

A 3-D MODEL FOR OXYGEN CONSUMPTION IN A RIVER USING COMPUTATIONAL FLUID DYNAMICS (CFD)

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Abstract - This work presents a three-dimensional Computational Fluid Dynamics (CFD) in house model to simulate the dispersion of organic substances along a river. The finite volume method is used to approximate the conservation of momentum and mass equations. A Cartesian coordinate system has been chosen to represent the river. Turbulence is taken into account by a zero-order equation model. The Streeter-Phelps model has been used to predict the dissolved oxygen along the river. Results show that the proposed methodology is a good tool for the evaluation of the environmental impact caused for pollutants emissions in rivers. The *in house* software, developed from the model in Fortran language, is very fast, especially when compared to other commercial CFD packages. Experimental comparisons for soluble chloride dispersion have been made for the Atibaia-River near REPLAN-Paulínia (major petroleum refinery in Brazil). The results show good agreement with experimental data.

INTRODUCTION

During many decades the growth of urban centers and industries occurred without any control. The consequences of this lack of organization are felt everywhere. The effects of human activities leading to the pollution of water, soil and air have been widely studied and discussed at many research centers. People are taking notice of the risks involved in the misuse of natural resources. Specifically, the

possibility of shortage of fresh water resources in the near future has increased. In some places, people already suffer water shortages. Some regions of the world experience daily rationing of drinking water. These facts have increased the interest of industries and environmental agencies in the development of research activities and programs aiming to reduce effluent emissions and in predicting the environmental impact of new emissions as well as to treat already polluted bodies of water.

There are many works in the literature about pollutant dispersion in rivers. Nokes and Hughes (1994) proposed a turbulent three-dimensional model to study turbulent dispersion in open channels containing arbitrary, but constant, dimensions. They proposed a semi-analytic technique to study the permanent discharge of a non degenerative effluent in a channel of known velocity and diffusivity distributions. The model assumed that no secondary fluxes were present.

Ye and McCorquodale (1998) proposed a three-dimensional model in order to simulate the momentum and mass transfer phenomena in a curved channel. In order to better describe the effects of secondary flow that appear in superficial sinuous channels, a slightly altered turbulence $k-\varepsilon$ model has been used to account for turbulence.

Several models can be found in the literature, some of which even analyze complex flows. The main contribution of the present work is that it proposes a three-dimensional model capable of predicting the dispersion of effluents in open channels using Computational Fluid Dynamics. The model is very fast, an unusual feature for CFD models. Due to this, it is possible to predict the dispersion of substances in long sections of rivers with some kilometers in extension, so the model can be used as a predictive tool to analyze and guide management decisions of future industrial installations near rivers.

Some of the results obtained using the software is presented in this work. This software is based on a three-dimensional model of the dispersion of an inert effluent using CFD techniques. Velocity and concentration profiles for the substance are estimated through the numerical solution of the discrete form of the conservation of mass and momentum equations. Results of a case study in which experimental data

were used for model validation are shown. As already mentioned, a distinctive feature of the software is its speed. For a thousand-meter long section of river, only about one minute of CPU time on a Pentium IV computer was required to generate the results. A commercial package would have taken several days to run a similar problem.

MODELING

The following hypotheses were assumed to the model:

- Flow is steady and uniform;
- The velocity distribution is independent of the downstream coordinate, z ;
- There is no secondary flow in the channel, so the downstream velocity (z direction) is the only non zero velocity component;
- There are no interactions between the river bed and the water.
- The dispersing plume is long and thin, so that the diffusion term in the z direction is negligible in comparison with the convective term in the same direction;
- The fluid follows is Newtonian;
- Physical properties, including global dispersion and volatility coefficients are constant.

The shape of the river is represented by a channel with a rectangular cross-section. Although simple, this shape is able to simulate a very large number of real cases. The model was developed for the Cartesian coordinate system.

The resulting equations for the model are:

$$\frac{\partial v_z}{\partial z} = 0 \quad (1)$$

$$0 = \frac{\partial}{\partial x} \left((\mu + \mu_T) \frac{\partial v_z}{\partial x} \right) + \frac{\partial}{\partial y} \left((\mu + \mu_T) \frac{\partial v_z}{\partial y} \right) + \frac{\rho g H}{L} \quad (2)$$

$$v_z \frac{\partial C_A}{\partial z} = \frac{\partial}{\partial x} \left((D + D_T) \frac{\partial C_A}{\partial x} \right) + \frac{\partial}{\partial y} \left((D + D_T) \frac{\partial C_A}{\partial y} \right) + R_A \quad (3)$$

In order to evaluate the turbulent viscosity and diffusivity, a zero-order equation model proposed by SPALDING (1961) has been used. The following equations are used:

$$\mu_T = \mu \kappa e^{-\kappa B} \left(e^Z - 1 - Z - \frac{Z^2}{2} \right) \quad (4)$$

$$D_T = \frac{\mu_T}{Sc_T \rho} \quad (5)$$

where: $Z = \frac{\kappa \bar{v}_z}{v^*} \quad (6)$

$$\kappa = 0,41 \text{ and } B = 5,0$$

In order to predict the spatial distribution of biochemical oxygen demand (BOD), the Streeter-Phelps model has been used. The term R_A on the mass-transfer equation is a reactional term:

$$R_A = v_z \frac{dC_{DBO}}{dz} = -k_d C_{DBO} \quad (7)$$

The spatial distribution of dissolved oxygen in the river is given by:

$$R_A = v_z \frac{dC_{Oxigênio}}{dz} = -k_d C_{DBO} + k_a (C_S - C_{Oxigênio}) \quad (8)$$

where: $k_d = 0,35 \text{ day}^{-1}$, $k_a = 1,05 \text{ day}^{-1}$ and C_S is the oxygen saturation concentration in the water.

The boundary conditions for the model are as follows:

- Velocity is equal to zero on the bed of the river: $v_z = 0$

- The shear stress is set to zero on the water surface: $\frac{\partial v_z}{\partial n_i} = 0$

- A substance concentration before the river is specified as an inlet condition: $C_A(x, y, 0) = C_{A0}(x, y)$

- The mass flow across the bed and the water surface of the river is set to zero: $\frac{\partial C_A}{\partial n_i} = 0$

where n_i is the i^{th} component of the outward boundary unit normal to the boundary.

NUMERICAL PROCEDURE

Basically, the numerical solution for the model is carried out in two steps. First, the velocity profile is calculated. Then, using these results, the concentration distributions of the contaminant in the river are obtained.

The velocity profiles are estimated solving numerically equation 2 using a finite volume procedure. The last term on the right side of equation 2 was determined iteratively using the volumetric flow rate of the river and of the effluent and the equation of mass conservation.

Using the estimated velocity profile, it is possible to estimate the concentration distribution in the river by solving the discrete form equation 3. The equation 3 has been used to predict the oxygen concentration too.

RESULTS

An *in-house* software has been developed based on the mathematical model. In order to verify the applicability of the model, the results of a case study on a river having the following dimensions and flow characteristics are shown:

The coefficient of diffusivity is within the range of values experimentally determined by Fischer (1967). The following results have been obtained for the velocity contour plot.

Table 1 – Data for a case example.

h [m]	3.00
W [m]	10.00
L [m]	1,000.00
Q_r [m ³ /s]	10.00
Q_e [m ³ /s]	0.10
D [m ² /s]	0.02
C_{A0} [mg/l]	0.50
C_{Ae} [mg/l]	5.00

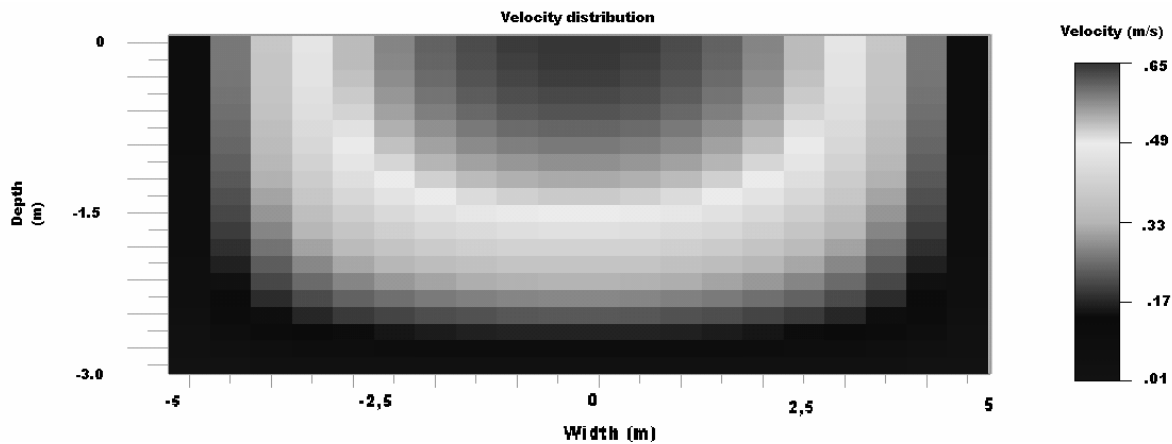
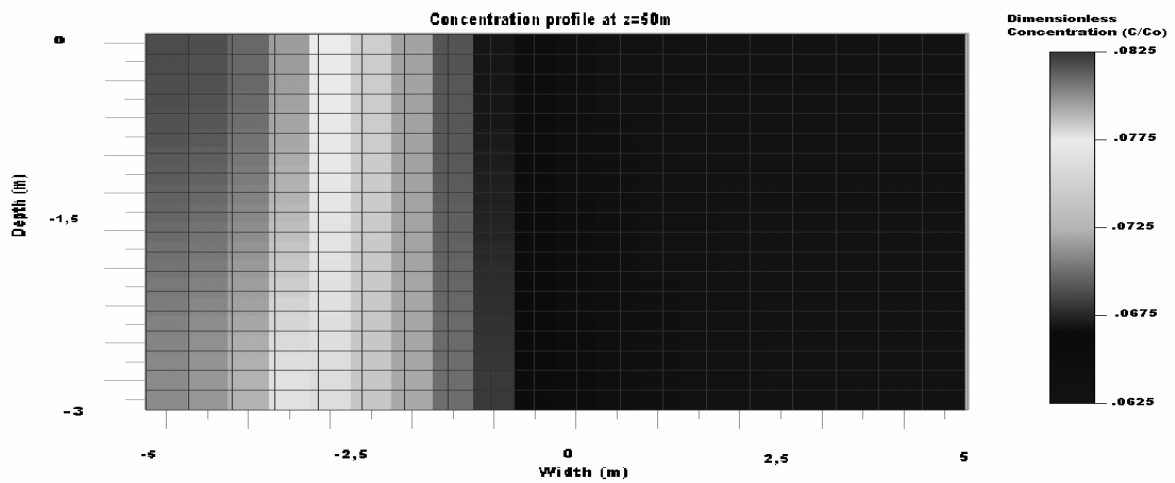
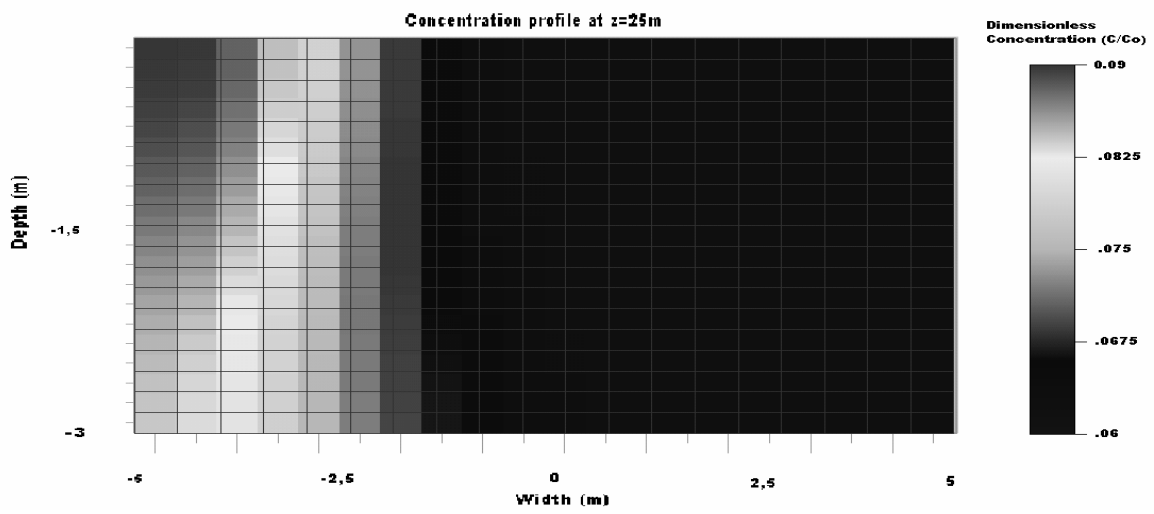
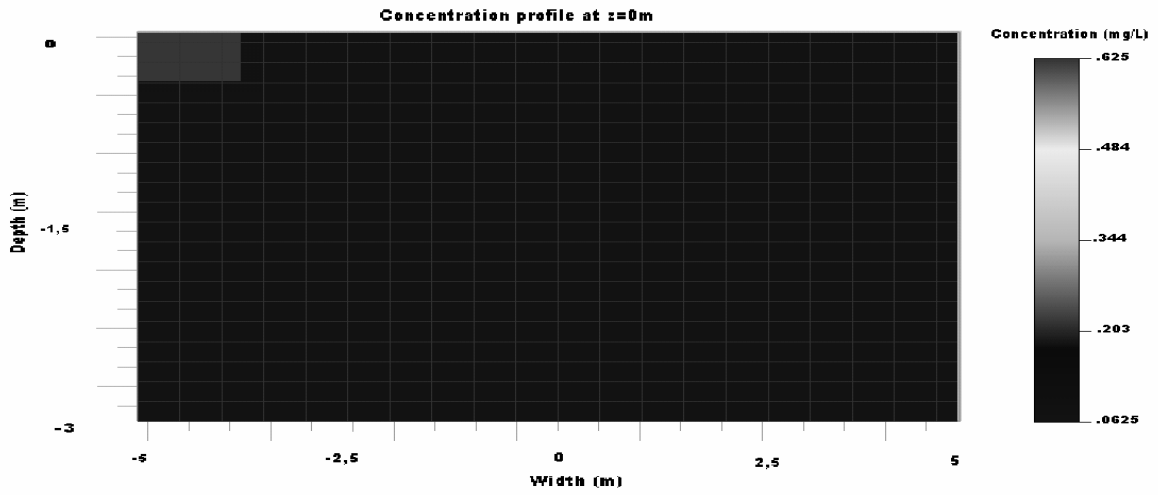


Figure 1 – Contour plot of velocity for the case study

The model indicates that the maximum velocity is at the centerline on the surface of the river. Some experimental publications have shown that the maximum velocity actually occurs just below the free surface of the river. This happens because, in practice, there are tensions at the free surface that were not taken into consideration by this model (e.g. those caused by wind). If need be, these can be considered in future refinements of the model.

Figure 2 shows the cross-sectional concentration profile located at 0, 25, 50, 100, 250 and 485 meters. The dark color indicates a high effluent concentration. The model shows the effluent being dispersed until it is diluted at a distance $L_D = 393m$, where the concentration at any point of the section is $(0.538 \text{ mg/L} \pm 1.0\%)$. In this work this distance is called the dilution distance.



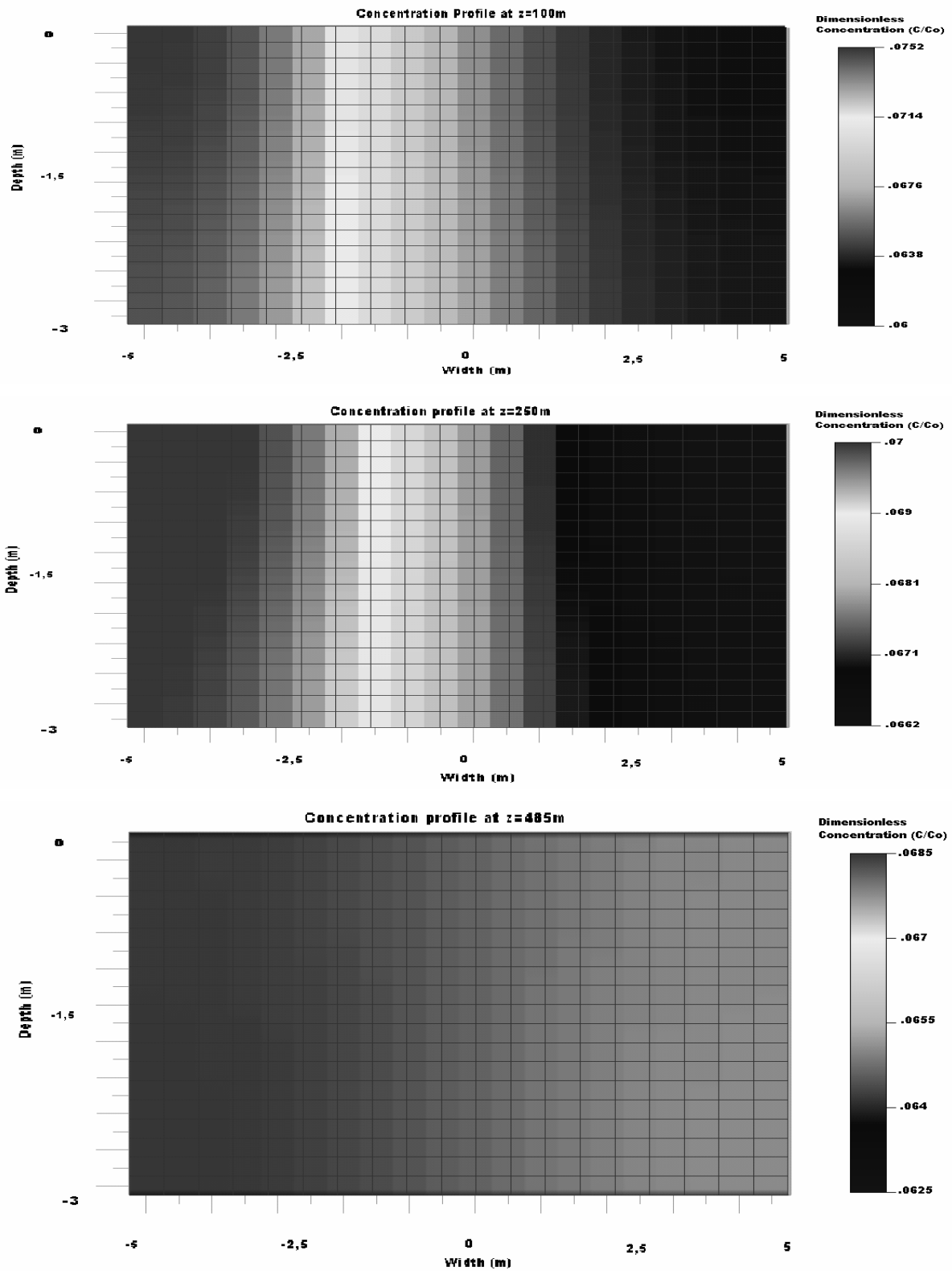


Figure 3 – Contour plots of dimensionless concentration downstream from a continuous effluent release into a river for the study case.

The following plot shows the effluent being dispersed at the free surface of the river. It should be observed that the range of variation in concentration Figure 5 is from 0.5 to 5 mg/l. This choice allows for a better visualization of the results. Otherwise, the variation would be visualized only very

close to the effluent emission. As already shown in Figure 4, the concentration does not vary considerably after 393 meters. The variation of concentration after this length is only because the biochemical oxidation.

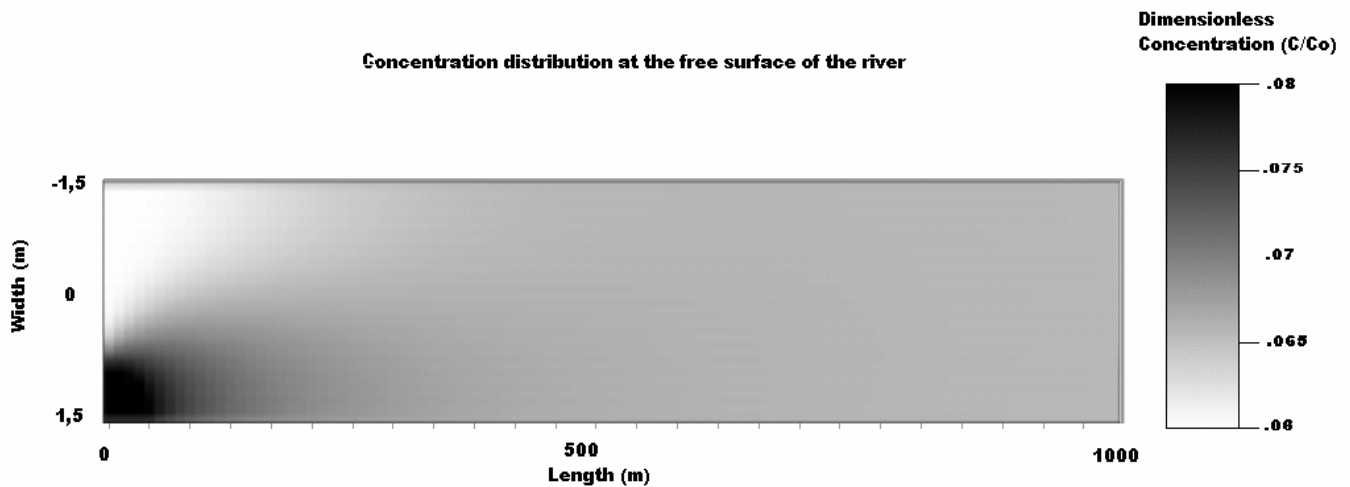


Figure 4: Contour plot of concentration at the river surface

The Figure 5 shows the consumption of oxygen at the free surface of the river. The preliminary results of oxygen consumption of the model indicate a very low consumption of oxygen for the organical substances. This results show a

necessity of the validation the kinetical constants of the model, since it is expected a high variation of the oxygen concentration. The dark color at figure 5 indicates the lowest concentration of oxygen.

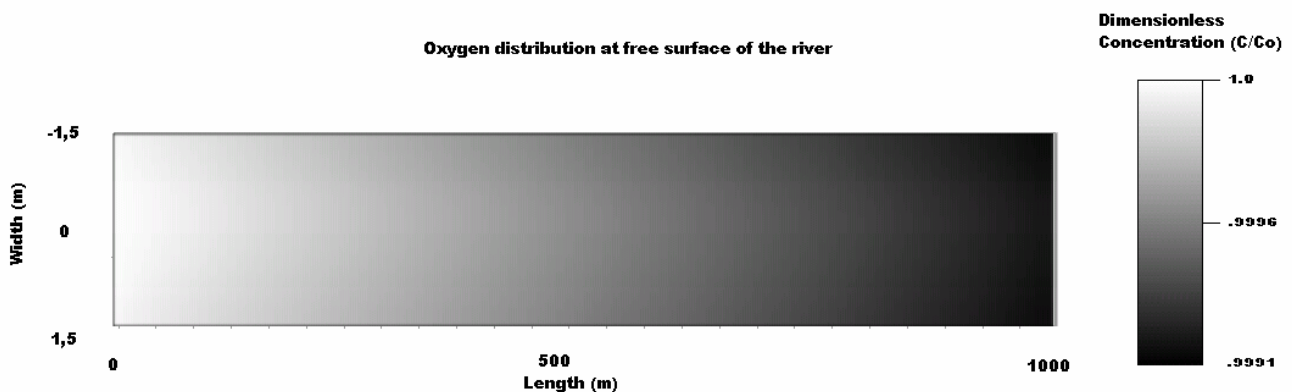


Figure 5: Contour plot of oxygen concentration at the river surface

Comparison with experimental data

The experimental data used in this work has been obtained from the Atibaia River, near the Petrobras Refinery, in Paulínia – São Paulo state in Brazil. In this river effluent is discharged from several

industries, including REPLAN, a major unit of the PETROBRAS Refining Industry. Figure 6 shows the distances from the river discharge point where the experimental data were collected.

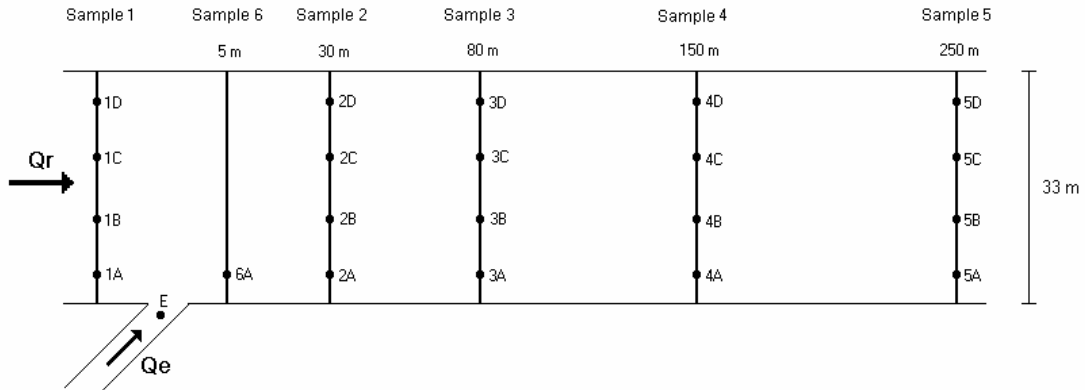


Figure 6 -- Schematic representation of the sample points

The approximate dimensions of the river were measured when the data were collected. The volumetric flow rate of the effluent was given by the refinery. These data are shown in Table 2.

Figure 7 compares the total chloride concentrations given by the model and the experimental data. The results show good agreement, specially considering the approximation for the geometry.

Table 2 – Data on the Atibaia River and REPLAN effluent.

W [m]	33.0
h [m]	3.0
L [m]	250.0
Q_r [m^3/s]	20.0
Q_e [m^3/s]	0.2

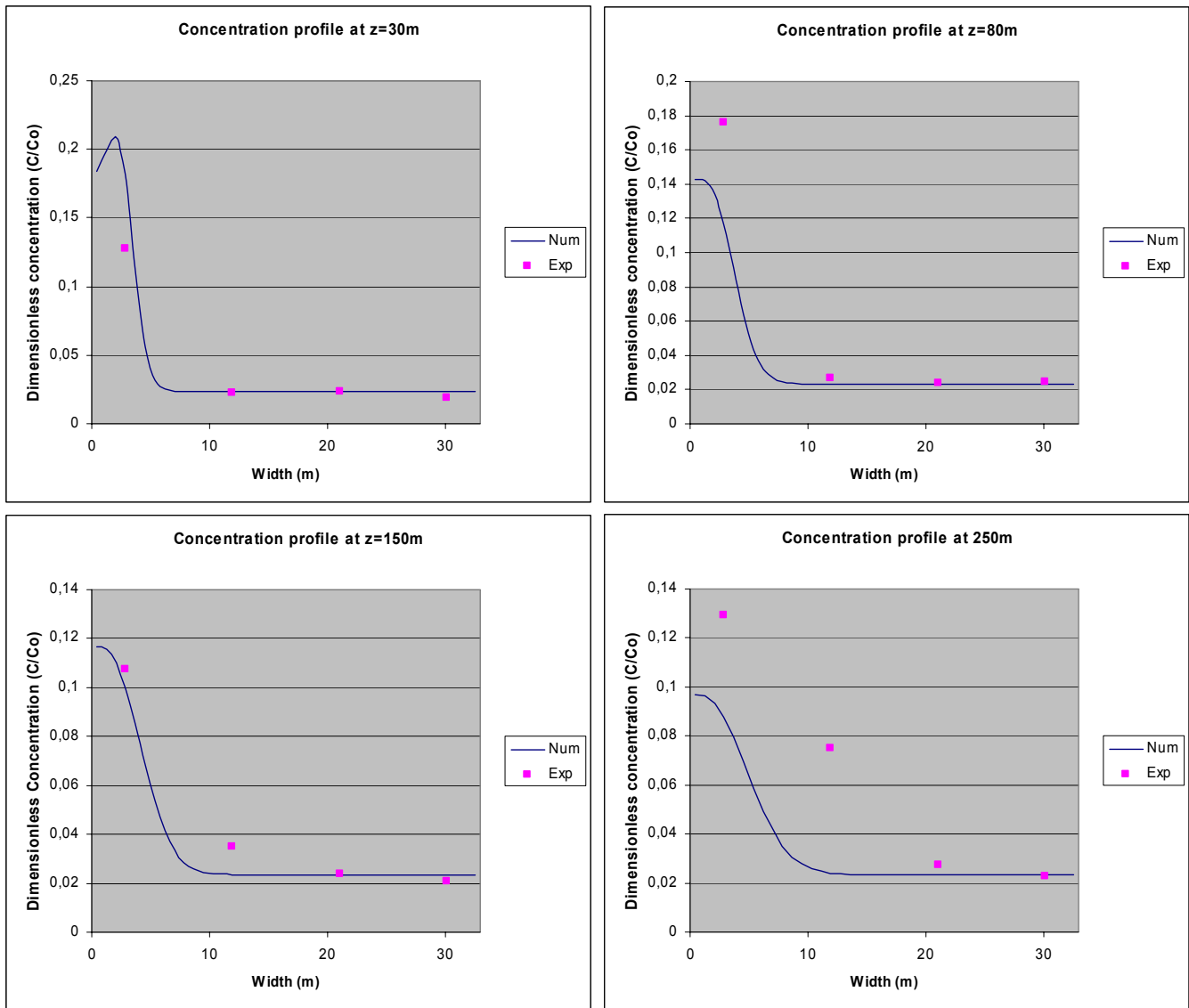


Figure 7 –Concentration of chloride at the free surface of the river for a segment 250m from the effluent discharge point. The points were located at: (a) 3m; (b) 11m; (c) 22m and (d) 30m from the river discharge point

CONCLUSIONS

The case study took less than one minute to give the output. This is not common in CFD codes at the time of writing of this paper. This same problem would require many days to be solved using commercial packages.

The results shown in this paper indicate that this new CFD model is capable of giving detailed information of the dispersion of soluble particles in a river, despite the simplifications considered. The comparison between experimental data and model results indicates that the model is suitable for predicting particle dispersion. There is a need, however, to validate the

model for oxygen consumption with experimental data. The computational time for the three-dimensional simulations did not exceed one minute for the case study. The model is very fast, making it a powerful tool for risk assessment.

Ye, J., McCorquodale, J.A., Simulation of curved open channel flows by 3D hydrodynamic model, *Journal of Hydraulic Engineering*, vol. 124, n° 7, July, 1998.

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