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Modeling contaminant transport with aerobic biodegradation in a shallow water body

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ABSTRACT:

The set of physical, chemical and biological characteristics in a water body determines its quality. In open systems, these components are not static but rather dynamic and interact particularly in such way that favor the establishment of physical, chemical and biological processes leading to changes in the water quality. A better understanding of these processes is useful in the formulation of water quality models, reactive substances mainly, being the most important and occurrence in nature.

The water quality modeling using consistent and simplified models aims to reproduce those interactions, so that their effects can be predicted.

This study focus on a conceptual model that includes both aerobic and anaerobic reactions. Nutrient uptake is described using the Michaelis-Menten expressions. A mathematical model is obtained consisting of a series of advective-diffusive-reactive transport equations.

The hydrobiological model was implemented in CFD software Flow-3D, introducing it in the corresponding subroutine of source code and compiling it, for later applied in the transport modeling of species in a shallow water body.

As a part of the model performance it was verified its capability to reproduce results obtained by Erwin and Celia (1992) in modeling two-species equations that describe contaminant transport with aerobic degradation using ELLAM (Eulerian Lagrangian Localized Adjoint Methods) in one dimension.

Later the model transport used in the previous comparing was applied in a shallow artificial lake in two dimensions. The CFD software Flow-3D uses volume finite approximations to solve equations and the technique VOF (Volume of Fluid) to calculate the free surface. In this stage results are consistent.

KEYWORDS: Biodegradation**,** Numerical Methods**,** Computational Fluid Dynamics**,** Quality water**,** Advective-Diffusive-Reactive transport equations

1 INTRODUCTION

The set of physical, chemical and biological characteristics are crucial to define a stream water quality. In open systems, such components are not remain static they have specific dynamics and interact so that favor the establishment of physical, chemical and biological processes that lead to changes in water quality.

In a balanced system the magnitude of these parameters are regulated naturally by self regulation or recovery mechanisms that maintained within certain levels of variation, which is known as the balance of the aquatic system.

The balance of an aquatic system can be altered by both natural factors or the incorporation of organic/inorganic material due to different human activities. Hydrobiologic modeling using simplified and consistent models attempt to reproduce these alterations, so that their effects can be predicted.

Regardless the extraordinary progress that has been observed in the development of models to simulate water quality, the high degree of complexity of the structure and dynamics of aquatic systems in addition to its stochastic nature, made necessary to particularize the model o be used in a specific study. Although most models are based in the same principles, some are more complex than others in terms of processes and mathematical formulation. Furthermore, it is very difficult to adapt models were formulated to certain conditions because, for instance, the lack of input data (very frequently encountered) that is required for use. Therefore, it is desirable that the water quality models, are structured according to the nature of the problem to be solved and the availability of information in the case is going to be applied. (Victorica de, J., 1996).

Hydrobiological models are mathematical representations of aquatic systems, that attempt describe: transport of nutrients such as nitrate, phosphate, oxygen, etc., transport of organisms (plants and animals), interaction between organisms and nutrients and interaction between different agents among others, it is important remark that models describe the behavior of aquatic organisms as populations individually (Massol, A., 2012).

It is clear that the cleaning process of aquatic contamination is far more effective with a better understanding of the mechanisms of transport, chemical and biological reactions and remediation. Although recently the progress in developing models for the transport phenomena has increased (R. Erwin and Celia, 1992), the reaction terms describing potentially complex chemical and biological phenomena are not well understood yet.

The potential application of these models on microbial biodegradation to address remediation problems has recently increased, in that context, this research work presents results of first, second and non-linear equations of one and two species, and is focused on the implementation in future of a hydrobiological model in a commercial CFD software.

The CFD FLOW-3D software uses a volume finite method in structured meshes, it derives directly from the integral form of the conservation laws for fluid motion and, therefore, naturally possesses the conservation properties, however, it is known that sometimes this kind of schemes present some difficulties in fluid/reaction modeling concerning to mass conservation and non-physical oscillations. In order to assure that the CFD software used is capable to solve correctly transport problems, this study led a series of numerical exercises comparing the results of a particular problem obtained by applying an

alternative methodology , ELLAM method and the finite volume method.

The search for alternative formulations to address these problems is important, as is desirable the application of numerical techniques to the solution of problems of practical interest. The key to implementing numerical methodologies to improve the efficiency of numerical methods is to recognize the changing nature of the equation of advection-diffusion-reaction (Celia et al., 1990). Therefore, it is very unlikely to get acceptable solutions a numerical method that fails to meet these conditions.

Herrera (1985) and Celia et al., (1990) presented a methodology for the general solution of equations of second order. This procedure leads to numerical approximations that automatically change to the extent that the partial differential equation is fluctuating. This methodology is referred to as Localized Adjoint Methods (LAM) and is not restricted to the spatial dimension (Herrera, 1985), so it can be applied to the processing of the time derivative, with a suitable choice of the weight function. This scheme is developed in Celia et al., (1990), where LAM philosophy is combined with the method of characteristics to give rise to the formulation of the method attached Eulerian-Lagrangian localized. The main success of these procedures is systematic and comprehensive treatment of the boundary conditions, keeping the conservative property. Also reduce significantly the temporal truncation error and the restrictions imposed by the Peclet and Courant numbers.

The CFD software tested has a default chemistry model and it correspond to the form:

$$\frac{\partial C_n}{\partial t} = k_1 c_i^r c_j^s \pm \cdots\cdots k_2 c_k^t c_l^u \tag{1}$$

which can describes zero, first and second linear order reactions. The software has great ability to shape up to 99 reactions represented in equations to ten terms, however, the standard model reactions are not able to simulate nonlinear terms. Therefore, this research team, with the assistance of Flow Science Inc. staff proceeded to modify the subroutine corresponding source code, programming nonlinear differential equation and compiling the program.

One way to verify if the programming of the equations was adequate, consisted in comparing the results of one-dimensional modeling of two species, in this case: oxygen and organic carbonic reported by Erwin and Celia, 1992. The comparison was very successful. After that, we implemented such equations in a shallow water model in 2-D over an artificial lake. The results are consistent with the one-dimensional model.

The results obtained in this work are satisfactory. On one hand, certain parameters of the chemical model was calibrated with assistance from the firm Flow Science Inc. and on the other hand, it was verified its ability to reproduce data given from methods whose primary kindness is the speed and stability of the solutions. As stated, this study is the basis of a better understanding for the implementation of a hydrobiological model 2D/3D in several kind of water bodies.

2 MODEL EQUATIONS

Here models that couple the transport, diffusion/dispersion, and reaction terms, they allow to incorporate many specific models currently in use.

2.1 One dimensional modeling of one kinetics of first order without biomass growth

The model used for single-species advection-diffusion-reaction transport equation is:

$$\frac{\partial C_1}{\partial t} + V\frac{\partial C_1}{\partial x} - D\frac{\partial^2 C_1}{\partial x^2} = -k\ C_1 \tag{2}$$

was applied to simulate two species with the standard model Flow 3D. Where C is the particular scalar, V is the fluid velocity, D is the diffusion molecular coefficient. A mesh sizes were used and time to comply with the restrictions of Courant and Peclet numbers.

2.2 One dimensional modeling coupling one kinetics without biomass growth

The model used for two-species advection-diffusion-reaction transport equation is:

$$\frac{\partial C_1}{\partial t} + V\frac{\partial C_1}{\partial x} - D\frac{\partial^2 C_1}{\partial x^2} = -k\ C_1^1 C_2^2 \tag{3}$$

As in section 2.1, C_n is the particular scalar, V is the fluid velocity, D is the diffusion molecular coefficient.

2.3 One dimensional modeling coupling two kinetics non-linear without biomass growth

Consider the two species equations that describe contaminant transport with aerobic degradation, they can be written as:

$$\frac{\partial C_1}{\partial t} + V\frac{\partial C_1}{\partial x} - D\frac{\partial^2 C_1}{\partial x^2} + \delta_1\left(\frac{v_m^1 x}{k_h^1 + C_1}\right)C_1 = k_{1-2}\left(\frac{v_m^2 x}{k_h^2 + C_2}\right)\delta_2 C_2 \tag{4}$$

$$\frac{\partial C_2}{\partial t} + V\frac{\partial C_2}{\partial x} - D\frac{\partial^2 C_2}{\partial x^2} + \delta_1\left(\frac{v_m^2 x}{k_h^2 + C_2}\right)C_2 = k_{2-1}\left(\frac{v_m^1 x}{k_h^1 + C_1}\right)\delta_1 C_1 \tag{5}$$

In these equations (Erwin and Celia, 1992) , v_m^i, is the maximum uptake rate for the species i, K_h^i, is the half-saturation constant for species i, k_{ij} is the yield ratio coefficient for species i when species j is limiting, X is a measure of biomass and δ_i equal to 1, if species i is limiting the reactions and zero otherwise.

2.4 Bidimensional modeling coupling two kinetics non-lineal without biomass growth in a shallow water model

Once we compared our simulations with the results obtained by different studies (Erwing and Celia, 1992; Arroyo, V., 2005), we had the confidence to deploy it to a artificial lake in two dimensions through a shallow water model. The same parameters of sections 2.2 and 2.3 were used here.

3 RESULTS AND DISCUSSION

The purpose to model one kinetics of first order without biomass growth were, first, test the default chemical model of the CFD software starting for more simple cases, and second, to see firsthand how react the kinetic. So, the equation (2) is written as follows. The results of 2.1 apart were:

$$\frac{dC_1}{dt} = -0.01C_1 \tag{6}$$

Initial conditions:$C_1(x,0) = 0\ mg/l$. Boundary conditions:$C_1(0,t) = 10\ mg/l,\ C_1(100,t) = 0\ mg/l$, length ($l$) = *100 m*, $k_1 = -0.01\ day^{-1}$, *D=0.2 m²/day*.

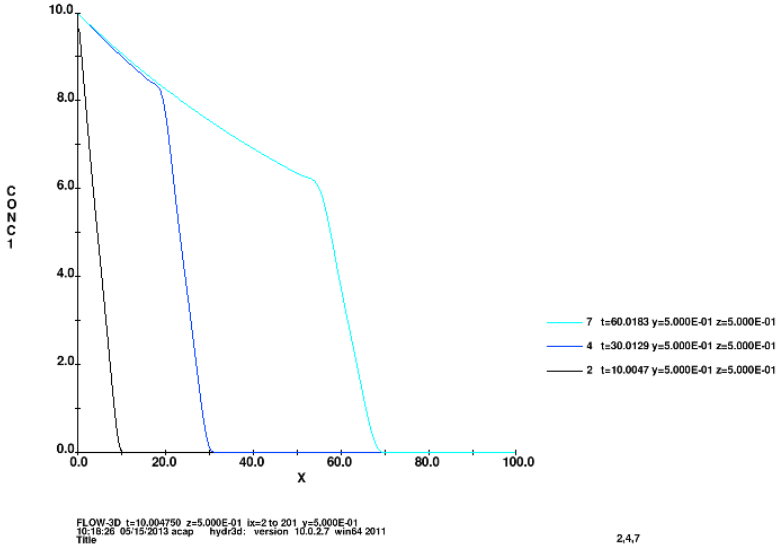


Figure 1 Development of specie C_1 behavior through time for 2.1

the results show that the dominant physical phenomenon is advection, diffusion is low. In this same purpose it is presented the modeling the section 2.2, just added a second specie with a constant value (C_2 = *3mg/l*) all simulation time. The equation (3) is written as:

$$\frac{dC_1}{dt} = -0.025C_1^1C_2^2 \qquad (7)$$

Initial condition: $C_1(x,0) = 0\ mg/l$, $C_2(x,0) = 3\ mg/l$. Boundary conditions: $C_1(0,t) = 10\ mg/l$, $C_1(100,t) = 0\ mg/l,\ C_2(x,t) = 3\ mg/l,$ *length = 100 m*, $k_1 = -0.025\ day^{-1}$, *D=0.2 m²/day*.

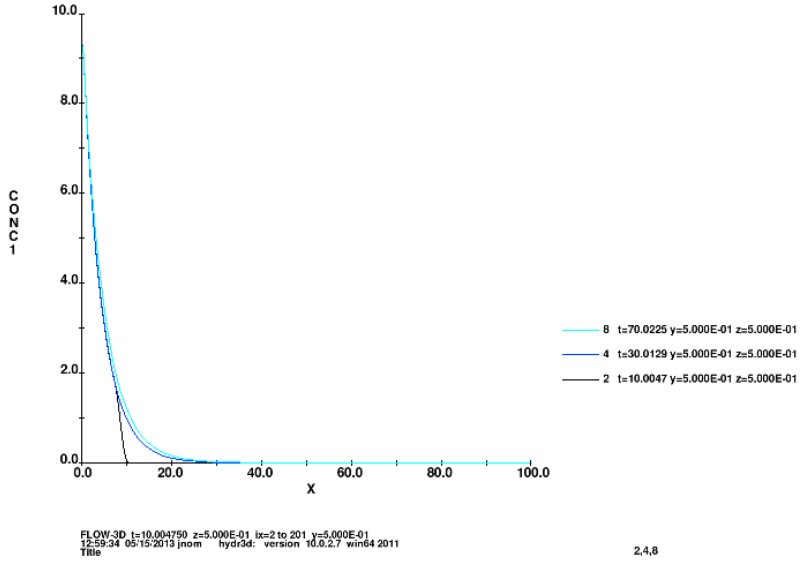


Figure 2 Development of specie C_1 behavior through time for 2.2.

In literature is possible to verify that results in last cases was correct. In the next section it is going to show the results corresponding to 2.3 and 2.4 points. Consider two species, C_1 is taken as oxygen and C_2 is organic carbon they are relating as in eq. (4) and (5). D = 0.2 m^2/day, $k_h^1 = k_h^2$ = 0.1 mg/l, $V_m^1 = V_m^2$ = 1days^{-1}, $k_{1\text{-}2}$ = 2.0, $k_{2\text{-}1}$ = 0.5, t = *68 days*. X is taken to be fixed at 0.2 mg/l. Initial conditions are assigned as: $C_1(x,0)$ = 3.0mg/l, $C_2(x,0)$ = 0.0 mg/l. Boundary conditions are: $C_1(0,t)$ =3.0 mg/l, $C_2(0,t)$=10.0 mg/l. Length domain is 100 m. In order to maintain the international system of units, the units *mg/l* were converted to kg/m^3. To facilitate comparison between results, the values shown in this studio should be are multiplied by 1000. The results of Erwing and Celia (1992), are shown next.

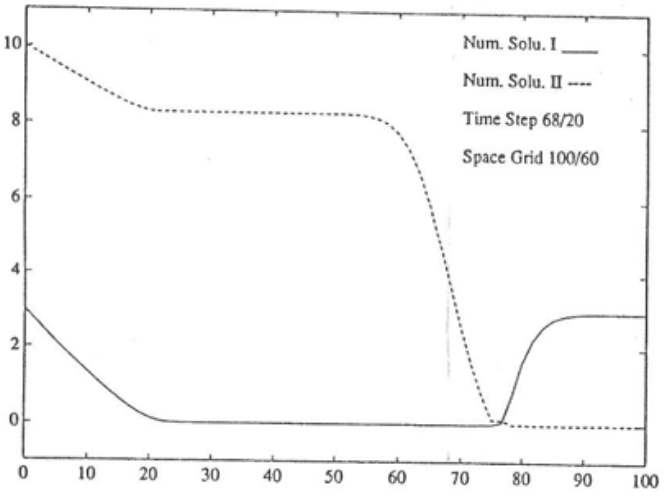


Figure 3 Results obtained for this case by Erwin and Celia (1992) with ELLAM method.

There are studies showing that the finite difference schemes are not stable because its solutions oscillate and to obtain a numerical solution (without the appearance of spurious oscillations or numerical diffusion) is necessary to meet the requirements of Courant and Peclet numbers, Cr<1 and Pe <2, which would imply use very fine meshes, and that the time steps are very small (Arroyo, V. 2005).

CFD software used is based on a finite-volume scheme, therefore, this verification is quite relevant to test the stability of the solutions thrown by this. The results are shown below.

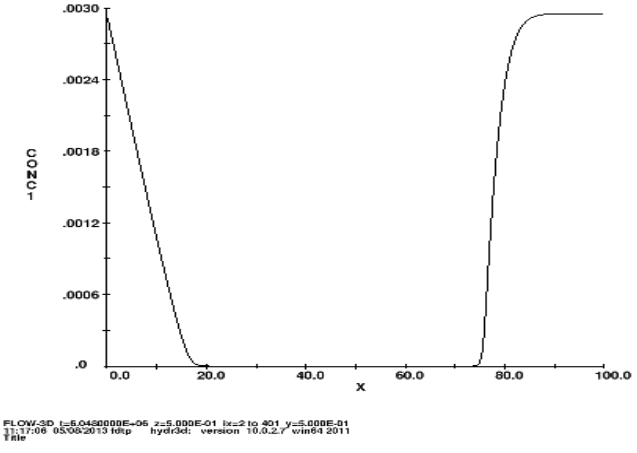


Figure 4 Results of convection-diffusion-reaction transport for oxygen (C_1)*

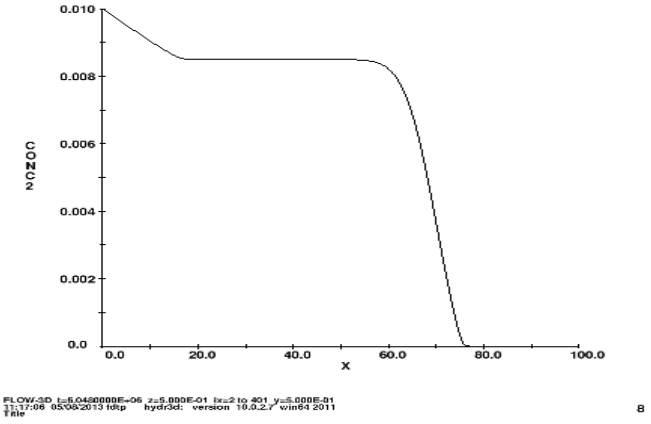


Figure 5 Results of convection-diffusion-reaction transport for organic carbon (C_2)*

*Values in kg/m^3

As can be seen the numerical values of the solutions obtained in this work and the reference work fit in an adequate way. The solution in finite volume used a Courant number of 0.3125 and Peclet number of 1.25.

Previous tests show that the software Flow-3D™ reproduces adequately the scalar transport phenomena, also some analytical solutions (Arroyo, V. 2005), by the above, the software was used to simulate the degradation of organic carbon in an artificial lake using a water shallow model. The lake would receive wastewater from a nearby park and it was considered that the movement in the lake promote aeration and thus the degradation of organic carbon, such movement is accomplished by means of two sources and a sink. These sources provide a flow rate of 1.5 m^3/s each one while the sink extract 3m^3/s, through pumping by this mechanism was possible the water level remained constant, artificial lake depth was 1.3 m .

Two scenarios were modeled, in the first through the two sources were discharged simultaneously dissolved oxygen and organic carbon, the second was made pursuant to a policy of pumping, which alternated injection of oxygen and the organic carbon, although this variables are not revised exhaustively because the main purpose is just coupling the reactive equations transport to a hydrodynamic model.

The approximate dimensions of water body are: horizontal length 218 m, 330 m in transversal extent and a depth of 1.30 m. We tested different sizes of mesh, finally selected one which is not so fine but it got good results in the shortest time, even though the fine meshes can capture motion in more detail, the computation time is too long. Selected mesh was 105 x 165 x 2 elements. The case was run on a dell precision 690 workstation with 2 quad-core processors 2766 mhz, a time of 86400 seconds equal to 24 hours.

The following diagram shows how the artificial lake and the position of the sources and sink, respectively: x_{S1}=50.12 m, y_{S1}=284.12 m; x_{S2}=152.47 m, y_{S2}= 62.21 m, x_{SK} =30.02 m, y_{SK} = 160.00 m. As in the section 2.3, C_1 is taken as oxygen and C_2 is organic carbon they are relating as in eq. (5) and (6). D = 0.2 m^2/day, $k_h^1 = k_h^2$ = 0.1 mg/l, $V_m^1 = V_m^2$ = 1days^{-1}, $k_{1\text{-}2}$ = 2.0, $k_{2\text{-}1}$ = 0.5, t = *1 day*. X is taken to be fixed at 0.2 mg/l. Initial conditions are assigned in all domain: $C_1(x,0)$ = 3.0mg/l, $C_2(x,0)$ = 0.0 mg/l, and in each source $C_1(x,0)$ =1.5 mg/l, $C_2(x,3)$=5 mg/l. It is a confined body water.

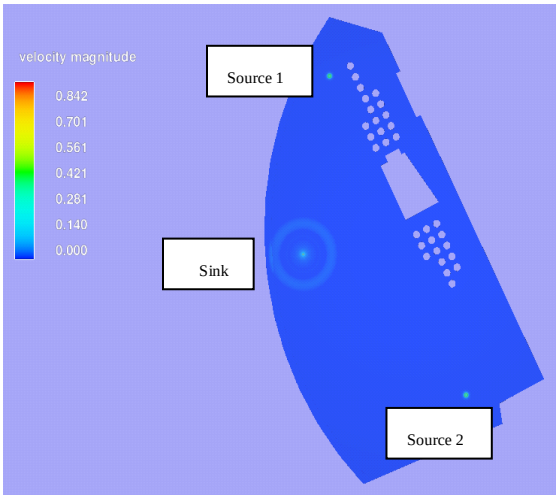


Figure 6 Schematic figure of the artificial lake with its sources and sinks

As was told before, the first exercise of 2D modeling was discharge at same time through sources oxygen and carbon organic, it can be seen that the reaction of scalars occurred mainly in the first 8 hours (figures

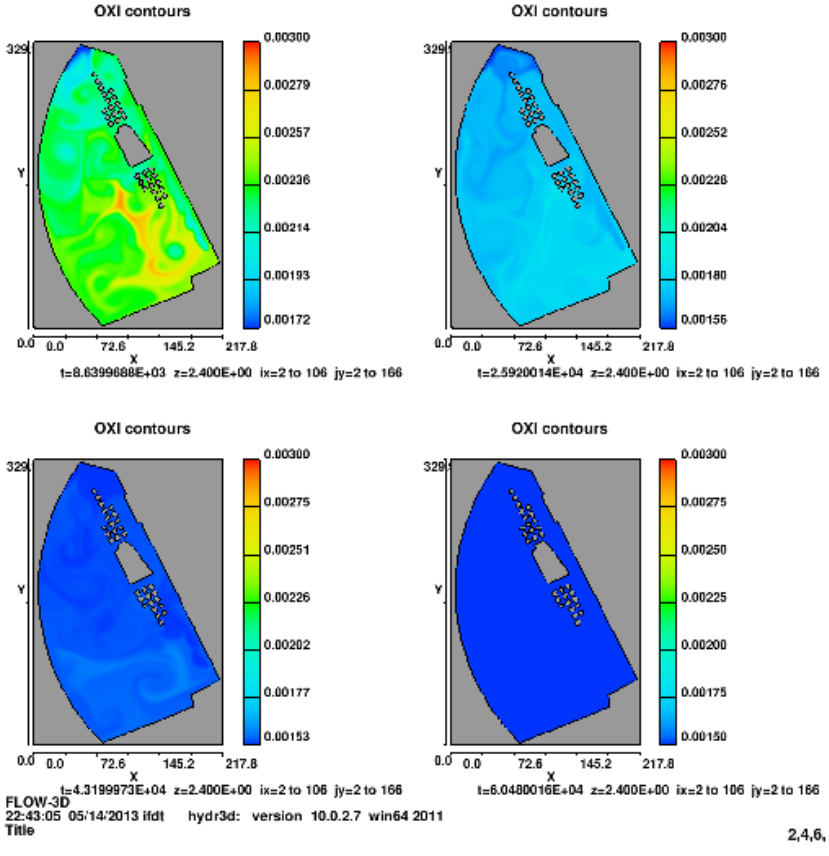


Figure 7 Development of C_1 trough time when both scalars were injected simultaneously

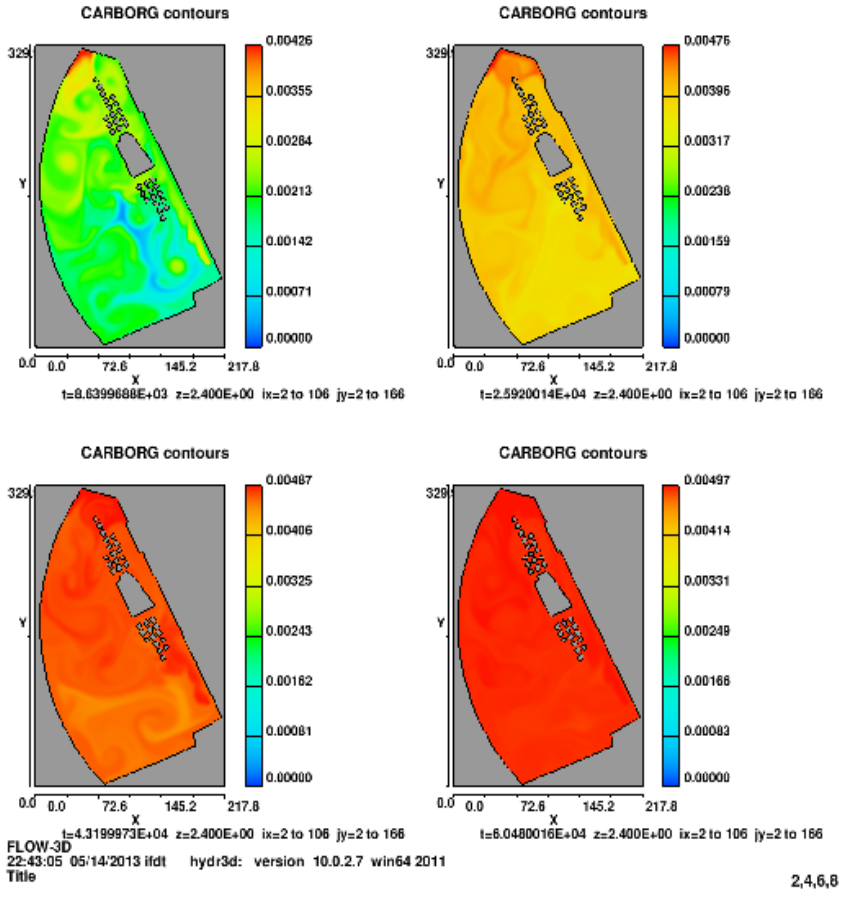


Figure 8 Development of C_2 trough time when both scalars were injected simultaneously

7 and 8) after that, the concentrations of both scalars reach its discharge value C_1=0.0015 *mg/l*, C_2=0.005 *mg/l*, almost uniformly throughout the body of water. The reason could be that last approximately 8 hours to circulate the total volume of the water, the scalars stabilize at a value close or equal to the discharge because the water is circulated throughout the simulation time with same concentration. To avoid this situation and for that the degradation of organic matter was more effective, was proposed inject alternately oxygen and organic carbon according to a policy of pumping (figure 9). This was allowed that two scalar react almost all the time, without accumulating as happened in the first case.

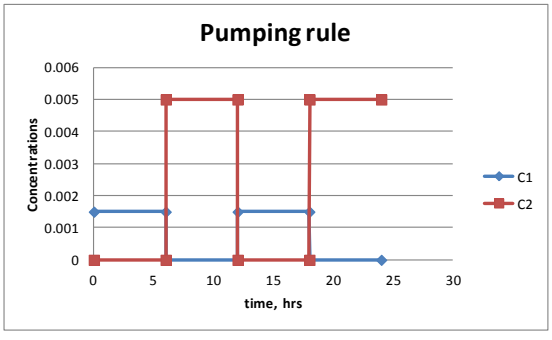


Figure 9 Pumping rule of scalars for second case of 2D modeling

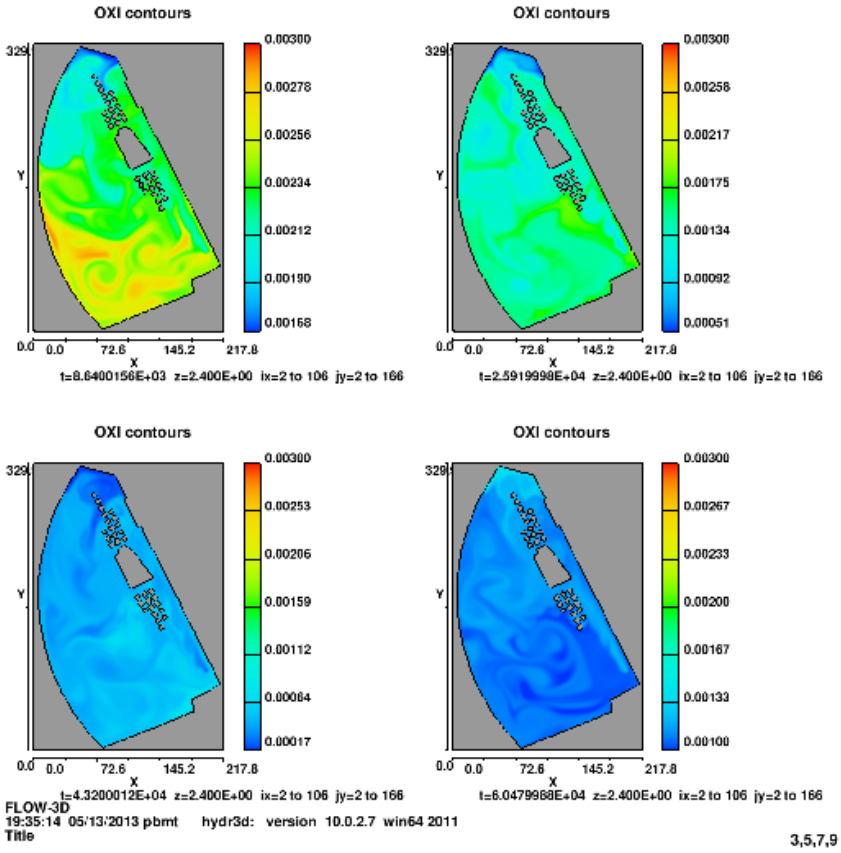
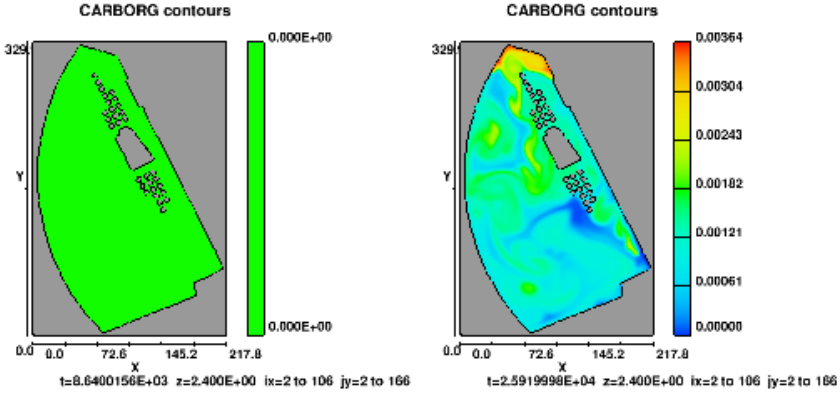


Figure 10 Evolution of reactive C_1 in lake when scalars were injected alternatively.



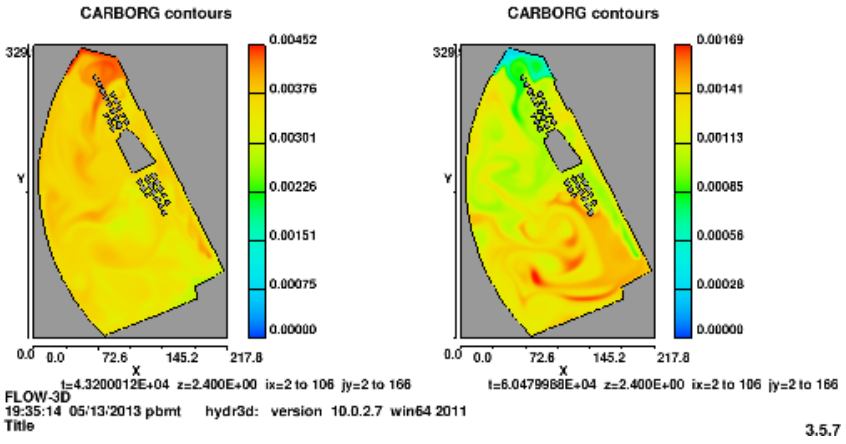


Figure 11 Evolution of reactive C_2 in lake when scalars were injected alternatively.

4 CONCLUSIONS

The results of the present study are satisfactory. The CFD Software is a reliable tool to reproduce both analytical solutions and also more stable schemes, such as ELLAM a lagrangian method that uses unstructured meshes (finite element) whose main characteristic is the speed to obtain solutions.

At first, it was made every attempt to use the default chemical model brings software (eq. 1) to model nonlinear relationships. This was done by means of graphs and interpolation curves of 4th, 5th and 6th grade, however, the polynomials obtained did not efficiently to the plots, especially near zero, so that the solutions oscillated widely, no matter the software CFD used can adjust the numerical parameters and search for a stable solution, the results of the kinetics differed markedly. There was a clear improvement when with advisory of Flow Science Inc, the authors programmed the complete differential equations (eqs. 4 and 5) in the corresponding subroutine and compiling the software, results can be seen comparing figures 3 with figures 4 and 5.

In the resulting plots a slow movement throughout the lake, with flow patterns move dissolved oxygen and organic carbon concentrations (Figures 7, 8, 10, and 11).

Through the results of modeling of nonlinear chemical-biological processes was concluded that it was better to discharge the scalars through a policy of pumping to lake instead pouring simultaneously, permitting in that way the reacting and degradation of the pollutants. For example, in first case of modeling the lake, in a time t = 25 920 s, the two variables have reached their limit in most of the domain C_1 = 0.0018, C_2 = 0.004 (see figure 7b and 8b), while for the second case at the same time C_1 = 0.001, C_2 = 0.0012 (see figures 10b and 11b), it is interesting because the low level of oxygen C_1 indicates interchange between reactants, as organic carbon C_2 consumes oxygen at a rate of 2:1 in this study.

Finally, this study allow to gain experience and good background to implement a hydrobiological model 2D/3D in water bodies, which will be developed at a later stage of this study.

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