

Particle-tracking method applied to transport problems in water bodies

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Abstract

In this work a particle-tracking model was implemented and applied to simulate the instantaneous injection of a dye tracer in the Setubal Lagoon, Santa Fe, Argentina. It focused on the study of the water quality problem generated in point sources of contaminated water through a rainfall drainage system. This problem is difficult to treat with the so-called Eulerian methods. The interpolation for the field velocity, the number of particles used in the simulations, the representation of boundary conditions and the mesh size for the calculation of concentrations are discussed. A field experiment using tracers is described in order to compare the numerical results and the simulations with real data. The diffusion coefficients calculated from the experiment and the hydrodynamic modelling give the necessary inputs for the simulations using the particle-tracking modelling of the measured four clouds. The results support the main advantages of this method in terms of strict mass conservation, good representation of high concentration gradients and point sources and as a consequence, a good representation of the maximum concentration and the general form of the clouds.

Keywords: particle-tracking, Lagrangian, dispersion, Setubal.

1 Introduction

Point sources in water quality problems, like rainfall runoff outlets, are difficult to represent in the so-called Eulerian methods, and the particle-tracking method may represent a good alternative for solving this kind of transport problems. In a pioneer work Chorin [1] employed the particle-tracking method, solving the Navier-Stokes equations, for determining the vorticity field of the two-



dimensional flow around a circular cylinder with high Reynolds numbers. Since then, the particle-tracking models have been applied to a wide range of engineering problems, for example, cohesive sediment transport (Vinzón and Paiva [2]); simulation of solute transport in coastal waters (Periañez and Elliot [3]). This method is included into the Lagrangian class, where the contaminant is transported as a consequence of the random movement of a large number of discrete particles. The method is free of oscillations as well as of numerical diffusion, and therefore it is also free of negative concentrations and mass loss. These problems frequently appear in the traditional finite differences or finite elements Eulerian methods, when the transport is dominated by advection, or the sources are too small related to the hydrodynamic mesh size, mainly around the sources or where strong concentration gradients take place. Particle tracking methods are particularly suited for this kind of problems (Periañez and Elliot [3]). The mesh for the calculation of the concentration is independent of the mesh used to solve the hydrodynamics, which makes it suitable for the representation of point or linear sources. The main disadvantage of the method lies in the fact that the number of particles (NP) used to represent the contaminant should be sufficient to represent the concentrations in the mesh, and then the solution may not be a smooth function, due to the stochastic nature of the dispersion stage. Nevertheless, increasing the NP can result in a significant increase of the computational time.

In this work we implemented a particle model for the passive substance transport and applied it to the case of the instantaneous injection of a dye tracer in the Setubal Lagoon, Santa Fe, Argentina. A tracer experiment was accomplished in order to evaluate the characteristic transport parameters of the receiving water body, e.g. the dispersion coefficients. The experiment involves the instantaneous release of a dye tracer and the recovery of the cloud downstream. The particle-tracking method is discussed, pointing out its main advantages and disadvantages, as well as some details of its application. The case study is described, and the modelling results are compared with field data.

2 Random walk particle-tracking method for non-homogeneous turbulence

Mathematically, the transport process can be expressed, in a one-dimensional domain, as follows:

$$x^{n+1} = x^n + \left(U + \frac{dD}{dx} \right) \Delta t + z \sqrt{2D \Delta t} \quad (1)$$

where x^{n+1} and x^n are the positions at integer time indexes $n+1$ and n , respectively, z is a random number having normal distribution with zero mean and unit variance, U is the fluid velocity and D is a non-homogeneous diffusion coefficient. The second term on the right hand of equation (1) includes the particle advection ($U \Delta t$), and a “drift” term, as a result of the non-homogeneous dispersion, due to the spatial variation of the dispersion coefficient. The third term in Eq. (1) represents the random displacement of the particles. Hathhorn [4]



has demonstrated the equivalence of results using the random number z normally as well as uniformly distributed. If one adopts a uniform distribution, this may imply a considerable computational time saving. Therefore the normally distributed random number z in the range $(-0.5, 0.5)$ can be obtained by a commonly computer generated random number r in the range $(0, 1)$, with mean 0.5 and standard deviation $\sqrt{1/12}$. In this case, the Eq. (1) must be expressed as:

$$x^{n+1} = x^n + \left(U + \frac{dD}{dx} \right) \Delta t + (2r - 1) \sqrt{6 D \Delta t} \quad (2)$$

The presence of sources is represented by the injection of a finite NP , at a rate corresponding to the simulated substance discharge. The mass of each particle i is represented by a mass quantity MP_i . The particles move at each time interval Δt due to the combined effect of advection and dispersion. When choosing the time and space steps we imposed the condition that the maximum particle path could not be greater than the cell size, thus avoiding the extrapolation of the velocity corresponding to the original position of the particle, beyond its neighbourhood. This is an important condition for non-uniform field velocities.

For a continuous source the mass is injected at each time interval under a certain rate $M/\Delta t$, and for an instantaneous source all the mass M is available at $t = 0$. In this work, the concentrations are evaluated by counting the number of particles in each grid cell, multiplying them by the mass of each particle, dividing the total mass by the cell volume and assigning this concentration value to the cell centre. The most important factors to be considered to achieve good simulations of the concentration distribution are the NP , the velocity interpolation procedure and the boundary condition prescription.

2.1 Computation of the particle velocities

For the advection of passive substances, the velocity of each particle is considered equal to the stream velocity where the particle is located, obtained by interpolation over the hydrodynamic mesh at each time step. The selected algorithm for the interpolation is a key feature of the model (Narayanan *et al.* [5]). In this work we implemented linear, bilinear and second order interpolations, based on Taylor series expansion. Using Molenkamp's classical experiment, it was observed that a second order interpolation is more accurate than the bilinear scheme, while the linear method produced a completely erratic path of the particles and, as a consequence, unacceptable errors for the advective transport.

2.2 Initial and boundary conditions

The model requires the prescription of initial and boundary conditions. The initial condition is given by the nature of the problem. For our case, a two-dimensional horizontal transport problem where the initial condition is an instantaneous linear source of dye tracer, an NP proportional to the mass injected is considered at a single point where the source is located. As regards the open boundaries, the particles are considered lost when they leave the domain. For closed boundaries, the prescribed condition is zero flux through the boundary.



3 Case study: Setubal Lagoon (Argentina)

The Setubal Lagoon is located in the alluvial valley of the Parana River (60°20'W and 60°40'W, 31° 20'S and 31° 37'S), province of Santa Fe, Argentina. It is part of a complex system composed of lagoons and creeks connected to this river. Most of the lagoon bottom is almost flat and strong bathymetric gradients are observed at the outlet reach. Its width ranges from 2000m, with a mean depth of 3m, to 300m and depths of up to 25m. The bottom is composed mainly of silt and clays and, to a less extent, of fine sand. On the right margin (RM) of the lagoon, along 5 km, Santa Fe city (360,000 inhabitants) is situated. Along this coast there are storm drains, and mixing of the rainfall water with sewer discharges causes environmental concerns, since the lagoon beaches are used for recreational purposes and a water intake for the city water supply is located downstream. Figure 1 shows the location of Setubal Lagoon and the position of the main storm drainage pipes. Several studies have been done related to the water quality problem of the Setubal Lagoon. Tessi *et al.* [6] described the high bacterial contamination indexes in the waters and sediments at the beaches, which match the maximum values established by the European standards (WHO [7]) and were adopted as a policy by the local Government. These facts motivated the need of studying the contaminant dispersion dynamics.

A dye tracer experiment was performed with this objective, and the tracer clouds were simulated using a 2-DH particle-tracking model. The hydrodynamics of the lagoon was calibrated and used for simulating the flow occurring during the experiment.

3.1 Tracer experiment

At the point indicated in Figure 1, an instantaneous tracer injection was done, using two tracers, Amidorhodamine G (Acid Red 50, colour index 45220) and Uranine (Acid Yellow, colour index 45350). At 11:21 a.m., 1.0 kg of Amidorhodamine G and 1.0 kg of Uranine, dissolved into 70 litres of water, were released from a boat. Based on previous results from the hydrodynamic model (Trento *et al.* [8]), five cross sections (*A*, *B*, *C*, *D* and *E*) were established for measurements, at about 1000, 2700, 4200, 6000 and 8000m from the injection point. At each cross section, the boat moved forward and backward, using DGPS for positioning (with an estimated error of about 5m). For the tracer cloud detection, water was continuously pumped through two serial fluorimeters, one equipped with filters for detection of Amidorhodamine G and the other for Uranine. Considering the low depth of the lagoon (about 3m), the measurements were carried out only at middle depth, expecting a complete mixing in the water column. A vertical profile for each cloud was measured in order to verify this hypothesis.

Water samples (400) were also collected for laboratory analyses. The minimum detection limit of the tracer under laboratory conditions was 0.05 ppb (0.05 mg/m³), while for the on site detection it was ~0.2 ppb. The results obtained from the laboratory analyses were complemented with the on site



measurements. The samples were collected at 10s intervals at the cross sections *B* and *C* and every 20s at the cross sections *D* and *E*. As the laboratory analyses showed that the cloud at cross section *A* was poorly measured, it was not taken into account. Furthermore, only the tracer Amidorhodamine G was considered, since the tracer Uranine showed significant losses. These losses can be related to the long storage time (approximately 3 months) between the experiment and laboratory analyses. The clouds were thus measured in a Eulerian way, recording the curves as the substance passed through a particular cross section for each cloud. In order to reconstitute the clouds in a Lagrangian way, the flow velocity was then determined as the distance and time between the maximum concentrations of two consecutive clouds. The new coordinates of each cloud point were evaluated according to $X_i' = X_i + u_x (t_i - t_0)$ and $Y_i' = Y_i + u_y (t_i - t_0)$ where X_i' , X_i , and u_x are the new and original coordinates and velocity in the East-West direction; Y_i' , Y_i , and u_y are the new and original coordinates and velocity in the North-South direction; t_i is the i -th sampling time and t_0 the time corresponding to the occurrence of the maximum concentration in the cloud.

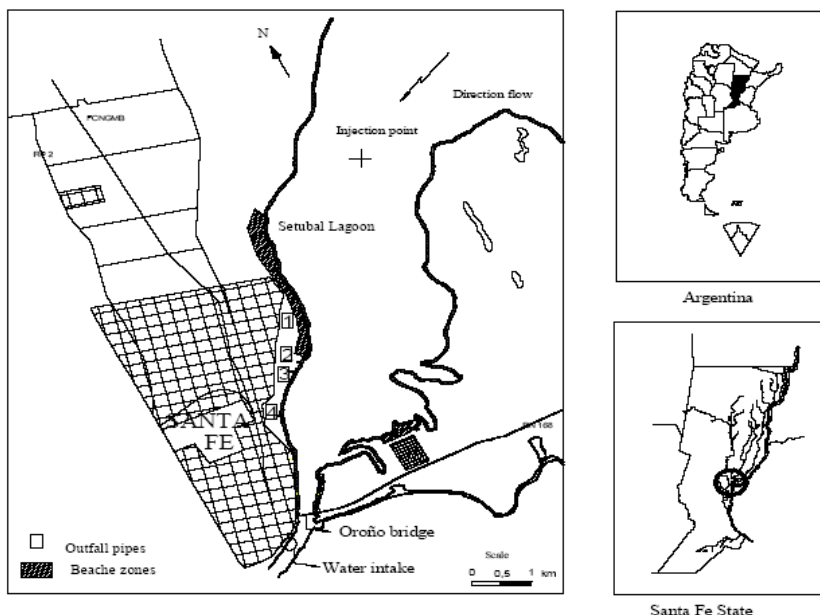


Figure 1: Geographic location of the Setubal Lagoon and the main four storm water pipes.

3.2 Dispersion coefficients from the field data

According to Holley and Jirka [9], for natural flows it is more adequate to adopt a “longitudinal” axis, following approximately the mean longitudinal flow direction, and a “transverse” axis, orthogonal to it, than a geographic coordinate

system (North-South Y axis and East-West X axis). Considering the longitudinal and transverse concentration distributions, if they follow a Gaussian profile, it is possible to adopt the method of the moments (Harleman [10]) to determine the longitudinal and transverse dispersion coefficients. The symmetrical form of the clouds B, C and D indicated a Gaussian behaviour, thus justifying the use of this method. Once the longitudinal (S_L^2) and transverse (S_T^2) variances were obtained, the dispersion coefficients for each cloud were evaluated using the following relationships:

$$D\varepsilon = \frac{\Delta S_L^2}{2T_d} \tag{3}$$

$$D\eta = \frac{\Delta S_T^2}{2T_d} \tag{4}$$

where ΔS_L^2 and ΔS_T^2 are the differences in the longitudinal and transverse variances between two successive clouds, respectively, and T_d is the effective diffusion time, or time associated to the transit of their maximum concentration. These results are shown in Table 1.

Table 1: Effective diffusion time (T_d), longitudinal (D_ε) and transverse (D_η) dispersion coefficients.

	<i>X</i> (m)	<i>Y</i> (m)	<i>C</i> _{max} (ppb)	<i>T</i> _d (s)	<i>Dist</i> (m)	<i>S</i> _L ² (m ²)	<i>S</i> _T ² (m ²)	<i>D</i> _ε (m ² s ⁻¹)	<i>D</i> _η (m ² s ⁻¹)
Injection	1950	8846	----	----	----	----	----	----	----
Cloud B	1539	6246	25.19	10200	2632	7355	468	0.36	0.023
Cloud C	1595	4798	12.67	15900	4063	24289	542	0.76	0.017
Cloud D	1344	3006	6.64	21060	5871	60472	456	1.43	0.011
Cloud E	848	1098	2.21	26310	7953	----	----	----	----

4 Numerical simulation of the clouds

The hydrodynamic model is two-dimensional, vertically averaged and based on finite differences (Borche Casalas [11]). The modelling domain was defined in order to cover the area of the tracer experiment. It was divided into 3456 square elements of 100m lengths. The adopted time interval according to a stability condition was 15s. The bathymetry was surveyed for the modelling purpose in a mesh that ranged from 25m to 100m. The surface slope, the wind velocity and the discharge for the hydrodynamic conditions occurring during the tracer experiment were measured, resulting in 0.025 cm/km, 6 kmh⁻¹ in the NE direction, and 1560 m³s⁻¹, respectively. With these data, the Manning coefficient *n* was adjusted in a value of 0.028 sm^{-1/3}. Figure 2 shows the bathymetry and the velocity field computed and used for the transport model. The dispersion coefficients considered were those evaluated from the tracer experiment, shown in Table 1. The coefficient obtained for the reach C-D was also considered for the reach D-E. The time step for the transport was 30s. The interpolation of the velocity and depth for each particle position was obtained following the bilinear scheme. The boundary condition at the lagoon margins was of zero flux. The

tracer mass, $M=1000$ g, was represented by 25000 particles of equal mass, while the concentrations of each cloud were calculated over a mesh with $\Delta x = \Delta y = 50$ m. The choice of that particle number is a compromise between the mesh size and the representation of the maximum concentrations observed in each cloud.

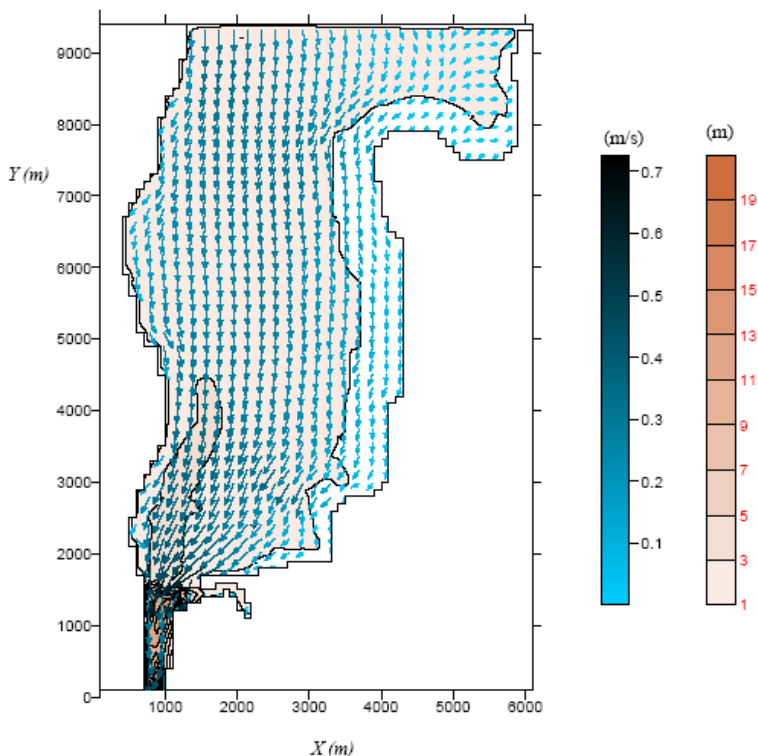


Figure 2: Bathymetry and velocity field obtained with the hydrodynamic model for the flow conditions occurring during the tracer experiment.

The results obtained with the transport model are shown in Table 2, in terms of the coordinates X and Y of the centre of mass of each cloud and their corresponding maximum concentrations. Cloud E has a smaller width than the preceding clouds probably due to the stretching produced when entering in the convergent South part of the lagoon. Considering the variances calculated from the model results for cloud E , starting at the injection point, $\sigma_e^2(t)=83065 \text{ m}^2$ and $\sigma_{\eta}^2(t)=239 \text{ m}^2$, the dispersion coefficients would be $D_e=1.579 \text{ m}^2\text{s}^{-1}$ and $D_{\eta}=0.004 \text{ m}^2\text{s}^{-1}$. Considering the variances between successive clouds, a negative value D_{η} would be obtained for cloud E . We verified a non-linear relationship for variance and time for the transverse direction, indicating that the dispersion process is not “Fickian” at this particular reach of the lagoon. The positions of

the clouds *B*, *C*, *D* and *E*, measured and computed, displayed in Table 1 and Table 2, respectively, are shown in Figure 3. The differences in the position of the centre of mass were 32, 37, 27 and 51m. It is important to stress that the measured clouds were actually re-constructed from the passage curves, as explained before. This means that the velocities at all the cloud points were considered uniform and equal to the mean velocity of the whole cloud in the foregoing reach. Table 3 shows a comparison of the maximum concentrations calculated, where we also included all the interpolation schemes (linear, bilinear and second order), which show non-significant differences between them.

Table 2: Results of the numerical simulation: coordinates of the centre of mass and maximum concentrations for clouds *B*, *C*, *D* and *E*.

	X (m)	Y (m)	Cmax (ppb)
Injection Point	1950	8846	
Cloud B	1525	6275	24.48
Cloud C	1625	4775	13.20
Cloud D	1325	3025	6.81
Cloud E	816	1058	1.49

In order to compare the model results using the dispersion coefficients obtained experimentally and those calculated according the classical equations by Elder [12] for turbulent flows in channels, the model was implemented using the following expression for longitudinal ($D_e = 5.93 u_* H$) and transverse ($D_\eta = 5.93 u_* H$) dispersion coefficients, where u_* is the shear velocity ($= \sqrt{\tau_0 / \rho}$), τ_0 is the bottom shear stress and ρ the fluid density. The result of this application is also included in Table 3. The results are similar to those previously obtained. In this case the differential advection is only significant in the flow direction, as the transverse velocity gradients are low, and thus it would match the Elder's hypothesis of turbulent diffusion in the transverse direction.

Table 3: Maximum calculated and measured concentrations (ppb) with the interpolation schemes (linear, bilinear and second order).

Cloud	Velocity Interpolation Scheme			Elder coef. and Bilinear Velocity Interpolation Scheme	Maximum Measured Concentrations
	Linear	Bilinear	Second Order		
B	23.98	24.48	24.37	25.16	25.19
C	14.36	13.20	13.15	17.10	12.67
D	6.83	6.81	6.69	10.65	6.64
E	1.81	1.49	1.44	1.62	2.21

5 Conclusions

The particle-tracking method allows a strict mass conservation and the representation of high concentration gradients without spurious oscillations or numerical diffusion. The method is also flexible for calculating the results in a



grid independent from the hydrodynamic method. This also represents an advantage for the kind of applications of interest, where generally the size of the cloud or plume is smaller than the size of the mesh used for solving the velocity field. Besides considering an adequate size for this post-processing grid, compatible with the scale of the transport problem, special care must be taken in the number of particles selected for the simulation. The relative error of the solution decreases in a quadratic way with the increase of the number of particles, and therefore it is convenient to identify an optimum number of particles to be employed. It was shown by an example that decreasing the number of particles and checking the relative differences between their solutions can achieve this.

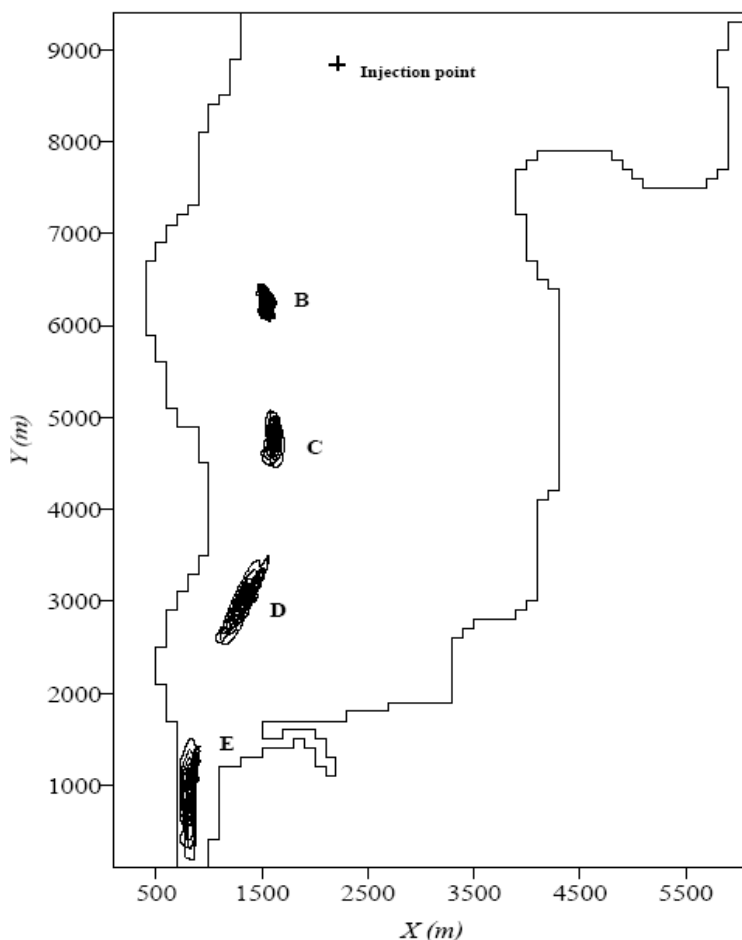


Figure 3: Comparison between the solution of the numerical model (dashed lines), and measured clouds (continuous lines) due to an instantaneous injection.

The method was applied to the case of a point tracer injection held in Setubal lagoon, Santa Fe, Argentina. The flow in this case showed a strong dominance of the longitudinal dispersion related to the transverse one. The model was implemented considering the longitudinal and transverse dispersion coefficients, and from theoretical results. The obtained results, in both cases, represent in an adequate way the concentration of the centre of mass and the general shape of the clouds.

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References

- [1] Chorin, A.J., Numerical study of slightly viscous flow, *J. Fluid Mech.*, v. 57 (4), pp. 785-796, 1973.
- [2] Vinzón, S. & Paiva A.M., Modelling the Sediment Concentration Profiles at the Amazon Shelf, *Fine Sediment Dynamics in the Marine Env., Proc. In Marine Science*, 5, J. Winterwerp & C. Kranenburg (eds.), Elsevier, 2002.
- [3] Periañez R. & Elliot A.A., Particle-tracking method for simulating the dispersion of non-conservative radionuclides in coastal waters, *J. Env. Radioactivity*, v. 58, pp.13-33, 2002.
- [4] Hathhorn W., Simplified approach to particle-tracking methods for contaminant transport, *J. Hydr. Eng.*, v. 123 (12), pp. 1157-1160, 1997.
- [5] Narayanan C. D. Lakehal & Yadigaroglu G., Linear stability analysis of particle-laden mixing layers using Lagrangian particle-tracking, *Powder Technology*, v. 15, pp. 122-130, 2002.
- [6] Tessi M. A., Lura M. C., Godoy P. G., Minetti M. L., Rafaghelli de Ramon R. C. & Mir A., Bacterias Indicadoras de Contaminación en las Aguas y Sedimentos de la Cuenca Del Paraná Medio (Zona Santa Fe-Paraná), *Rev. Fac. Ing. Química, Santa Fe*, v. 40, pp. 81-98, 1972 (in Spanish).
- [7] World Health Organization, *International Digest of Health Legislation*, v. 27 (4), pp 709-918, 1976.
- [8] Trento, A., Vinzón, S., Borche, A., Alvarez, A. & Venturini, V., Modelación Bid. del Transporte de Colif. Fec. en la Laguna Setúbal (Argentina), in *Proc. XVII Cong. Latin. Hidr.*, Guayaquil, Ecuador. v. 3, pp. 353-364, 1996 (in Spanish).
- [9] Holley E.R. & Jirka G. H., Mixing in Rivers, *Technical Report E-86-11*, US Army Engineer Waterways Exp. Station, Vicksburg, Mississippi, 1986.
- [10] Harleman, D.R.F., *Transport Processes in Environmental Engineering, lecture notes*, Parsons Hydrodynamics Lab., MIT, Cambridge, 1988.



- [11] Borche Casalas, A., Modelo Matemático de Correntología do Estuario do Rio Guaíba, *Caderno de Rec. Híd. No. 12*, IPH/UFRGS, 68 pp, 1985 (in Portuguese).
- [12] Elder, J. W., The dispersion of marked fluid in turbulent shear flow, *J. Fluid Mech.*, v. 5 (4), pp. 544-560, 1959.

