Software for Modeling Multiple Emissions in a River

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Abstract – This work presents a software based on a three-dimensional model for the dispersion of effluents in rivers using CFD techniques. There are several models can be found in the literature, some of which even analyze complex flows. They are however restricted to small river sections. The main contribution of this work is that it proposes a new software 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. Moreover, multiple emissions can be analysed by the model, allowing its use as a predictive tool to analyze and guide management decisions on future industrial installations near rivers. Results for the dispersion of an inert emission in a river near Campinas were used to validate the model. This software is Windows 98/NT/2000 based, and it was developed using Visual Fortran, Visual Basic and Matlab.

Keywords – Environmental engineering, CFD, River section, Finite volume method.

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. Nowadays 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 to be used 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 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 flows were present in the river. Ye and McCorquodale (1998) proposed a three-dimensional model to predict the momentum and mass transfer phenomena in a curved channel. In order to better describe the effects of the 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 flows in complex geometries. They are however very time expensive due to the dimension of the river. This disadvantage highlights the main contribution of this work, since it proposes a very fast three-dimensional model capable of predicting the dispersion of effluents in very large open channels using Computational Fluid Dynamics. The fast speed of this software is 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.

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 were used to validate the model.

Modelling

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 nonzero 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 are constant, including the dispersion coefficient, which assumes an average constant value, determined by experimental techniques.

A channel with a rectangular cross-section represents the shape of the river. 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:

$$\frac{\partial v_z}{\partial z} = 0 \tag{1}$$

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

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

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:

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

$$D_T = \frac{\mu_T}{Sc_T \rho} \tag{5}$$

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:

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

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

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

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. Since the geometry of the river has a fixed height and width, there is no recirculation flow and the velocity profile is constant.

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 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. Table 1 presents the river dimensions and the flow rate of the river and the emission.

Figure 1 presents a schematic representation of the case study. The emissions points are located in 0 m, 100 m, 150 m, 260 m and 380 m from the begin of the domain. The effluent is discharged in the top of the river in Points 1, 2 and 3. In Points 4 and 5, the effluent is discharged at the bottom of the river. All the emissions points have the same flow and concentration of substance.

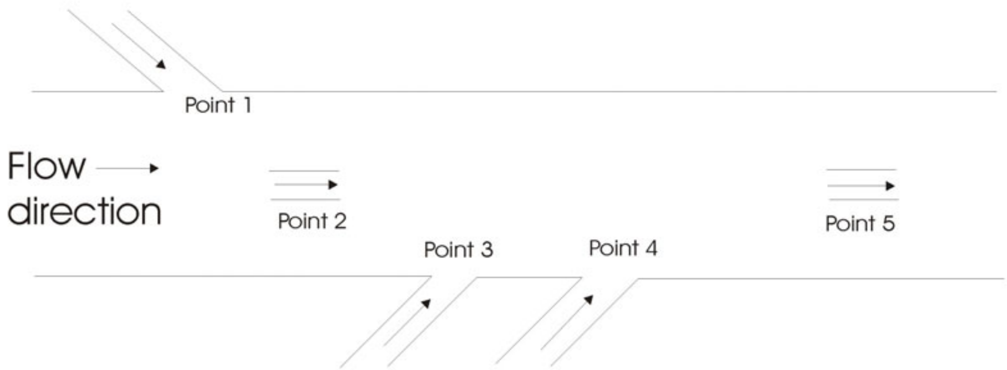

Figure 1: Schematic representation of the case study

Figure 3 shows the cross-sectional concentration profiles located at 0, 25, 50, 125, 175 and 275 meters. The red color indicates a high effluent concentration. Figure 4 shows the effluent being dispersed at the free surface of the river. It can be observed the effect of all the emissions points in these figures.

Figure 2 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 if needed.

Table 1 – Data for a case example

h [m]	3.00
W [m]	10.00
L [m]	500.00
River flow [m^3/s]	20.00
Effluents flow [m^3/s]	0.30
Coefficient of dispersion [m^2/s]	0.02
Concentration of substance in the begin of the domain [mg/l]	0.50
Concentration of substance in the effluents [mg/l]	5.00

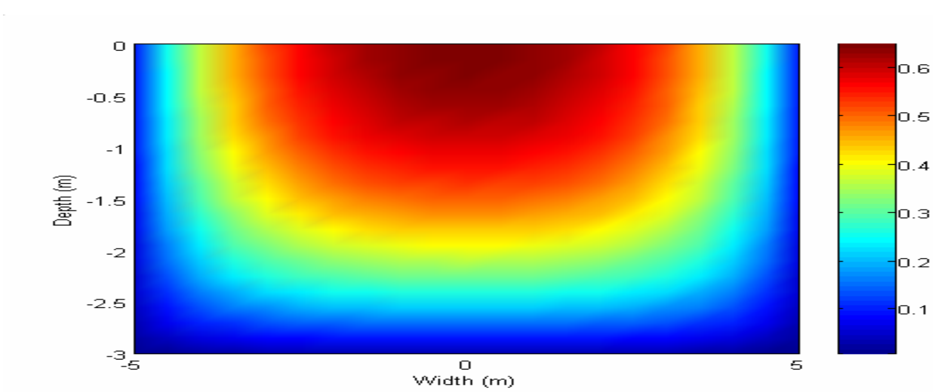

Figure 2 – Contour plot of velocity for the case study

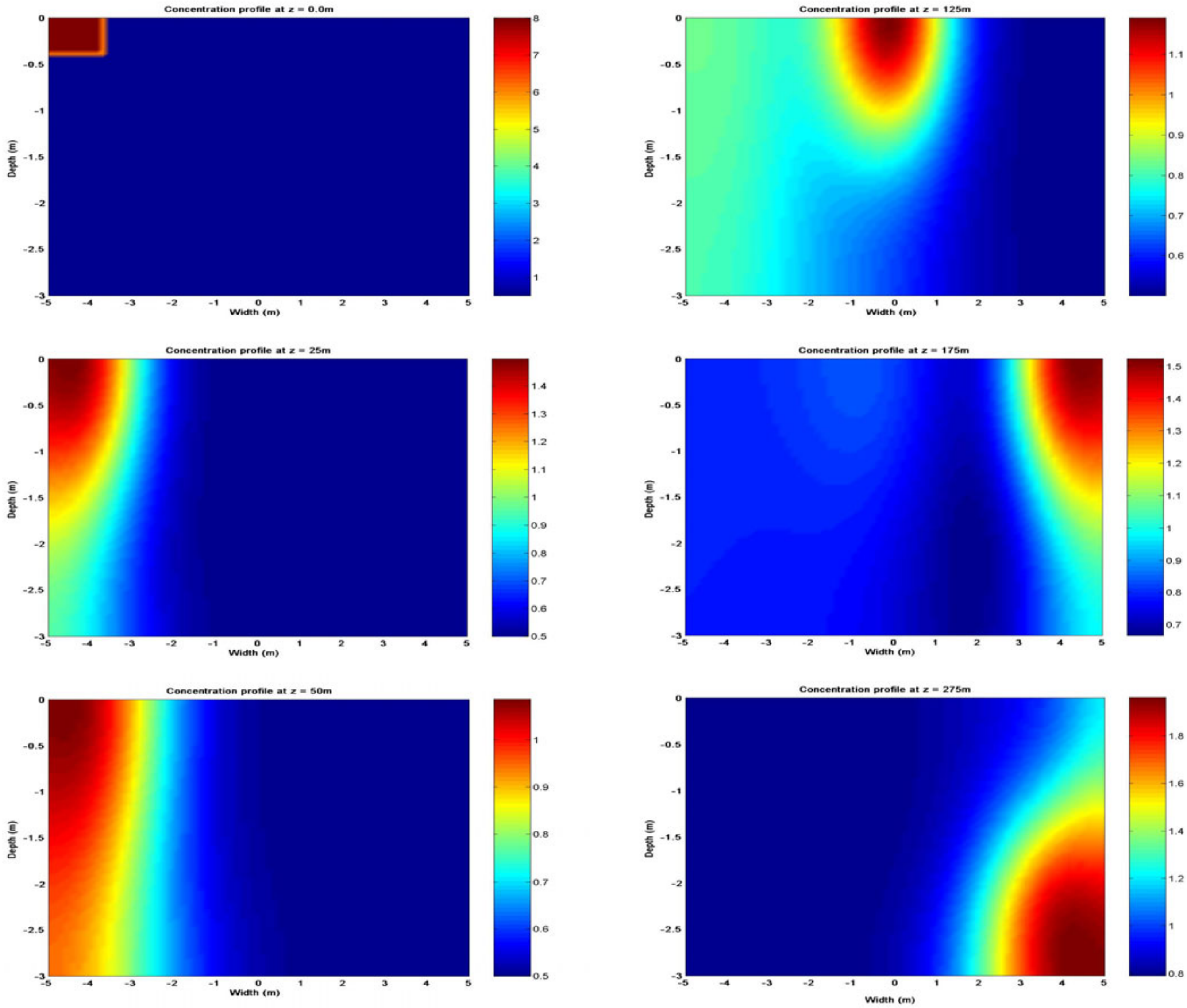

Figure 3 – Contour plots of concentration downstream from a continuous effluent release into a river

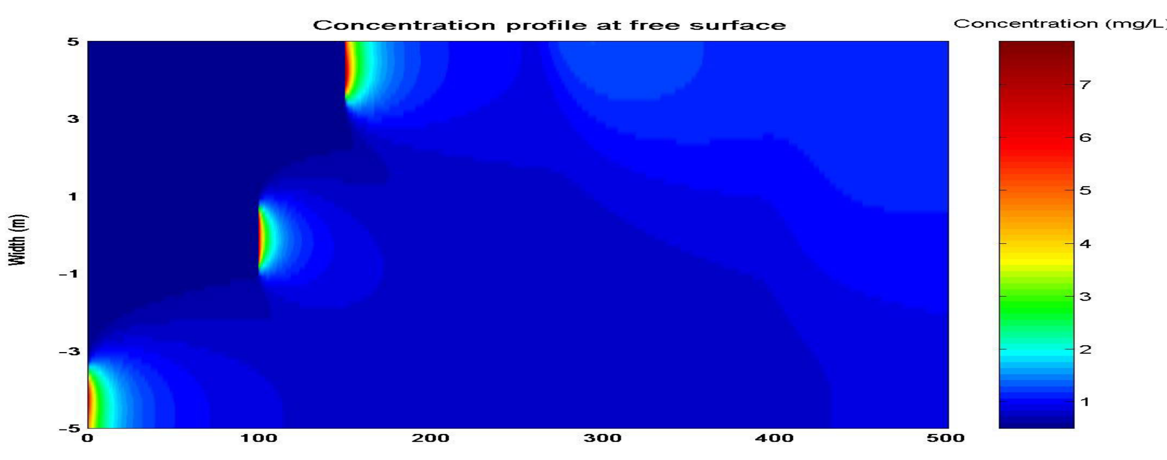

Figure 4: Contour plot of concentration at the river surface

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.

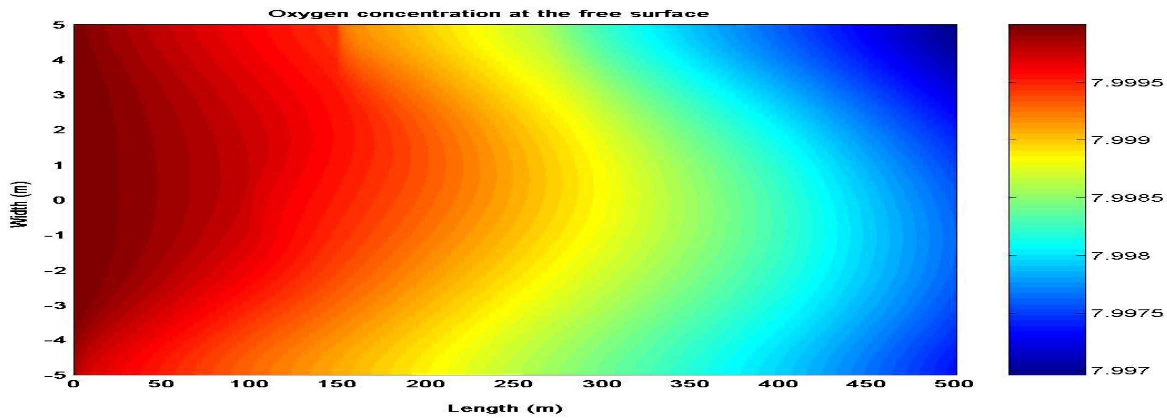

Figure 5: Contour plot of oxygen concentration at the river surface

Comparison with experimental data

The experimental data used in this work has been obtained for the Atibaia River, near Rhodiaco Company, in Paulínia – São Paulo state in Brazil. This river receives multiple effluent discharges from several industries. Figure 6 shows the distances from the river discharge point where the experimental data were collected.

The approximate average width of the river is 33 meters and its approximate average depth is 3 meters. The company informed the volumetric flow rate of the effluents. These data are shown in Table 2.

Figure 7 compares the total sodium 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.

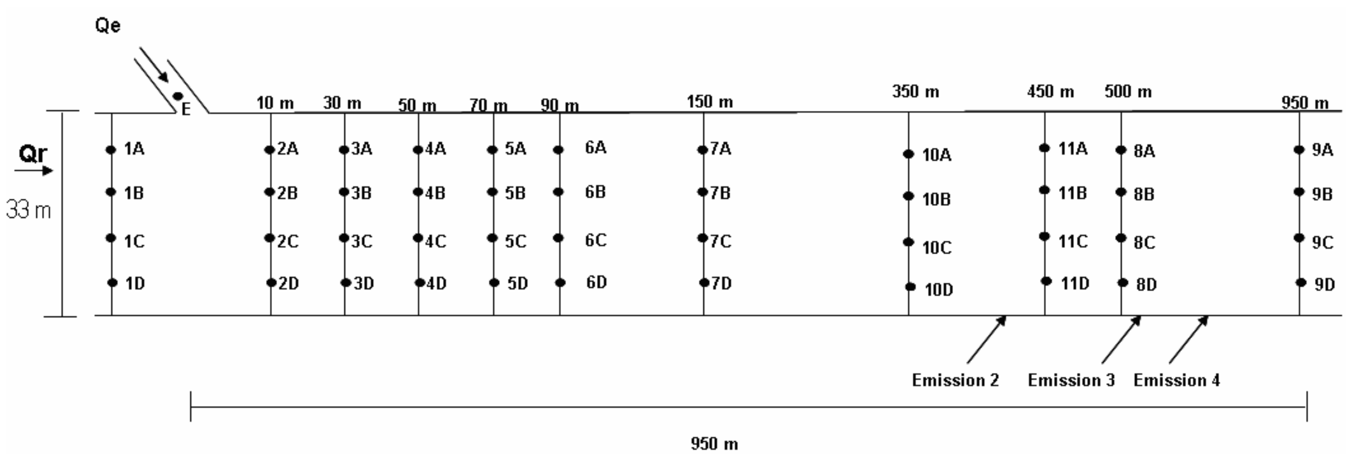

Figure 6 -- Schematic representation of the sample points

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

W [m]	h [m]	L [m]	Q_r [m^3/s]	Q_e [m^3/h]
33.0	3.0	950.0	10.8	195

Table 3: Data for the additional emissions points.

	Distance from emission 1	Flow rate
Emission 2	437 m	2320 m^3/h
Emission 3	540 m	1380 m^3/h
Emission 4	635 m	310 m^3/h

Table 3 shows the location and the flow of the additional emissions points along the system. These emissions points have a very low sodium concentration and a high flow rate. Consequently, these discharges contribute for the dilution of the sodium.

A mesh with 10 millions volumes in the downstream direction and 70x70 volumes for the other directions was used, totaling 49 billions control volumes. The model took about sixteen hours for the simulation. This same problem would require many days on a cluster if commercial packages were used.

Software

This software was developed to be used on the environment Windows 98/NT/2000. It was developed using three programs that interacts with each other. The mathematical model was developed in Visual Fortran, the programs interface was in Visual Basic .NET and the graphical results were given by Matlab outputs.

The software first receives input data that is configured by the user. The program generates the numerical and graphical outputs. The necessary inputs are river dimensions; number of effluents; river and effluents flow rates; river and effluents concentration of substances and coefficient of dispersion of the substance. The outputs of the model are dilution concentration of the substance, the distance where the dilution concentration is reached and the velocities and concentrations profiles along the 3D river directions.

The language of the software is Portuguese, for this first version. Figure 8 shows the main software Windows interface. In this figure, it can be observed the interface for data insertion. The results given by the software are shown in the place marked for a red circle.

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 substances 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 pollutants dispersion. There is a need, however, to validate the model for oxygen consumption. The computational time for the three-dimensional simulations did not exceed 24 hours for the cases presented in this paper. The model is very fast, making it a powerful tool for risk and environmental impact assessment.

A very important contribution of this paper is that it estimates the turbulent dispersion coefficient from the experimental data collected at the river, avoiding its estimation of this parameter from an empirical correlation.

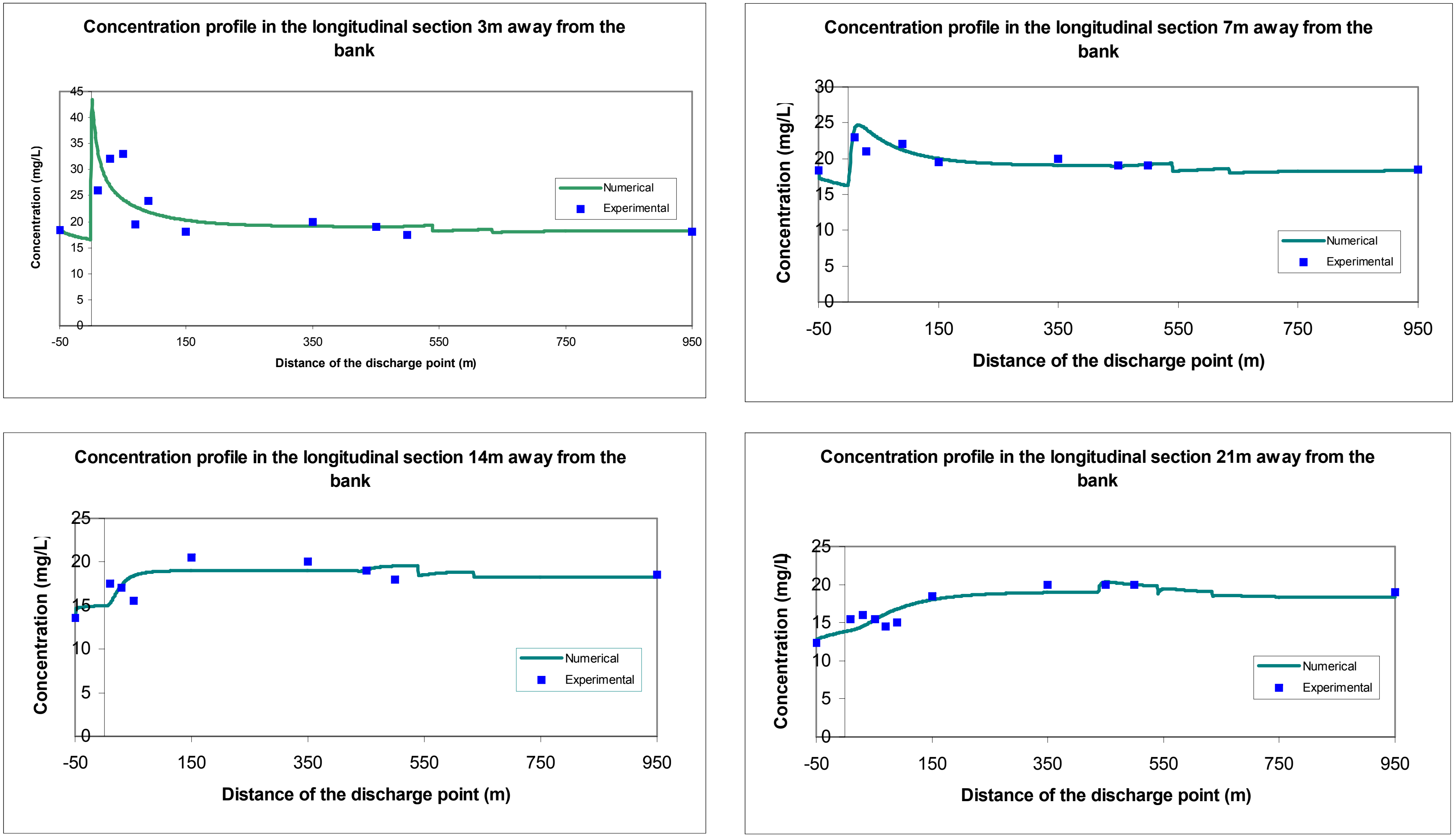

Figure 7 –Dimensionless sodium concentration at the free surface of the river for the segment of 950m from the effluent discharge point. The points were located at: (a) 3m; (b) 11m; (c) 22m and (d) 30m from the river discharge point according to Figure 6.

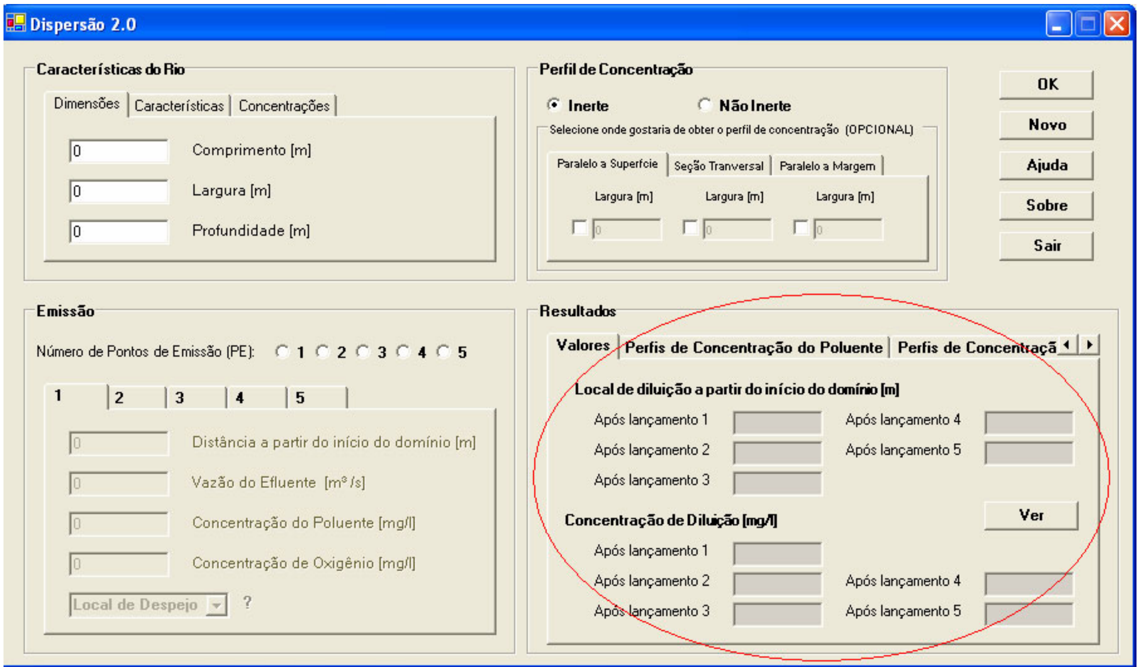

Figure 8: Graphical interface of the software

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