Modeling multiple emissions in a river

M.B. Machado[1], L.T. Furlan[2], E. Tomaz[3], J.R Nunhez[4]

[1,3,4]Faculdade de Engenharia Química, Departamento de Processos Químicos, Unicamp – Universidade Estadual de Campinas, Cidade Universitária Zeferino Vaz, 13083-970, Campinas, SP, Brazil

[2]PETROBRAS/REPLAN, Rodovia SP-332, Km 132, 13140-000, Paulínia, SP, Brazil

E-mail: furlan@petrobras.com.br, E-mail: machadomb@yahoo.com.br, E-mail: nunhez@feq.unicamp.br

Abstract - This work presents a three-dimensional Computational Fluid Dynamics (CFD) *in house* model to simulate the dispersion of soluble substances in a river. The finite volume method is used to approximate the momentum, mass and species conservation 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 concentration of organic substances and dissolved oxygen along the river. The model can also predict the impact of multiple effluents discharges. Results show that the proposed methodology is a good tool for the evaluation of the environmental impact caused for pollutants emissions in rivers. The software has been developed from the model and use the Fortran language. It is very fast, especially when compared to available commercial CFD packages. Experimental comparisons for soluble chloride dispersion have been made for the Atibaia-River near REPLAN-Paulínia (major petroleum refinery in Brazil). Despite approximations imposed to the shape of the river, the results show good agreement with experimental data.

Keywords – environmental engineering, CFD, river, finite volumes

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 misusage 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. In particular, the prediction of the impact of emissions in rivers requires a reliable simulation tool in environmental engineering.

River water quality models need to represent the physical, chemical and biological transformations which occur inside the river itself. It would be desirable to predict the oxygen and pollutant concentrations after the river received many emissions.

There are many works in the literature about pollutant dispersion in rivers. Nokes and Hughes (1994) proposed a three-dimensional turbulent model to predict turbulent dispersion in open channels containing arbitrary, but constant, dimensions. They proposed a semianalytic 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 flows were present in the river.

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-ε 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 this work is that it proposes a three-dimensional model capable of predicting the dispersion of effluents in very large open channels using Computational Fluid Dynamics. The model is very fast, an unusual feature of CFD models. Due to this, it is possible to predict the dispersion of substances in long sections of rivers with some kilometers in extension. This allows the model to be used as a predictive tool to analyze and guide management decisions of future industrial installations near rivers.

This software is based on a three-dimensional model for the dispersion of effluents in rivers using CFD techniques. Velocity and concentration profiles are estimated through the numerical solution of the discrete form of the mass, momentum and species conservation equations. If necessary, the developed model can consider the presence of multiple effluents discharges along the river. This flexibility allows for the simulation multiple discharges points in different locations of the river bank.

Results for the dispersion of an inert emission in a river near Campinas have been used to validate the model.

The model is very fast. A thousand meters of a river of width of 10 meters and depth of 3 meters takes only about one minute of CPU time on a Pentium IV. The river is discretized in 44,100,000 control volumes. A commercial package would take 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 the Newtonian Fluid law;
- Physical properties, including global dispersion coefficient, 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:

$$\frac{\partial \mathrm{v}_z}{\partial \mathrm{z}} = 0 \qquad (1)$$

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

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

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

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

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

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

$\kappa = 0{,}41$ 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 of first order:

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

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

$$R_A = v_z \frac{dC_{Oxygen}}{dz} = -k_d C_{BOD} + k_a\left(C_S - C_{Oxygeno}\right) \qquad (8)$$

where: k_d = 0,35 day^{-1}, k_a = 1,05 day^{-1} and C_S is the oxygen saturation concentration in the water. In the equations 7 and 8, C_{BOD} and C_{Oxygen} are the values obtained in the transversal section immediately before the actual section.

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 ith component of the outward boundary unit normal to the boundary.

NUMERICAL PROCEDURE

The numerical solution for the model is carried out in two steps. First, the velocity profile is estimated. 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 is determined iteratively using the volumetric flow rate of the river and of the effluent and the mass conservation equation.

Using the estimated velocity profile, it is possible to predict the concentration distribution in the river by solving the discrete form of the equation 3. Equation 3 has been also used to predict the oxygen concentration. The effect of multiple effluents discharges points can be considered in the program.

RESULTS

In order to show the applicability of the model, a case study is shown.

A diffusivity coefficient within the range of experimental values presented by Fischer (1967) was chosen to account for the effluent dispersion. Table 1 presents the river dimensions and the flow rate of the river and the emission.

Figure 1 shows the velocity contour plot of a cross section of the river.

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 yet taken into consideration by this model (e.g. those caused by wind). These effects can be accounted for in future refinements of the model.

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

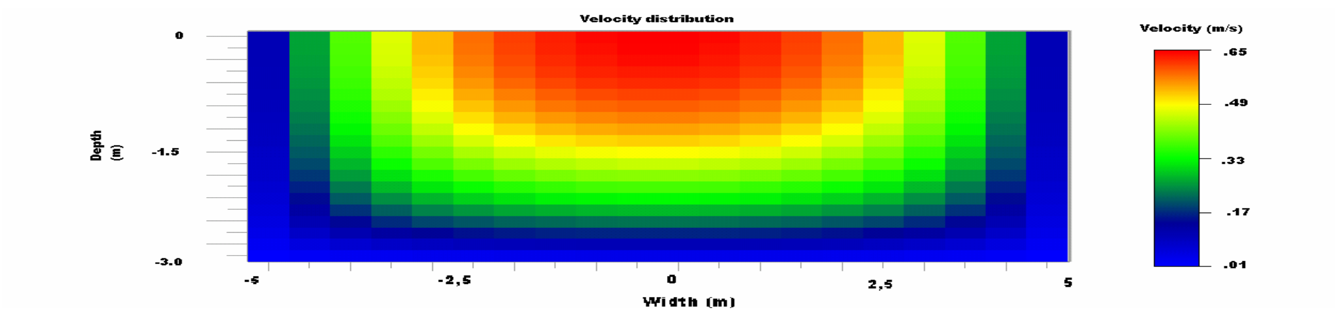
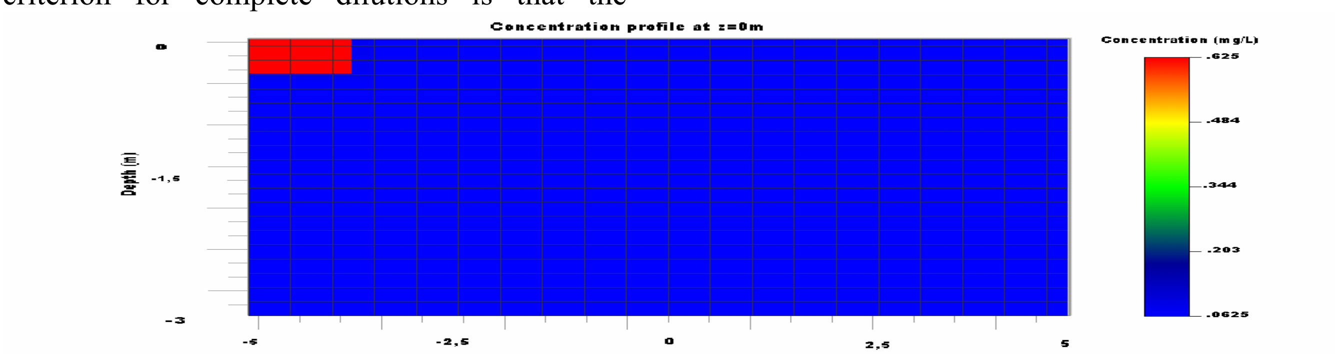


Figure 1 – Contour plot of velocity for the case study

Figure 2 shows the cross-sectional concentration profiles located at 0, 25, 50, 100 and 250 meters. The red color indicates a high effluent concentration. The model shows the effluent being dispersed and indicates it is diluted at a distance L_D = 393 meters. The criterion for complete dilutions is that the concentration at any point in across sectional section does not vary in more than 1%. In our case, it is (0.538 mg/L ± 1.0%). In this work this distance is called the dilution distance.



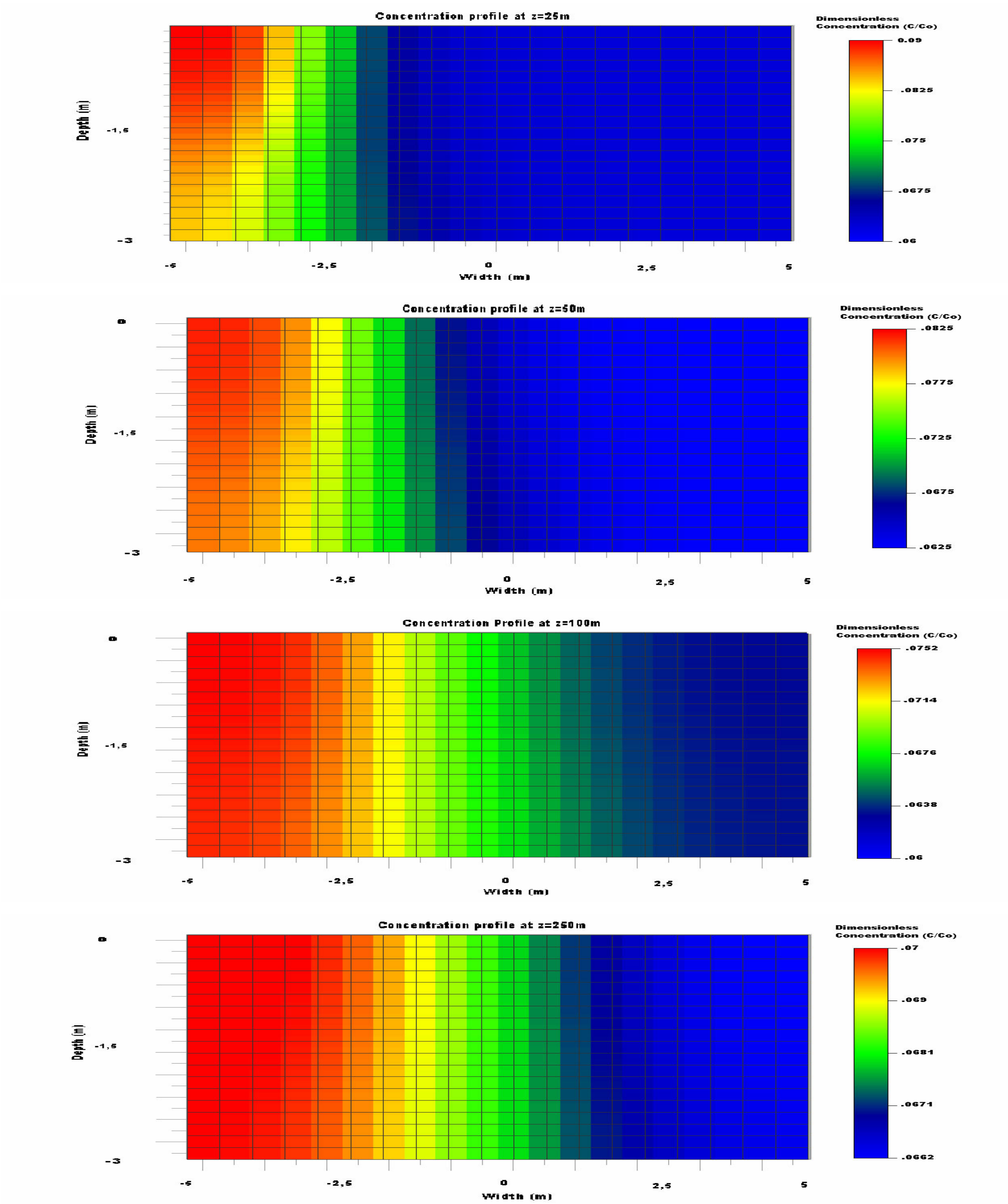


Figure 3 – Contour plots of dimensionless concentration downstream from a continuous effluent release into a river for the study case.

Figure 4 shows the effluent being dispersed at the free surface of the river. The concentration does not vary considerably after 393 meters. The variation of concentration after this length is only due to biochemical oxidation.

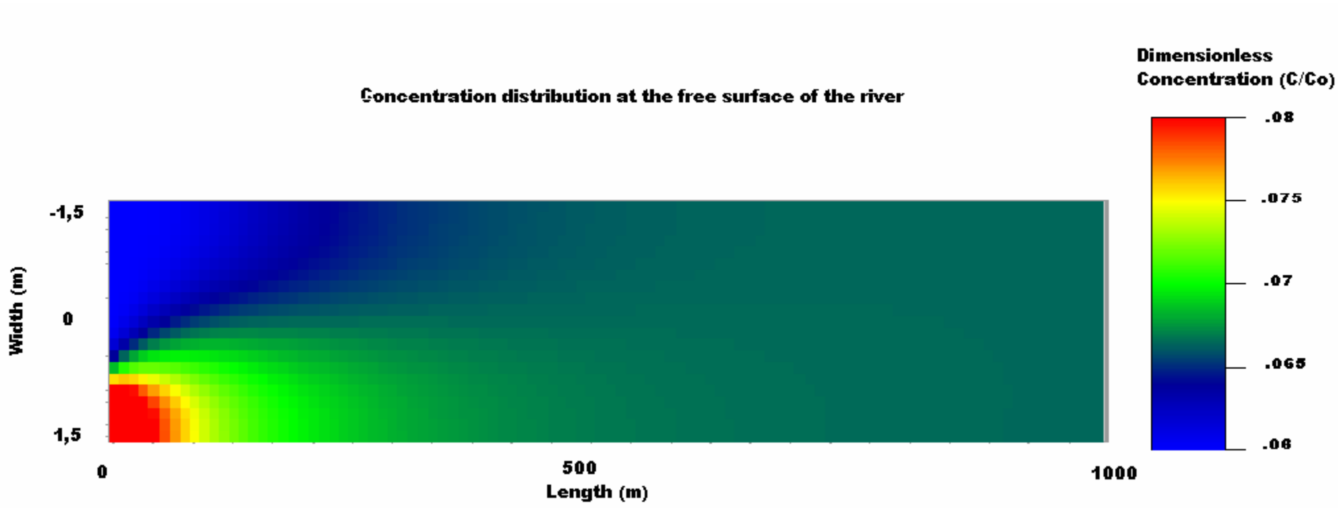


Figure 4: Contour plot of concentration at the river surface

Figure 5 shows the oxygen consumption at the free surface of the river. These preliminary results for the oxygen consumption indicate a very low consumption of oxygen for the organic substances. These results need to be validated.

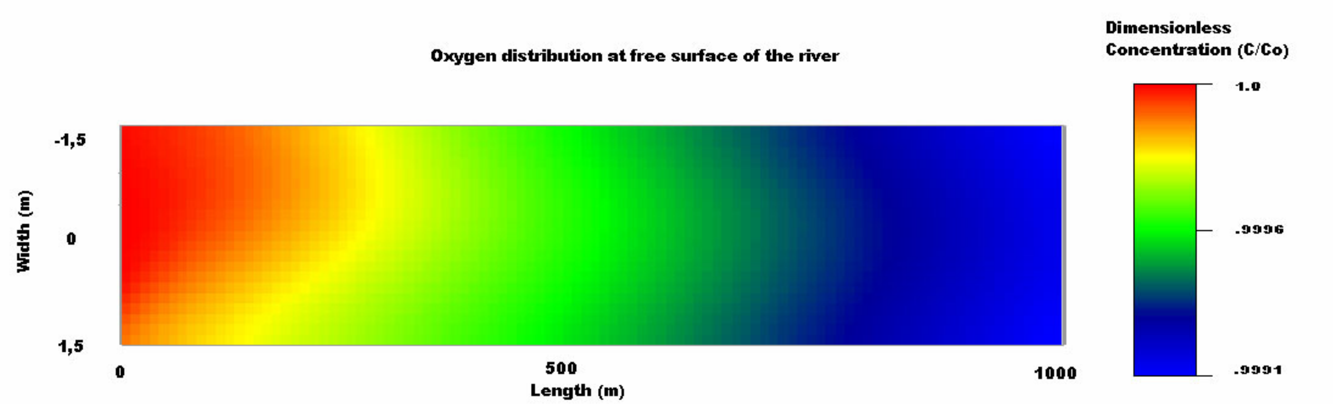


Figure 5: Contour plot of oxygen concentration at the river surface

Multiple effluents discharge points

The developed program can predict the impact of multiple effluents discharge. Figure 6 indicates three different discharge points at 0m, 200m and 400m in order to show the flexibility of the model.

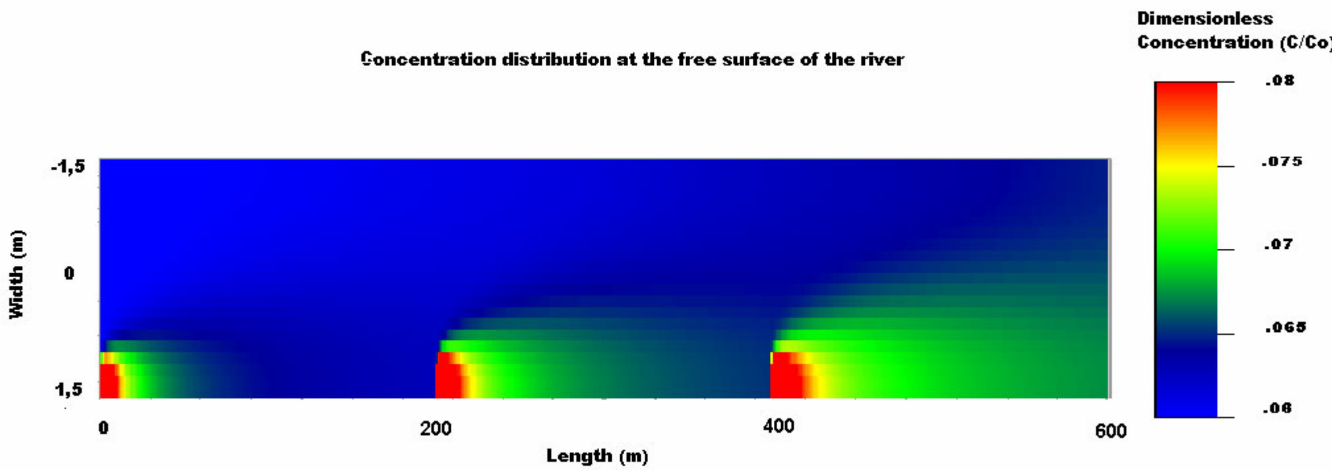


Figure 6: Contour plot of concentration at the river surface with multiple discharge points

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. This river receives multiple effluent discharges from several industries, including REPLAN, the major PETROBRAS Refining Industry unit. Figure 7 shows the distances from the river discharge point where the experimental data were collected.

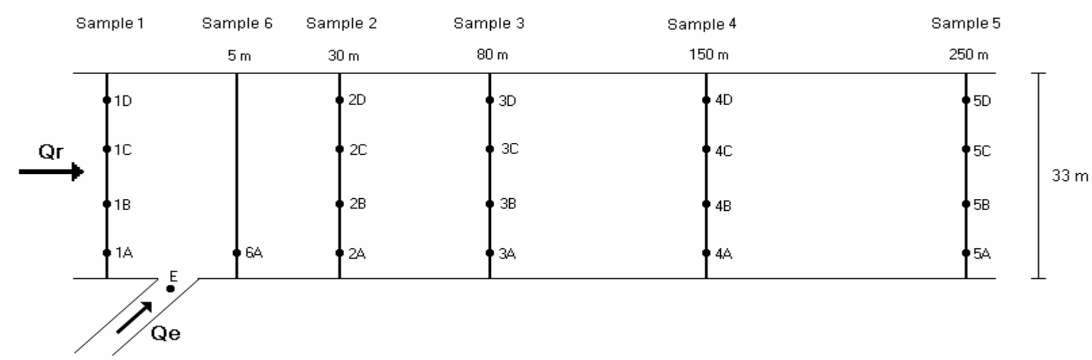


Figure 7 -- Schematic representation of the sample points

An approximate width of 33 meters and depth of 3 meters was considered for the simulations. The volumetric flow rate of the effluent was given by the refinery. These data are shown in Table 2.

Figure 8 compares the total chloride concentrations given by the model and the experimental data. The results show good agreement, especially considering the approximations used for the geometry of the river bed.

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

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

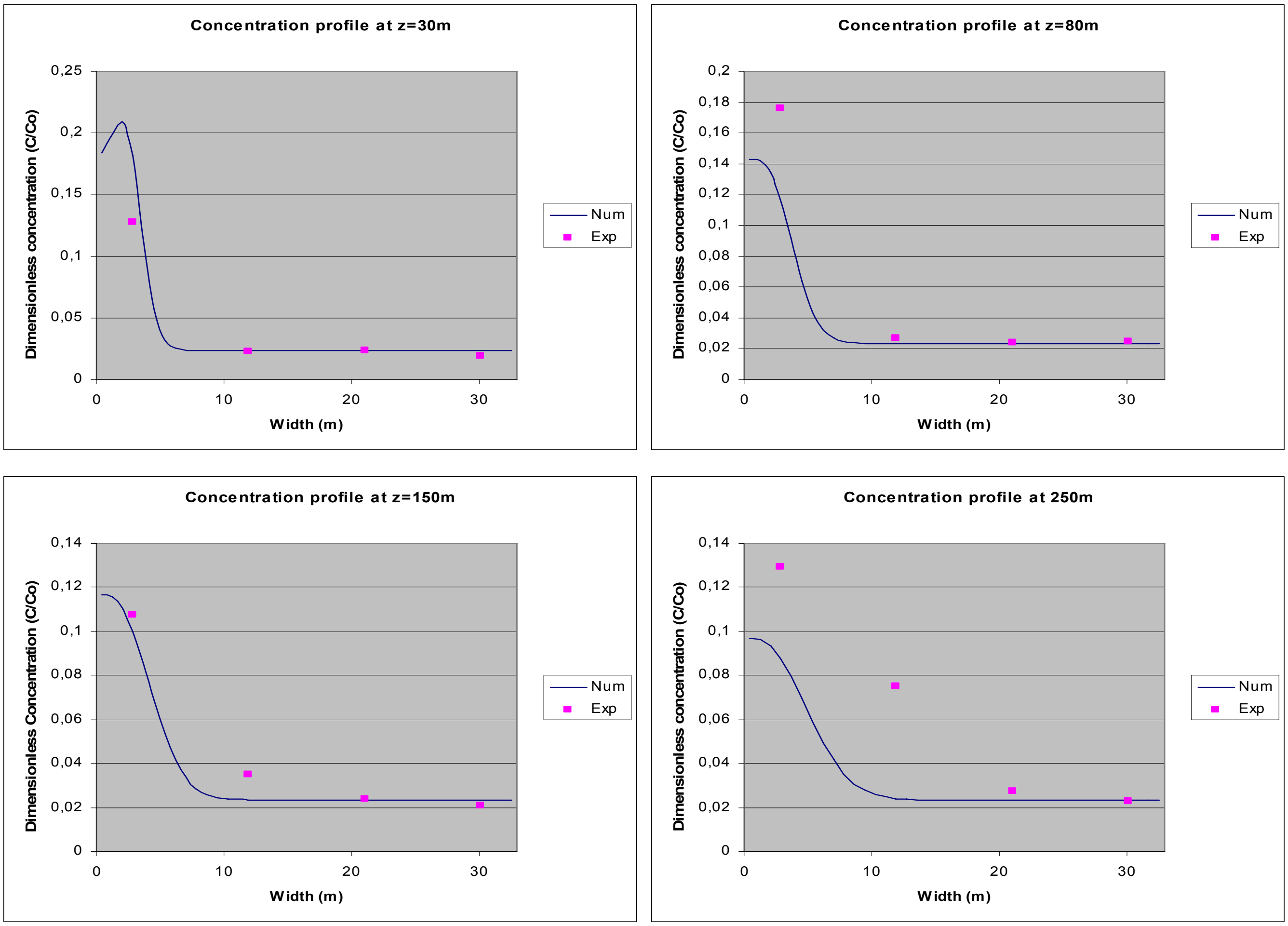


Figure 8 –Dimensionless chloride concentration at the free surface of the river for the segment of 250m from the effluent discharge point. The points were located at: (a) 3m; (b) 11m; (c) 22m and (d) 30m from the river discharge point.

The model took less than one minute to run this case and it used 44,100,000 control volumes. This is not common in CFD codes at the time of the writing of this paper. This same problem would require many days and a cluster to be solved using commercial packages.

CONCLUSIONS

The results shown in this paper indicate that this new three-dimensional, turbulent CFD model is capable of giving detailed information of the dispersion of soluble particles in a river, despite the simplifications applied in the shape of the river. The comparison between experimental data and model results indicates that the model is suitable for predicting particles dispersion. There is a need, however, to validate the model for oxygen consumption. The computational time for the three-dimensional simulations did not exceed one minute for the cases presented in this paper. The model is very fast, making it a powerful tool for risk assessment.

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