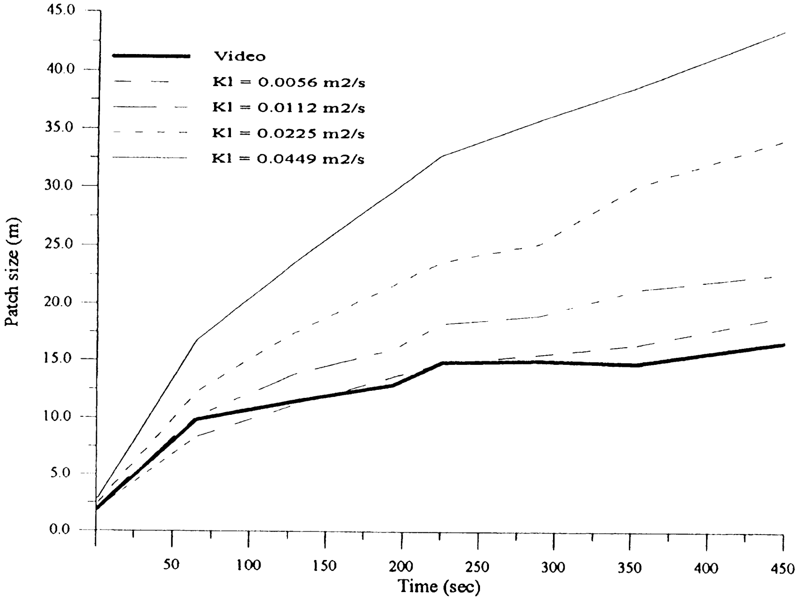

Figure 4. Simulation of the tracer cloud size

5 Summary and conclusions

A general 3D model for the dispersion of pollutants has been developed, based on a Lagrangian formulation. The model allows to describe the evolution of marine discharges both in the near and far-field.

The model has been validated with a series of simple analytical cases showing a good agreement, and has been finally used to simulate two real cases: the Besòs (Barcelona, Spain) marine outfall discharge and the dispersion of a tracer cloud released in the surf-zone. In this latter case, for a K_L = 0.0056 m^2/s, a good fit of the modelled results to the experimental ones is observed.

The model requires a thorough calibration process, but the first results illustrate the possibility of considering the model a useful engineering tool to verify existing outfall designs and to predict future or hypothetical situations.

Acknowledgements

This work was jointly sponsored by the FANS project (in the framework of the MAST-III Programme under contract no. MAS3-CT95-0037) and the Spanish CICYT (CYTMAR Programme, project MAR96-1856). The authors are also grateful to F. Collado and EMMSA for their collaboration.

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