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Tridimensional Simulation of Pollutant Dispersion in Water Bodies

P.C.S. Jucá and C.R. Maliska
Computational Fluid Dynamics Laboratory - SINMEC
Mechanical Engineering Department - UFSC
88040-900 - Florianópolis, SC , Brasil

ABSTRACT

This work presents a numerical model for the simulation of tridimensional dispersion of chemical and thermal pollution in water bodies. Among the strategies used for eliminate pollutants, the dispersion in water bodies is frequently employed. The prediction of this dispersion is, therefore, of extreme importance for establishing the environmental regulations related to the disposal of pollutants in water bodies. The tridimensional model advanced here uses boundary-fitted grids and a finite-volume technique. As a test problem the dispersion of a thermal jet issued into a cross-flow is calculated, demonstrating that the complex phenomenon of the interaction of the buoyant jet and the cross-flow is correctly predicted. The influence of the bottom over the dynamics of the jet is investigated. The results demonstrated that the existing numerical techniques can be used to model the complete field in environmental flows.

1. INTRODUCTION

Due to the technological evolution of the human kind, new points of residuals (toxic or non toxic) are added to the ecological system daily, and the elimination and/or dispersion of these residuals can't be left to the processes supplied by the natural ecosystems. In particular, the hidrosphere receives a great quantity and diversity of residuals in many ways, mainly in the form of waste waters. The potential damage that each residual can offer to local ecosystems depends upon factors that range from quantity, concentration, presence of others sinergetics compounds and, mainly, on its own nature.

The dispersion process of pollutants is usually done discharging them in large water bodies or rivers, through structures that can promote an adequate mixing, and consequent dilution of the pollutant to acceptable levels. This process is closely related with the geometry, relative position of the discharging structure and, of course, the dynamic behavior of the discharge imposed by the momentum and buoyance forces present in the process, see (Jirka and Doneker, 1991).

When a pollutant discharge occurs in a water body, basically three different flow regimes can be observed. The region near the discharge, where the momentum forces dominates the flow, is called near field and the flow behaves like a simple jet characterized mainly by the physical parameters of the discharging point and of the ambient conditions of the receiving water. In special, if the pollutant is something which can modify the local density, buoyance forces are present and become dominant far from the discharging point, imposing the dynamics of the flow. This is called the far field region. An intermediate (field) region can be observed, were the momentum forces and buoyance forces are comparable. Although there are no physical parameters that can clear split these regions, (Dunn et al., 1975), point out some characteristics of each one.

In a buoyant jet discharged in a water body, the type of problem solved as example in this work, different but interdependent basic physical processes can be identified. The ability of the model in incorporating these phenomena will be a measure of its confidence. The governing physical phenomena, see Fig. 1, present in a buoyant jet discharge are:

a) the entrainment of ambient fluid;

b) the interaction between the discharge and the cross-flow ambient water and wind currents;

c) superficial exchanges of mass and heat;

d) interaction with physical boundaries (bottom and shores);

e) estratification of the receiving water body and

f) the lateral and vertical dispersion due to momentum and buoyance forces.

The prediction of all these interactions is a challenging task for the environmental analist.

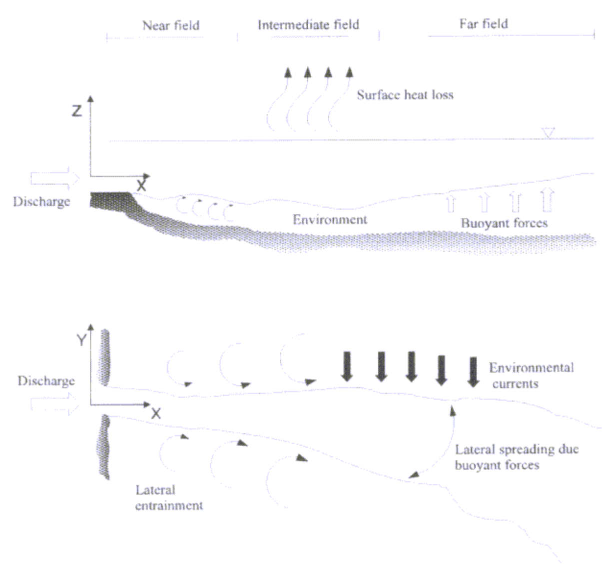

Fig. 1 - Physical processes in a buoyant jet discharge

2. THE APPROACH USED IN THIS WORK

The effluent dispersion in water bodies can be studied using hydraulic or mathematical modelling. Field studies can also be employed to enhance the knowledge of the phenomena to support the construction of more sophisticated models.

Hydraulic modelling have been used in the past years in a large diversity of sites and situations and the basics of this techniques is reported by Kobus, (Kobus, 1980). These models are expensive to build and maintain, but easy to operate. The most severe restriction is that they are dedicated to specific physical site and can't be easily modified to deal with other different sites. Moreover, scalling are never fully satisfied. Pinheiro (Pinheiro, 1993) presents a review of the state-of-art of the physical modelling of the discharge of jets and plumes in inland waters.

The mathematical approach can be done by phenomenological modelling, integral or differential (numerical) and stochastic models, as reported in (Fisher et al., 1979), (Adams, 1981), (Schatzmann, 1979). A discussion about the basics of each one and the main difficulties involved in reproducing with fidelity the physical phenomena can be seen in (Jirka, 1975).

Among the mathematical methods, the differential approach seems, at least in the few past years, the most promissing one. This is the method that require less simplificating hipothesis over the governing equations and so can reproduce with more fidelity the physical phenomena. The price to be paid is the complexity of the equations to be solved and of the computational code associated with the numerical solution. The differential models solve the PDE's that governs the transport of momentum, energy and concentration in a choosen domain, once the boundary conditions for each variable is well known and established.

Most of the early developed mathematical models were dedicated to each region and only a few, according to (Fisher et al., 1979), (Jirka et al., 1975), (Adams et al., 1981), and (Dunn et al 1975), deal with the complete field. However, only complete field models can fully predicted the phenomena, as pointed out by (Dunn et al., 1975).

The adequate treatment of the different scales of time and length involved in the physical phenomena present in the three different regions were one of the challenging aspects in developing complete field models. Nowadays, the existing numerical approaches can treat the domain through variable spaced meshes, adequating the refinement to the scales of each sub-domain. Boundary-fitted coordinate (BFC) also allows easy treatment of boundary conditions and improves the ability of the model to deal with different discharge geometries or sites.

There are several numerical methods avaiable in the open literature that can be applied for these problems. In this work it's used a finite-volume method, using BFC with structured meshes. The starting model for thermal discharge was proposed by (Maliska et al., 1987). Following, (Dihlmann et al., 1989), developed models for simulating atmospheric plumes dispersion and (Jucá et al., 1989), proposed a 3D model applied to thermal and pollutant dispersion. This work presents a 3-D model to deal with the discharge of pollutants in water bodies and is a continuation of the efforts to improve numerical codes for simulation of environmental flows. In particular, heat rejection from thermal plants are considered, taking into account the complexity introduced in the flow dynamics when buoyance forces are present.

3. THE MATHEMATICAL MODEL

The physical phenomena involved in a buoyant jet discharge in a water body are governed by the mass conservation principle, the Navier-Stokes equations, energy conservation equation and equations for the conservation of the chemical species. In a general curvilinear coordinate system (ξ,η,γ) these equations can be written as

$$\begin{aligned}\frac{1}{J}\frac{\partial(\rho\phi)}{\partial t} &+ \frac{\partial}{\partial\xi}(\rho U\phi) + \frac{\partial}{\partial\eta}(\rho V\phi) + \frac{\partial}{\partial\gamma}(\rho W\phi) = -\hat{P}^{\phi} + \hat{S}^{\phi} \\ &+ \frac{\partial}{\partial\xi}\left[\left(\alpha_{11} J \mu_{ef}\frac{\partial\phi}{\partial\xi}\right) + \left(\alpha_{12} J \mu_{ef}\frac{\partial\phi}{\partial\eta}\right) + \left(\alpha_{13} J \mu_{ef}\frac{\partial\phi}{\partial\gamma}\right)\right] \\ &+ \frac{\partial}{\partial\eta}\left[\left(\alpha_{21} J \mu_{ef}\frac{\partial\phi}{\partial\xi}\right) + \left(\alpha_{22} J \mu_{ef}\frac{\partial\phi}{\partial\eta}\right) + \left(\alpha_{23} J \mu_{ef}\frac{\partial\phi}{\partial\gamma}\right)\right] \\ &+ \frac{\partial}{\partial\gamma}\left[\left(\alpha_{31} J \mu_{ef}\frac{\partial\phi}{\partial\xi}\right) + \left(\alpha_{32} J \mu_{ef}\frac{\partial\phi}{\partial\eta}\right) + \left(\alpha_{33} J \mu_{ef}\frac{\partial\phi}{\partial\gamma}\right)\right]\end{aligned} \qquad (1)$$

In the Eq. (1) U,V,W are the contravariant components of the velocity vector given by

$$\begin{aligned}U &= (u\xi_x + v\xi_y + w\xi_z)\, J^{-1} \\ V &= (u\eta_x + v\eta_y + w\eta_z)\, J^{-1} \\ W &= (u\gamma_x + v\gamma_y + w\gamma_z)\, J^{-1}\end{aligned} \qquad (2)$$

where the α_{ij} are the components of the metric tensor and J the jacobian of the coordinate transformation. The ϕ represents the dependent variables for each conservation equation. For $\phi = 1, u_1, u_2, u_3$, T or C_i the mass conservation equation, momentum in x, y and z cartesian coordinates directions, energy and concentration of chemical species are recovered, respectively. Γ represents the diffusivity transport coefficient, being zero for the mass conservation equation and equals to the viscosity for the Navier-Stokes equation. For the energy equation Γ is equal to k/c_p and for a chemical specie it's the product of the density times the mass diffusivity.

The source term P^ϕ is zero for the mass and energy conservation equations. For the Navier-Stokes equations it's given by

$$\hat{P}^{u_i} = \left[\frac{\partial \overline{p}}{\partial \xi} \overline{\xi}_i + \frac{\partial \overline{p}}{\partial \eta} \overline{\eta}_i + \frac{\partial \overline{p}}{\partial \gamma} \overline{\gamma}_i \right] \tag{3}$$

where the subscript indicates partial derivative in the the "i-th" cartesian direction. The source term S^ϕ is zero for mass, energy and species conservation equations. For the Navier-Stokes equations it's written as

$$\hat{S}^{u_i} = \frac{\mu}{3} \left[\frac{\partial (\nabla . \vec{V})}{\partial \xi} \overline{\xi}_i + \frac{\partial (\nabla . \vec{V})}{\partial \eta} \overline{\eta}_i + \frac{\partial (\nabla . \vec{V})}{\partial \gamma} \overline{\gamma}_i \right] + \rho g_i \tag{4}$$

where the term related to the buoyance forces is present only in the case when non-isothermal flows are considered. For the discharges considered herein, the gravity vector was aligned with the z cartesian direction.

In this work the Boussinesq approximation to deal with the buoyance forces is not used. The density is variable in each term of the governig equations and the state equation employed was suggested by Gebhart and Mollendorf, 1977, relating density and temperature by

$$\rho = 999.9720 \left[1 - 9.297173 \times 10^{-6} \, (T - 4.029325)^{1.894816} \right] \tag{5}$$

Eq. (1) representing the system of partial differential equations governing the pollutant dispersion is integrated in time and in a 3D elemental control volume. The pressure-velocity coupling is handled using the SIMPLEC method of (Van Doormaal and Raithby, 1984) applied in the contest of the all speed flow methodology described by (Silva and Maliska, 1986). Fictitious control volumes are used for the applications of the boundary conditions. The resulting linear system of equations are of the form

$$\begin{aligned} A_p \Phi_p = {} & A_e \Phi_E + A_w \Phi_W + A_n \Phi_N + A_s \Phi_S + A_d \Phi_D + A_f \Phi_F \\ & + A_{ne} \Phi_{NE} + A_{se} \Phi_{SE} + A_{nw} \Phi_{NW} + A_{sw} \Phi_{SW} + A_{de} \Phi_{DE} + A_{fe} \Phi_{FE} \\ & + A_{dw} \Phi_{DW} + A_{fw} \Phi_{FW} + A_{dn} \Phi_{DN} + A_{ds} \Phi_{DS} + A_{fn} \Phi_{FN} + A_{fs} \Phi_{FS} + b_p \end{aligned} \tag{6}$$

for $\phi = 1, u_1, u_2, u_3$, T or C_i. An equation for pressure is derived from the mass conservation equation using the SIMPLEC method. Due to 3D nature of the problem, numerical details and expressions of the coefficients are not given. Details can be found in (Jucá, 1994), (Marchi, 1992) and (Maliska, 1995). The code Navier (SINMEC, 1992) was used as a starting point. To deal with turbulent flows a k-ε model and a simple algebraic model was implemented. In this paper, however, only results for laminar flows are considered.

4. TEST CASES

In order to check the confidence of the mathematical model and in the modified computational code, some of the hydraulic model studies carried out by (Carter et al., 1974) at Chesapeake Bay Institute are simulated. Carter used a 40x10x1 ft flume, with a retangular discharge opening oriented at right angles with respect to a uniform flow along the length of flume, as show in Fig 2.

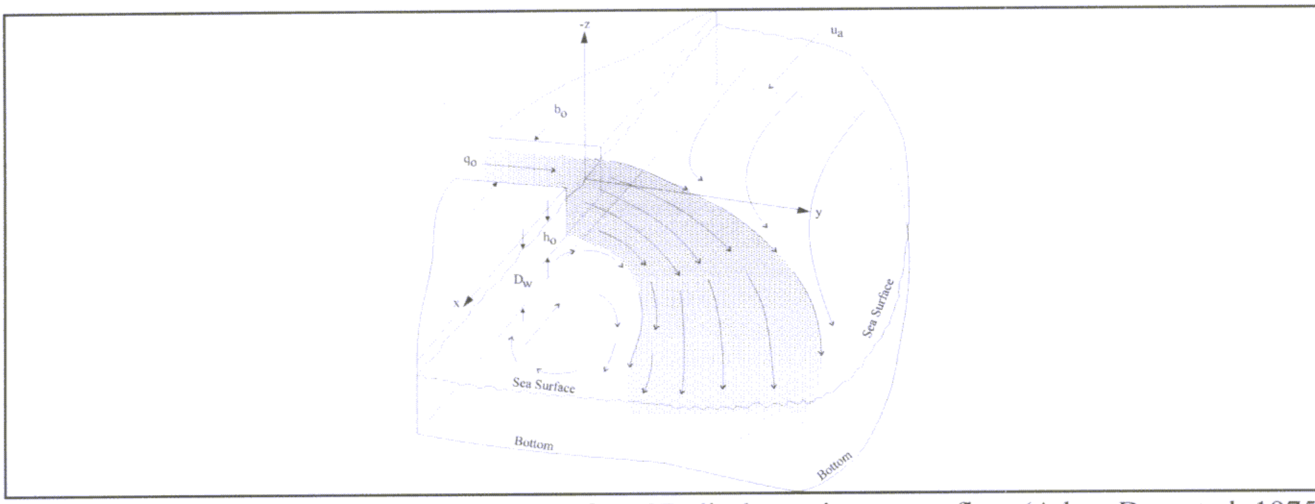

Fig. 2 - Esquematic drawing of a buoyant surface 3D discharge in a cross-flow.(Adap. Dun et al. 1975)

Three different runs were select to test the numerical model. Basicaly the runs selected were the same, except for the ratio of the depth of receiving water (D_w) to the outfall depth (h_0). The densimetric Froude number, defined as,

$$F = \frac{q_0}{\left(\frac{\Delta\rho}{\rho g h_0}\right)^{1/2}} \tag{7}$$

was taken about 8.9, where q_0 is the inlet velocity of the jet. The aspect ratio of the outfall (h_0 / b_0) was taken as 0.37. Other details of these runs are listed in Table 1. With all conditions kept constant and varying the D_w/h_0 relation, the near bottom influence in the flow dynamics can be analyzed. The Reynolds number were defined as

$$R_e = \frac{\rho \; q_0 \; h_0}{\mu} \tag{8}$$

For all runs the viscosity was taken as a constant and equals to 10^{-3} N/ms and the ambient density as defined by Eq. (5) for the ambient temperature of 20°C. The discharge temperature was 25.55 °C, what means a 10°F above the ambient temperature, as employed by (Carter et al., 1974).

The numerical domain was taken 2m wide and 3.82 long, with the depth defined in Table 1, for each run.The center of the discharging point was located 0.814 m downstream the ambient entrance section. Previous numerical tests had shown that this dimensions are sufficient far from the discharging point to avoid interference in the local flow dynamics. The discretization mesh was 70x45x5, 70x45x9 and 70x45x10 volumes for cases B, M, and G, respectively. The volumes were highly concentrated near the outfall. Upstream and dowstream volume distribution follow a suitable geometric relation.

Non-slip velocity boundary conditions were imposed to the walls and bottom of the flume. In the ambient entrance section a uniform velocity profile was imposed and in the exit section a local parabolic boundary condition. The water surface is coincident with (x,y) directions and at this boundary a local parabolic boundary condition for the u_1 and u_2 cartesian velocity components was imposed. No mass was allowed to leave the domain at this boundary, imposing a zero value for W, the contravariant component of the velocity vector.

Table 1 - Test run cases parameters

TEST	D_w (m)	D_w / h_0	h_0 (m)	b_0 (m)	h_0 / b_0
B	0.0509	0.96	0.0530	0.0198	2.6769
M	0.1015	1.94	0.0524	0.0198	2.6462
G	0.2539	4.76	0.0533	0.0198	2.6923

TEST	q (m/s)	U_a (m/s)	(q / U_a)	F	R_e
B	0.241	0.054864	4.377	8.92	12,799
M	0.244	0.054864	4.428	9.08	12,767
G	0.238	0.054864	4.352	8.82	12,765

5. RESULTS

The center line position of the jet at the surface for the runs B,M and G can be seen in the Fig 3 to 5 plotted against the data from (Carter et al., 1974). In these figures the coordinates were made dimensionless with respect to the outfall depth (h_0). As can be seen, the model shows very good agreement for the runs M and G, while for the run B it predicts a centerline position more attached to the wall.

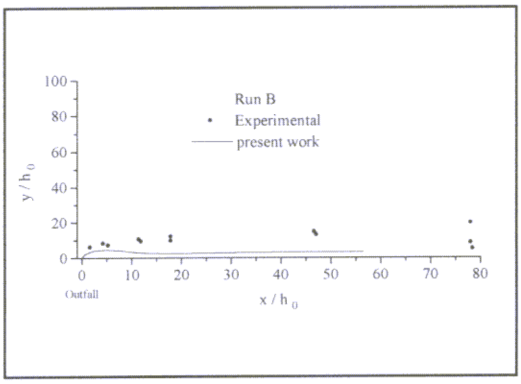

Fig. 3- Centerline position. Run B

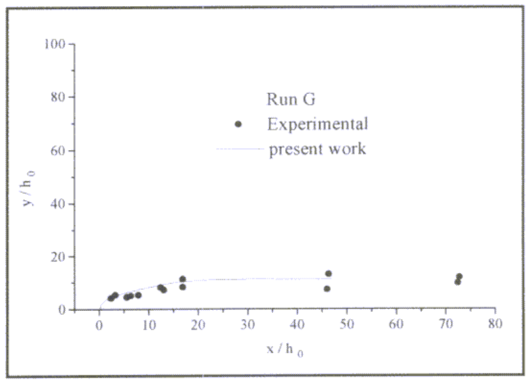

Fig. 4 - Jet centerline position. Run G

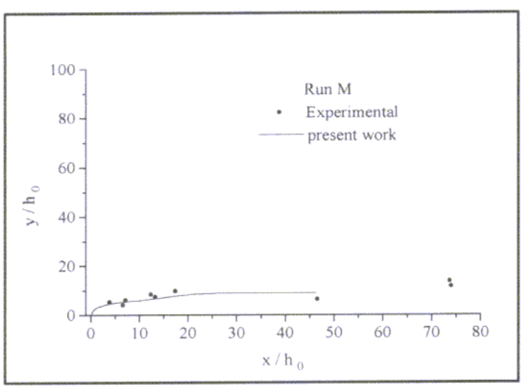

Fig. 5 - Jet centerline position. Run M

However, in Run B, as expected for the relation D_w/h_0 equal to one, a total deviation of the cross flow current near the outfall occurs. As a consequence a strong surface recirculation pattern is observed donwstream the outtfall, what causes the observed attachment of the center line to the wall. This recirculation can be seen, for the surface plane, in Fig 6.

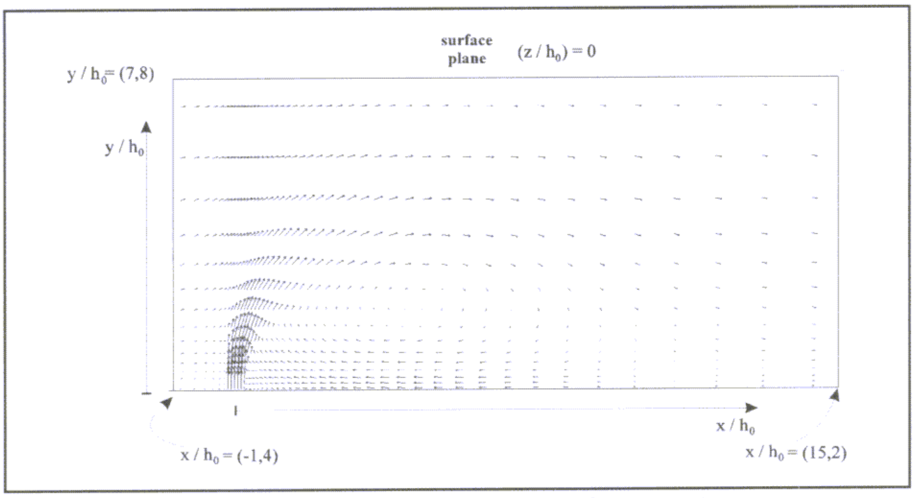

Fig. 6 - Surface flow pattern for Run B

For the runs M and G, where D_w/h_0 is greatter than unit, the crossflow is able to pass under the jet, what reduces the intensity of the recirculation in the superficial plane just downstream the outfall. However, the flow pattern that is established is more complex. Part of the crossflow passes under the jet and immediately after the outtfall, depending upon the magnitude of D_w/h_0, and part of it recirculates up to the surface and once there, due to the entrainment caused by the momentum forces in the jet, recirculates upstream. This flow pattern allows to the jet centerline to be more appart from the wall. This condition offers an intersting flow pattern showed in Fig 7. In a glance, we could suppose that a mass source is present just donwstream the outfall. Indeed a more appropriate 3D visualization shows that at this point the flow is coming up after have been deviated toward the botton by the jet. The upward flow separates in two parts. One recirculates upstream and other follows donwstream without any considerable contribution for the pollutant dilution.

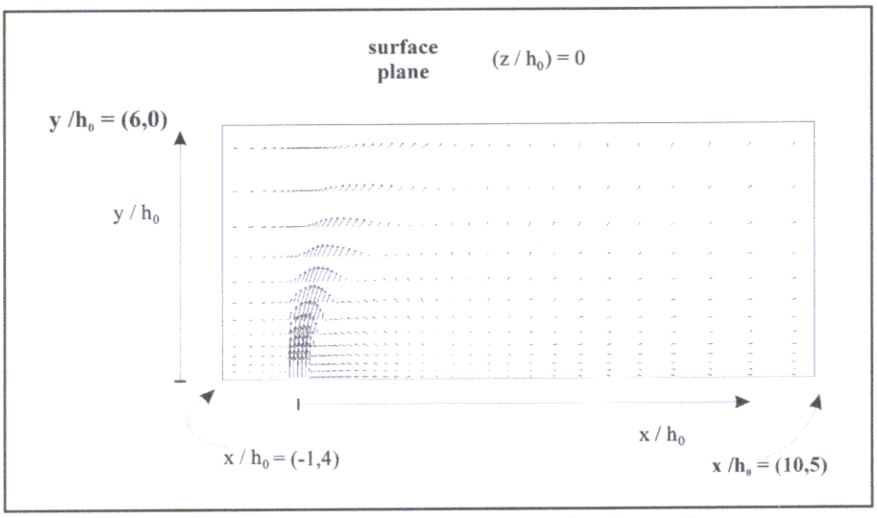

Fig. 7 - Surface flow pattern for Run G

Figs. 8 to 11 shows the centerline decay temperature for the 3 runs against the experimenal data from (Carter et al. 1974). The centerline decay temperature is defined as:

$$\frac{\theta_c}{\theta_0} = \frac{T_{centerline} - T_{amb}}{T_{outtfall} - T_{amb}} \tag{9}$$

In these cases a poor agreement was achieved, and a faster temperature decay is predicted in all the runs. However, the correct tendency is achieved in all cases. It should be noted, however, that the experimental data do not show a decay asymptotically to zero, but seems to reach a constant value far away from the outfall (S/h_0 = 80), what does not sound as physicaly correct. Unfortunatelly, the original data from Carter wasn't avaiable for a deeper evaluation.

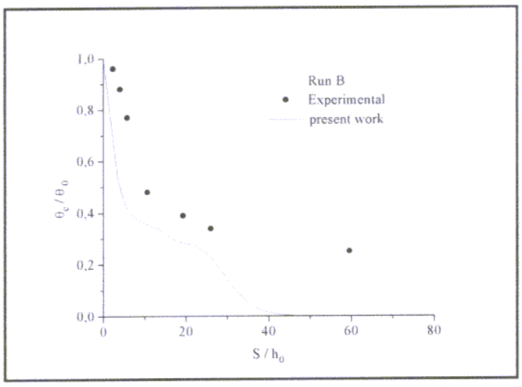

Fig. 8 - Temperature centerline decay.

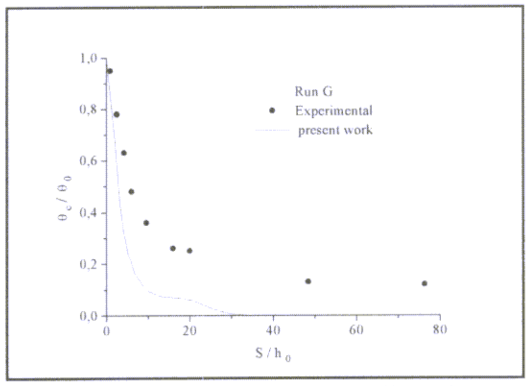

Fig. 9 - Temperature centerline decay

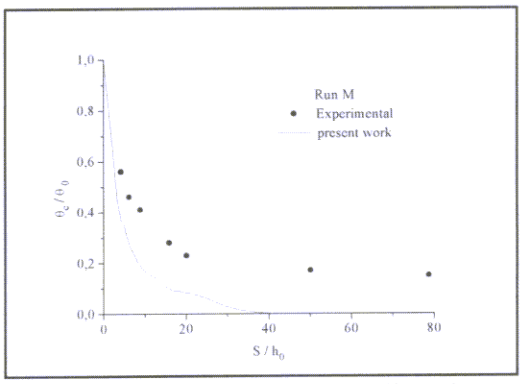

Fig. 10 - Temperature centerline decay

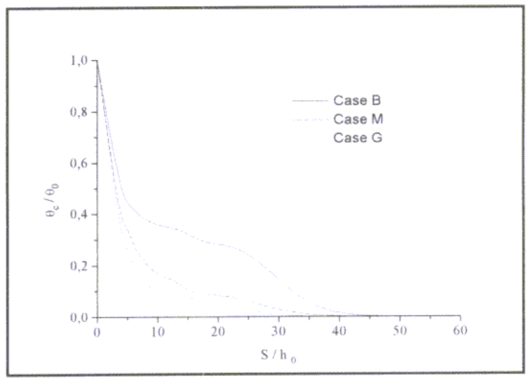

Fig. 11- Temperature centerline decay

Fig. 11 resumes all the results for the centerline temperature decay. These show that in the Run B, due the blockage of the cross-stream and the resulting strong recirculation just donwstream the outfall, the temperature decay is smoother than in the cases where the water body is deeper. In the last case the dilution occurs faster. This fact points out the importance of 3D modelling in the prediction of environmental flows.

Figs 12 and 13 shows the isotherms for the Runs B and G for the surface and for the z/h_0 = 1 planes. The comparison shows that in the deeper case the dilution is more efective and less close to the shore.

6. CONCLUSIONS

This paper described a 3D numerical model using a finite-volume technique in BFC for the solution of environmental flows. The iteraction of the jet issued from a wall with a cross-stream current

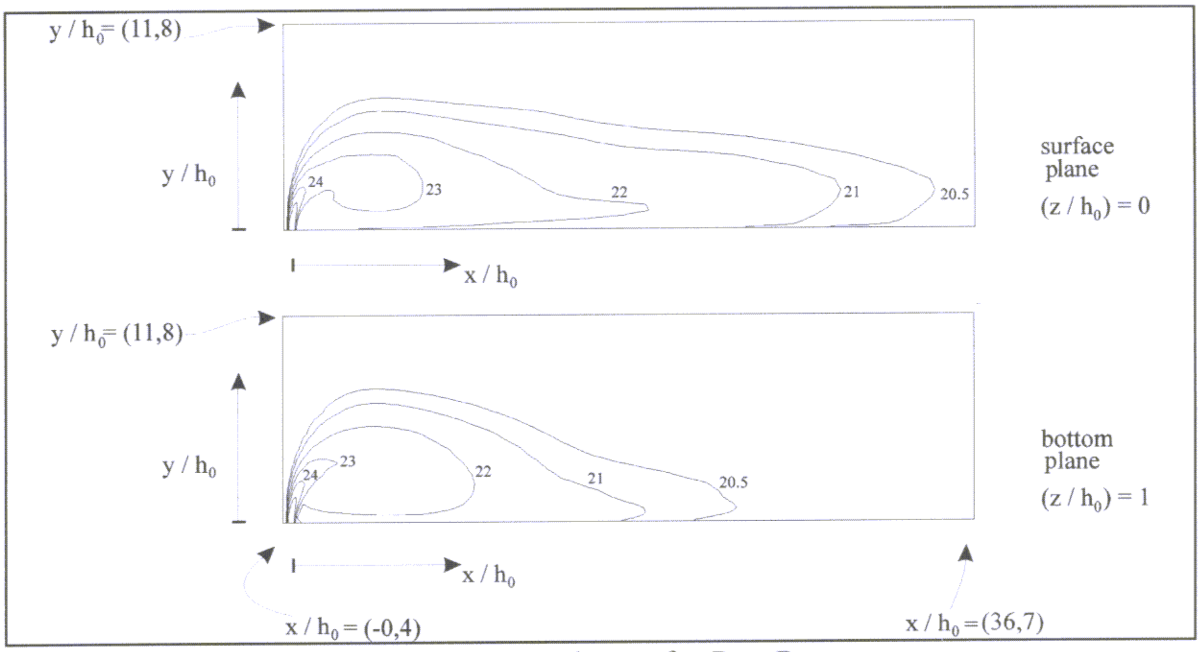

Fig. 12 - Isotherms for Run B

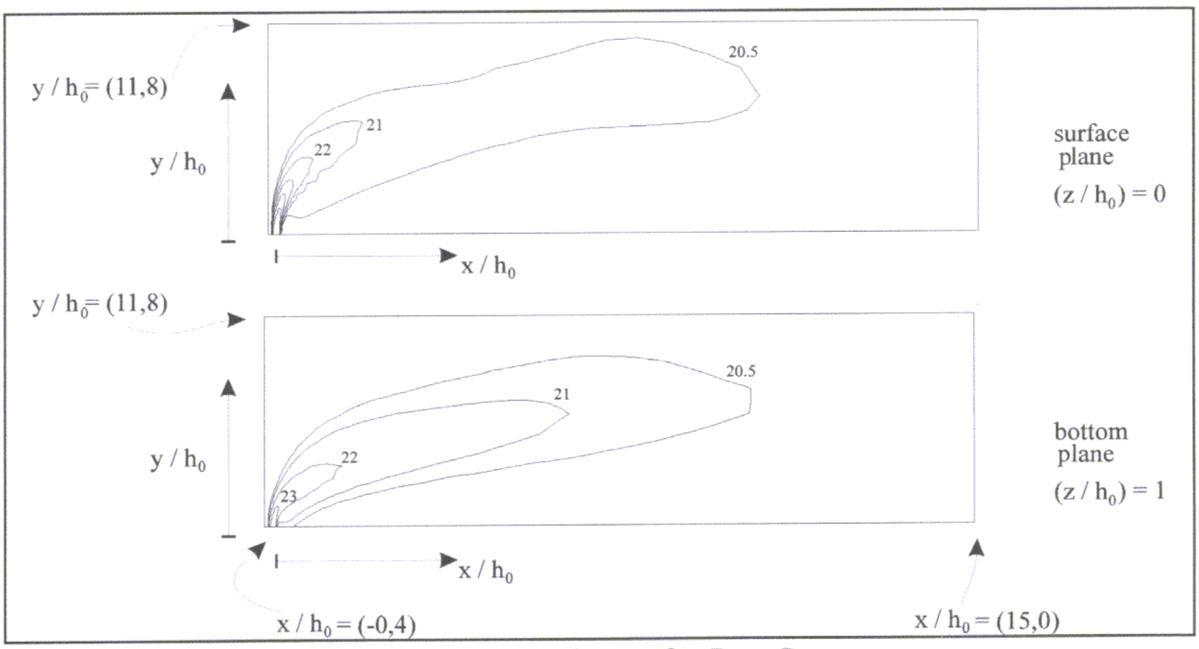

Fig. 13 - Isotherms for Run G

was solved. The results were compared with experimental ones, demonstrating the ability of the method in predicting complex flows. The problem solved also demonstrated that tridimensional analysis of certain environmental flows is necessary in order to capture the relevant features of the flow.

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