

## A STABILIZED FINITE ELEMENT METHOD FOR UNSTEADY POLLUTION DISPERSION IN RIVERS

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**Abstract.** *In this work a stabilized finite element method is proposed for the simulation of unsteady pollution in rivers. The pollution constituents transport is modeled using a set of one dimensional and transient convection-reaction-diffusion equations. The boundary conditions can vary on time, and all constituents can interact with each other dynamically. The proposed numerical method is validated using an analytical test case associated with the advection of a pollution front considering time periodic boundary conditions. The DO-BOD model was implemented and the numerical results for a real channel and river pollution problem is analyzed, comparing it to the experimental data.*

**keywords:** *river pollution, finite element method, DO-BOD model.*

### 1. Introduction

The understand of the dynamic characteristic of river pollution transport is fundamental in many environmental problems related to the transient dispersion of chemical or organic compounds. The transient behavior of the river flow influences the concentrations of chemical or biological compounds and its decay after its release from the sources positions. It can compromise the environmental health of the river, considering a admissible maximum concentration of a given specie at any time and any position in the stream. A steady-state analysis based in the time mean values cannot be used to describe this kind of situation.

The unsteady behavior of pollution problem is taken into account in many modern simulation tools, like EDP-RIV1 from USA-EPA or MIKE from DHI for instance. Considering this kind of problem, fast and robust numerical solution schemes have to be implemented in order to provide stable results, without introduction of excessive numerical viscosity.

The space and time dispersion of contaminants have been explored in some works concerning the implementations of numerical schemes. Fischer *et al.*, 1998 had proposed a group of criteria for the numerical simulation of unsteady contaminant transport in rivers. The absence of oscillations in the solution (stable schemes), reduced truncation error and reduced distortion of short-wavelength Fourier components are the main properties required to the numerical schemes.

### 2. Mathematical Formulation

In the present paper unsteady pollutant transport in an open channel (or river) is considered. A reference axis  $x$  along the stream is assumed, and the flow carries a set of species  $\{i = 1, N\}$  diluted in water at a concentration  $C_i(x, t)$ . The concentrations of the species are distributed through the river  $\Omega \equiv \{x \mid x \in [0, L]\}$ , where the transport problem is modeled by a set of unsteady advection-diffusion equations given by:

$$\frac{\partial(AC_i)}{\partial t} + \frac{\partial(uAC_i)}{\partial x} = \frac{\partial}{\partial x} \left( D_i A \frac{\partial C_i}{\partial x} \right) + AS_i \quad (1)$$

In this equation  $A(x)$  denotes the area of the river cross-section and  $u(x)$  is the local velocity of the stream (a plug flow is considered). The distribution of those variables in the stream direction is given from the hydrological and bathymetric river database. The variables  $D_i$  and  $S_i$  denote respectively the longitudinal dispersion coefficient and the source term related to the production or destruction of the specie  $i$ .

This general formulation can reproduce a great number of pollution problems in rivers. Detailed aspects of chemical or biological pollution dynamics can be taken into account for each constituent equation by means of the modeling of diffusion and source terms, (Porto, 1991).

Considering here our attention to organic pollution problems, the classical DO-BOD model will be used. This simple model for organic pollution in rivers takes into account only two species: The dissolved oxygen (DO) and the bio-chemical oxygen demand (BOD).

### 3. Numerical Method

This section present the numerical method used to solve the more generic transport equations Eq. (2). The methodology presented here is one of many variants of a class of methods known as Characteristic-Galerkin Procedure. This kind of methodology has been used with success as early as, Adey and Brebbia, 1974. The Characteristic-Galerkin method variant used in this work was first published by Löhner *et al.*, 1984 and is described in details in other works Löhner *et al.*, 1985 and O. C. Zienkiewicz, 2000b.

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right) + Q = 0 \quad (2)$$

If the equation above is represented in a reference system convected with the flow such that:

$$dx'_i = dx_i - u_i dt \quad (3)$$

Noting that for  $\phi = \phi(x'_i, t)$

$$\frac{\partial \phi}{\partial t} \Big|_{x_{const}} = \frac{\partial \phi}{\partial x'_i} \frac{\partial x'_i}{\partial t} + \frac{\partial \phi}{\partial t} \Big|_{x'_{const}} = u_i \frac{\partial \phi}{\partial x'_i} + \frac{\partial \phi}{\partial t} \Big|_{x'_{const}} \quad (4)$$

In this new coordinate system convected with the flow eq. (2) becomes simple:

$$\frac{\partial \phi}{\partial t}(x'(t), t) - \frac{\partial}{\partial x'} \left( k \frac{\partial \phi}{\partial x'} \right) + Q(x') = 0 \quad (5)$$

The time discretization of eq. (5) along a characteristic line, or a line convected with the flow results in eq. (6). In this equation  $\alpha$  is 0 for the explicit form, between zero and one for the semi-implicit form and equal one for the implicit form.

$$\frac{1}{\Delta t} (\phi^{n+1} - \phi^n|_{(x-\delta)}) \approx \theta \left[ \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right) - Q \right]^{n+1} + (1 - \theta) \left[ \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right) - Q \right]^n \Big|_{x-\delta} \quad (6)$$

Substituting the terms evaluated in  $(x + \delta)$  by Taylor series expansion shown in eq. (7), (8) and (9).

$$\phi^n|_{(x-\delta)} \approx \phi^n - \delta \frac{\partial \phi^n}{\partial x} + \frac{\delta^2}{2} \frac{\partial^2 \phi^n}{\partial x^2} + O(\Delta t^3) \quad (7)$$

Assuming  $\theta$  equal 0.5:

$$\frac{1}{2} \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right) \Big|_{(x-\delta)} \approx \frac{1}{2} \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^n - \frac{\delta}{2} \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^n \right] + O(\Delta t^2) \quad (8)$$

$$\frac{1}{2} Q|_{(x-\delta)} = \frac{Q^n}{2} - \frac{\delta}{2} \frac{\partial Q^n}{\partial x} \quad (9)$$

Now it is necessary to calculate a approximation for the distance traveled by the particle. There are many forms to calculate this distance, each one leading to different stabilization terms. The approximations employed in this work for velocity and distance are presented in eq. (10), (11) and (12).

$$\delta = \bar{u}\Delta t \quad (10)$$

$$\bar{u} = \frac{u^{n+1} + u^n|_{(x-\delta)}}{2} \quad (11)$$

$$u^n|_{(x-\delta)} \approx u^n - \Delta t u^n \frac{\partial u^n}{\partial x} + O(\Delta t^2) \quad (12)$$

Substituting the Taylor expansion presented in eq. (7), (8) and (9) and the estimative for velocity and traveled distance,  $\delta$ , we have:

$$\begin{aligned} \frac{1}{\Delta t}(\phi^{n+1} - \phi^n) &= -u^{(n+\frac{1}{2})} \frac{\partial \phi^n}{\partial x} + \frac{\Delta t}{2} u^n \frac{\partial u^n}{\partial x} \frac{\partial \phi^n}{\partial x} + \frac{\Delta t}{2} u^{(n+\frac{1}{2})} u^{(n+\frac{1}{2})} \frac{\partial^2 \phi}{\partial x^2} + \\ &+ \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^{n+\frac{1}{2}} - \frac{\Delta t}{2} u^{n+\frac{1}{2}} \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^n \right] - Q + \frac{\Delta t}{2} u^{n+\frac{1}{2}} \frac{\partial Q}{\partial x} \end{aligned} \quad (13)$$

where,

$$\frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^{n+\frac{1}{2}} = \frac{1}{2} \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^{n+1} + \frac{1}{2} \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right)^n \quad (14)$$

and,

$$u^{n+\frac{1}{2}} = \frac{u^{n+1} + u^n}{2} \quad (15)$$

In order to obtain the fully explicit form the terms evaluate in  $(n + \frac{1}{2})$  are approximated by terms in  $n$ . Equation (16) shows this for the velocity term and the diffusion term is treated in a similar way.

$$u^{n+\frac{1}{2}} = u^n + O(\Delta t) \quad (16)$$

For the fully explicit form:

$$\begin{aligned} \Delta \phi &= \phi^{n+1} - \phi^n = -\Delta t \left[ u^n \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right) + Q \right]^n \\ &+ \frac{\Delta t^2}{2} u^n \frac{\partial}{\partial x} \left[ u^n \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left( k \frac{\partial \phi}{\partial x} \right) + Q \right]^n \end{aligned} \quad (17)$$

### 3.1. Spatial Discretization

The spatial discretization of the equation above is possible without any stabilization problem using the Galerkin method. The method is conditional stable even for high Peclet number but this stability depends on the time step used Codina and Zienkiewicz, 2002.

Equation (18) present the interpolation of scalar inside de element, where,  $\tilde{\phi}$ , are the scalar values evaluated in the element nodes,  $\mathbf{N}$ , is the conventional finite element shape function. Utilizing time approximation given by (17) and the Galerkin method in it classical form O. C. Zienkiewicz, 2000a, Hughes, 1987 where the weighting function is the shape function  $N$ , it is possible to find (19).

$$\phi = \mathbf{N} \tilde{\phi} \quad (18)$$

$$\mathbf{M}(\tilde{\phi}^{n+1} - \tilde{\phi}^n) = -\Delta t[(\mathbf{C}\tilde{\phi}^n + \mathbf{K}\tilde{\phi}^n + \mathbf{f}^n) - \Delta t(\mathbf{K}_u\tilde{\phi}^n + \mathbf{f}_s)] \quad (19)$$

$\mathbf{M}$  is the mass matrix and can be treated in its condensed or lumped form Reddy, 1985, Lax and Wendroff, 1960. The treatment of mass matrix this way makes the solutions evident but introduces a new approximation to the problem. In this work the mass matrix is always treated in its lumped form.

The diffusion effect is represented by  $\mathbf{K}$ , this matrix is symmetrical and positive definite. But the convective term in this equation,  $\mathbf{C}$  is asymmetrical. The  $\mathbf{f}$  and  $\mathbf{f}_s$  terms represent the source and the source correction for high Peclet numbers.  $\mathbf{K}_u$  is a convection stabilization term for high Peclet numbers.

$$\begin{aligned} \mathbf{M} &= \int_{\Omega} \mathbf{N}^T \mathbf{N} d\Omega & \mathbf{C} &= \int_{\Omega} \mathbf{N}^T \frac{\partial}{\partial x_i} (u_i \mathbf{N}) d\Omega \\ \mathbf{K} &= \int_{\Omega} \frac{\partial \mathbf{N}^T}{\partial x_i} k \frac{\partial \mathbf{N}}{\partial x_i} d\Omega & \mathbf{f} &= \int_{\Omega} \mathbf{N}^T Q d\Omega \end{aligned} \quad (20)$$

$$\begin{aligned} \mathbf{K}_u &= -\frac{1}{2} \int_{\Omega} \frac{\partial}{\partial x_i} (u_i \mathbf{N}^T) \frac{\partial}{\partial x_i} (u_i \mathbf{N}^T) d\Omega \\ \mathbf{f}_s &= -\frac{1}{2} \int_{\Omega} \frac{\partial}{\partial x_i} (u_i \mathbf{N}^T) Q d\Omega \end{aligned} \quad (21)$$

### 3.2. Time step calculation

The algorithm presented above is conditionally stable with its stability depending on the time step used. So, it is necessary to deduce a safe way to estimate the time step limits. The factors that determine the stability are the element length, the velocity and the diffusivity coefficient. A dimensional analysis of these variables leads to the following form with time dimension, (22) and (23). These estimations take into account respectively the diffusive and convective effects.

$$\Delta t_d = \frac{h}{|U|} \quad (22)$$

$$\Delta t_c = \frac{h^2}{2k} \quad (23)$$

According to O. C. Zienkiewicz and Vázquez, 1999, the forms present in eq. (24) respect both the diffusivity and convective limits. A further discussion on the calculation of the time step is presented in Codina and Zienkiewicz, 2002.

$$\Delta t = \frac{\Delta t_d \Delta t_c}{\Delta t_d + \Delta t_c} \quad (24)$$

## 4. Results

### 4.1. Single reaction species

This section presents a comparison between the results obtained with the numerical method presented in the last section and the analytical solution for the case of a single reacting species. Twelve different conditions were simulated combining three different diffusivity coefficients, two decay coefficients and two initial conditions. Manson *et al.*, 2000 studied the same problem using another numerical method.

Analytical solution for (2) is possible for the case of a single reacting species with a sudden release of mass  $M$  in a steady flow and uniform channel area. Equation below presents the transient concentrations solution,  $c(x, t)$  obtained if the boundary conditions are given by the same equation when  $x$  equals 0.

$$c(x, t) = \frac{M}{A\sqrt{4\pi(D)t}} \exp\left(-\frac{(x-ut)^2}{4Dt}\right) \exp(-kt) \quad (25)$$

The solution above is gaussian in space traveling with the convection velocity and have a variance given by  $\sigma^2(t) = 2Dt$ . The channel velocity is constant and equal 1 m/s resulting from a  $10m^3/s$  flow in a channel with  $10m^2$ . Three diffusion coefficients were used in this test case, 1, 5 and  $100m^2/s$ . These coefficients are in accord with those present in real rivers. The decay coefficients used were equal to 0 and 0.693/day.

The numerical method is started with the distribution given by (25) with two initial variances  $\sigma^2 = 37,636m^2$  and  $\sigma^2 = 180,000m^2$ . The numerical domain used had 120000 m in length and was divided in 1200 elements with 100m each, the same element length used by Manson *et al.*, 2000. The simulation time is equal 14400 seconds.

Figures (4.1), (4.1), (4.1) and (4.1) compare the numerical and analytical results. These figures show the remarkable agreement obtained for this case and a estimative for the error dimension is only possible when the error in peak percentage is compared Tab. (1).

Table 1: Percentage error in peak

Case	D	k	$\sigma^2$	Error %
1	1	0.693	37636	0.099
2	5	0.693	37636	0.079
3	100	0.693	37636	0.082
4	1	0.693	180000	0.012
5	5	0.693	180000	0.045
6	100	0.693	180000	0.011
7	1	0.000	37636	0.097
8	5	0.000	37636	0.070
9	100	0.000	37636	0.081
10	1	0.000	180000	0.010
11	5	0.000	180000	0.035
12	100	0.000	180000	0.010

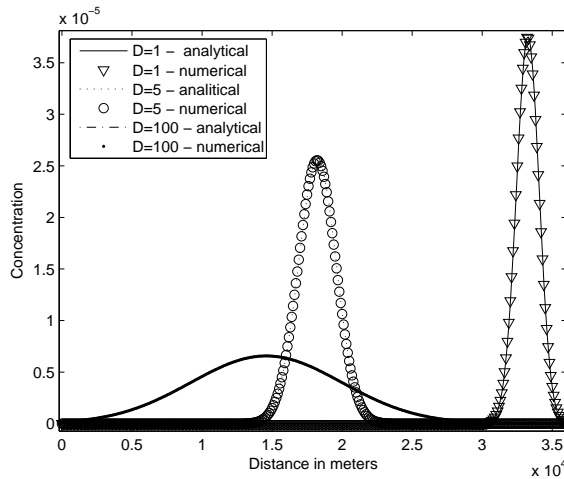


Figure 1: Analytical and numerical comparison for  $k=0.683$  and  $\sigma^2 = 37636m^2$

The good results obtained for this first case suggest that the CBC algorithm can be used to simulate more complex situations or a more long period of time. The computational cost is inexpensive considering that this is a one dimensional problem so no efforts were made to optimize or measure the simulation time.

#### 4.2. Transport of a contaminant cloud with no reaction

In the present section the CBC algorithm is used to simulate the evolution of a cloud of non-reactive component in a channel. In this problem the concentration is measured in two sections 5350 meters apart in the channel, for more information concerning this problem see French, 1986. The measurement in the first section is used as boundary condition for the numerical method. The channel velocity was measured as 0.59m/s. This

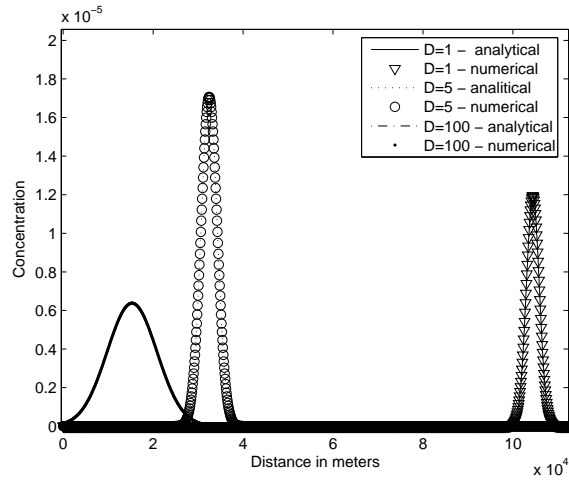


Figure 2: Analytical and numerical comparison for  $k=0.683$  and  $\sigma^2 = 180000m^2$

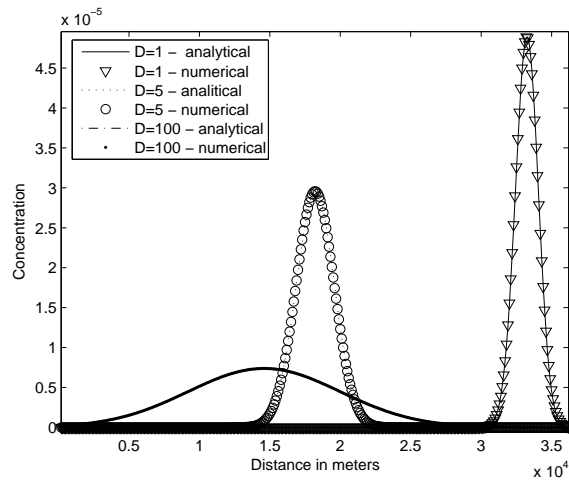


Figure 3: Analytical and numerical comparison for  $k=0.000$  and  $\sigma^2 = 37636m^2$

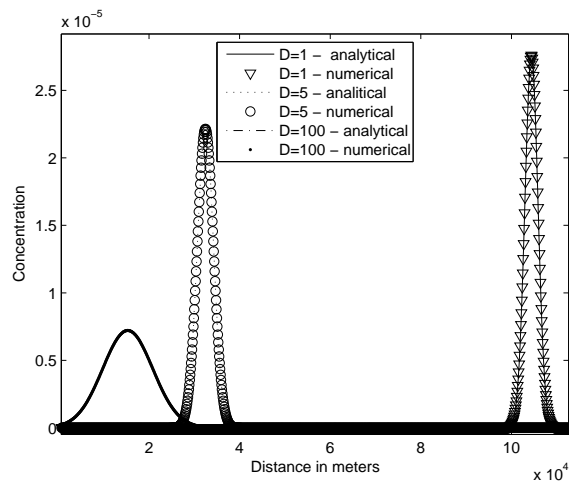


Figure 4: Analytical and numerical comparison for  $k=0.000$  and  $\sigma^2 = 180000m^2$

problem goal is estimate the diffusivity coefficient that best fits the numerical results with the experimental ones.

Table (2) show the measurements for the two sections.

Table 2: Concentration data for section 1 and 2

Section 1		Section 2	
Time in seconds	Concentration	Time in seconds	Concentration
0	0.00	32	0
3	0.26	37	0
6	0.67	42	0.07
9	0.95	47	0.22
11	1.09	52	0.40
13	1.13	56	0.50
15	1.10	60	0.58
17	1.04	62	0.59
19	0.95	64	0.59
24	0.72	68	0.54
29	0.50	75	0.44
34	0.31	84	0.27
39	0.21	94	0.14
49	0.08	104	0.06
59	0.02	114	0.03
-	-	124	0.025
-	-	134	0.02
-	-	144	0

The diffusivity coefficient that best fits the numerical with the experimental results is approximately  $30m^2/s$ , that is very close to the coefficient calculated by French, 1986 using a analytical method. It's important to say that in this case this diffusivity coefficient can not be considered the real diffusivity coefficient that exists in the river, in fact this coefficient is a estimative for the mean of this coefficient along the river. For this simplification and the difficulty to obtain accurate experimental measurements the numerical results can be considered satisfactory.

### 4.3. Multiple interacting species

In 1979 an emergency in a factory in New-Zeland leads to a large amount of milk discharged in the Waipa River. The milk was used as a water tracer transported in the river, data was measure for three fixed times along the river for BOD and DO. The data collected in this incident was compared with numerical estimative by Manson *et al.*, 2000 and McBride and Rutherford, 1984 using different numerical methods.

The experimental data provided by McBride and Rutherford, 1984 include spatial profile for BOD and DO along the river for three times 11 hours apart. In order to validate the CBS algorithm the data obtained for the second time will be used as time boundary condition and results obtained numerically for the last time will be compared with the results measured in the last time. The same velocity and depth profiles used by McBride and Rutherford, 1984 were used in this work (26) and (28), with  $x$  in kilometers. The re-aeration rate  $k_2$  was formulated according to the surface renewal model of O'Connor-Dobbins (27).  $k_1$  was considered as  $1/day$  based in McBride and Rutherford, 1984 and  $D$  was estimated as  $10m^2/s$  based in the same reference.

$$\begin{aligned}
 u &= 0.09 + 0.002x \quad \text{for } x < 30 \\
 u &= -0.4 + 0.018x \quad \text{for } x \geq 30
 \end{aligned}
 \tag{26}$$

$$k_2 = 3.74 \sqrt{\frac{u}{h^3}}
 \tag{27}$$

$$h = 6 - 0.08x
 \tag{28}$$

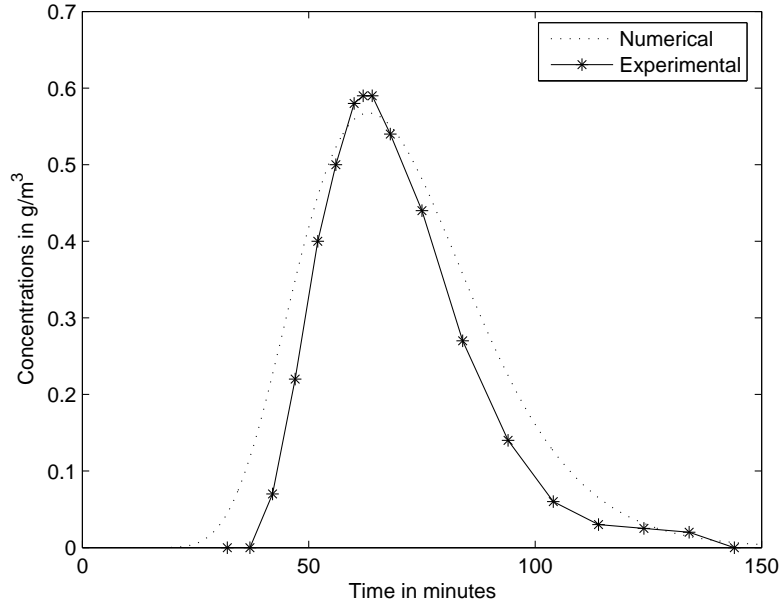


Figure 5: Analytical and numerical comparison for for concentration

For the aerobic condition when  $C > 0.1mg/l$  the Phelps assumption give by (29) was adopted for source and sink terms.

$$\begin{aligned} S_l &= -K_1L \\ S_C &= k_2(C_s - C) - \alpha k_1L \end{aligned} \quad (29)$$

in this equation  $L$ =river BOD;  $C$ =river DO;  $C_s$ =saturation river DO;  $k_1$ = the river deoxygenation coefficient,  $k_2(x)$ = the river reaeration coefficient and  $\alpha$  is the ratio of the river  $BOD_{ultimate}$  to BOD.

For anoxic condition when  $C < 0.1g/m^3$  the modifications to Streeter-Phelps given by (30) where used.

$$\begin{aligned} S_l &= -K_2C_s \\ S_C &= 0 \quad \text{if } \alpha k_1L > k_2C_s \\ S_C &= k_2(C_s - C) - \alpha K_1K \quad \text{if } \alpha k_1L \leq k_2C_s \end{aligned} \quad (30)$$

Figure (4.3) show the experimental data for BOD and DO used as boundary condition for the numerical problem and figure (4.3) show the comparison between the numerical and experimental data. Considering all the errors associated with the experimental measurement and all the assumptions made for estimate  $k_2$ ,  $k_1$ ,  $\alpha$  and the approximations for  $u$  and  $h$  the results can be considered satisfactory.

## 5. Conclusion and Discussions

In the first case studied in this paper the numerical method results were compared with an analytical solution for twelve cases varying three parameters, diffusivity, decay coefficient and initial state. The obtained results are in remarkable good agreement with the analytical solution and indicate that the CBC algorithm can be used in more complex situations and for simulate longer periods of time.

In the second case presented in this paper a comparison with experimental results is performed, a water tracer was throw in a channel and measured in two section for a period of time. The results for the first section were used as boundary conditions for the CBC method, the diffusivity coefficient were calibrated to approximate the numerical results in the second section with the experimental ones. It was noticed some difference between



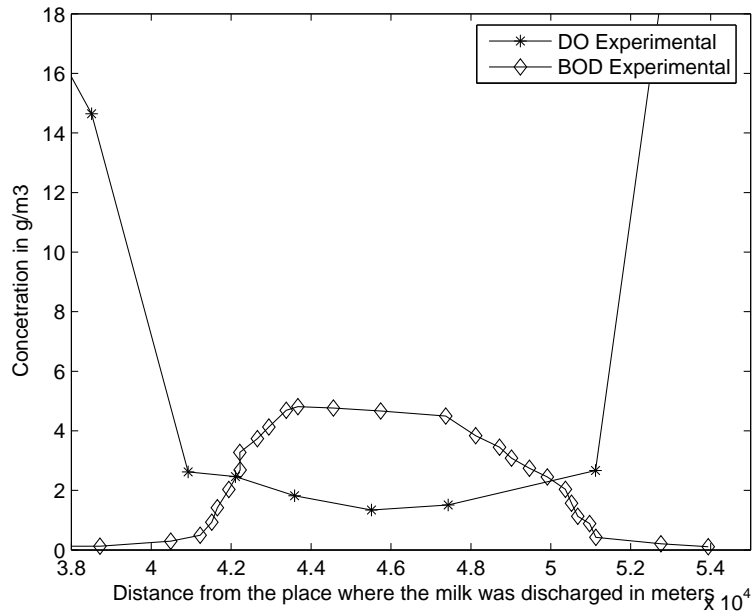


Figure 6: Experimental data for the second section

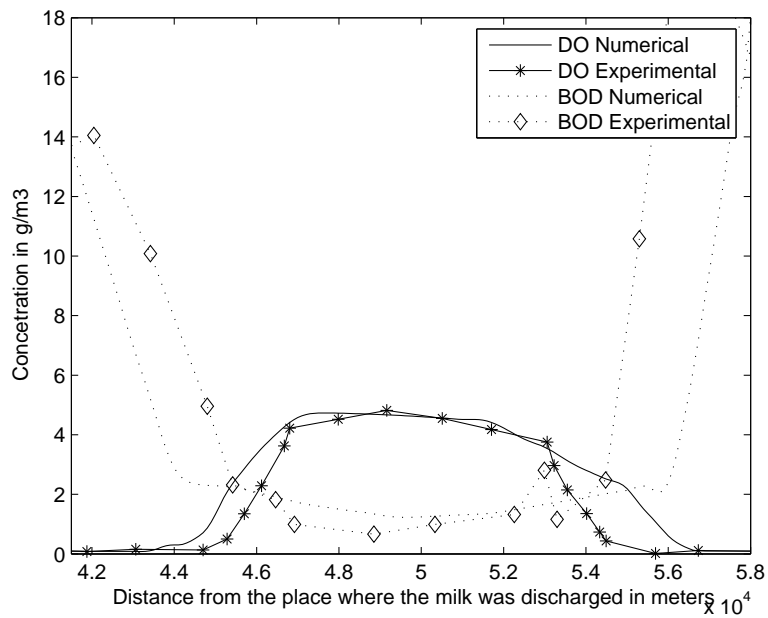


Figure 7: Numerical and experimental data for the last section

the results, but considering that the diffusivity coefficient was taken as constant along the river and always there exists errors associated with the experimental data the CBC algorithm behaved quite well.

The last case show a more realistically application where two species with reaction interact along a real river. For this case is difficult to estimate the CBS algorithm performance alone because the numerical method is influenced by many other parameter that should be calibrated or modeled and moreover there is a error associated with the experimental data collected. The best information provided by this case is the importance of good modeling for the decays coefficients and the right representation of the river domain and velocity as well as the measured data.

## 6. Acknowledgements

This section, if existing, shall appear before the references list.

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