ORGANIC MATTER DECAY MODELING FOR NUMERICAL SIMULATIONS OF HYDROELECTRIC RESERVOIR FILLING

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Abstract. *Brazil's great hydrographic potential makes hydroelectric power plants the base of our electric energy supply, and the consequent inundation of a hydrographic basin provokes many different problems for the water quality, due to biochemical phenomena, such as organic matter decomposition. This work presents a computational methodology for the determination of the organic matter decay on a hydroelectric reservoir filling, applied on numerical simulation of the ambient impacts caused by this process. The most influent parameter in water quality is oxygen concentration, therefore the organic matter decay modeling is associated to oxygen concentration balance, through a DO – CBOD model. The mass decomposition is calculated from the solution of simple differential equations, whose decay coefficient is function of parameters determined by the solution of hydrodynamic and transport equations, which are coupled by the oxygen density, or oxygen demand distribution. Because of the complexity of the code, special attention is given to the optimization of its construction, approaching terrain and phytophysiognomy data manipulation, mesh generation, and object oriented programming.*

Keywords*: Organic Matter Decay, Numerical Simulations, Hydroelectric Reservoir, Oxygen Demand.*

1. INTRODUCTION

The decomposition of drown organic matter in a reservoir can significantly change the chemical balance in water environments, and the most influent parameter in water quality study is oxygen concentration. This is an essential element for more complex forms of life, controls many chemical reactions by oxidation and indicates the general conditions of aquatic systems quality. This work will present a model built to provide a resource for quantification of oxygen concentration through an interaction model between BOD (biochemical oxygen demand) and DO (dissolved oxygen). BOD is an equivalence of vegetal mass density on the aquatic phase in oxygen demand, while DO is a balance of the oxygen absorbed by the aquatic system due to reareation (surface O_2 inflow) and organic decomposition (O_2 consumption), which is proportional to BOD concentration.

The BOD-DO balance in hydroelectric reservoir filling processes is associated with the hydrodynamic behavior, and this coupling is in the core of discussions on ecological equilibrium of lakes and reservoirs. Influenced by physical, chemical and biological factors, the living organisms react to hydrodynamic variations, determining interaction on nutrients recycling, on planktonic populations dynamics and organic production "(Legendre & Demers, 1984; Harris & Trimbee, 1986)". The importance of a BOD-DO model dwells in the fact that the energy and mass fluxes that characterize an ecosystem behavior are determined, among other factors, by transformations associated to organic matter production, consumption and decomposition processes. Besides, the interaction of the water column with the lake sediment and the organic matter oxidation constitute essential factors for nutrients liberation and maintenance of biogeochemical cycles in the aquatic ecosystems "(Jorgensen, 1988)". As the water issue is taking larger space on discussions of international organizations about the planet future, and since Brazil has a great hydrographic potential, making hydroelectric power plants the base of electric energy supply, the importance of the water problem is even bigger. Models of predictions on ambient impacts play an increasing role on the study and control of ecological systems wealth, especially in environments with human alterations. The objective of water quality models as management tools is much accentuated in systems that suffer anthropogenic influence "(Jorgensen, 1988)".

The hydrodynamic approach is necessary to simulate the changes on oxygen rates and distribution in the water during and after a reservoir filling. In this work the problem is mathematically modeled by the Navier-Stokes equations coupled to transport equations, in the 2DH form. The domain is discretized in a two-dimensional triangular mesh and the solution is numerically obtained by means of Finite Element Method. Since the focus is the filling process, and the consequent flooding, of a hydrographic basin, the terrain modeling deserves especial attention, as well as the mesh generation procedure, stages of the simulation that will be addressed in this paper.

The global approach of this simulation tool is traduced in a complex computational system, involving modules responsible for each stage of the simulation, such as terrain modeling, phytophysiognomic data manipulation, among

others, in the intent of reaching accurate prediction results. Additionally, the code development follows the Object Oriented concept, allowing a more dynamic and flexible programming.

2. SIMULATION ENVIRONMENT

First, it would be helpful to have a brief understanding over the system's structure. The simulation environment is composed of several modules that encapsulate specific tasks in the simulating process. A quick explanation on each module is shown below.

2.1. Terrain

Here the terrain data sets are handled. This is where the user defines the domain of simulation.

2.2. FEMesh2d

Responsible for two-dimensional triangular mesh assembling.

2.3. Phyto

The vegetation map of the terrain in study is manipulated in this module, as well as the phytophysiognomy data.

2.4. Decay

This module is responsible for the biomass decay modeling. It quantifies the organic mass transferred to the water, which impacts on the chemical elements percentages present in the reservoir water.

2.5. Simulator

In this module all the information handled in the other modules is collected for the simulation itself.

The modules can be accessed using a high level script language, based on MATLAB, which gives great power and flexibility to the user. Alternatively, the user can employ a simple Graphic User Interface (GUI) to perform common tasks. Figure 1 shows a simplified scheme of the whole system of simulation, where the data flux between the modules is represented by the arrows.

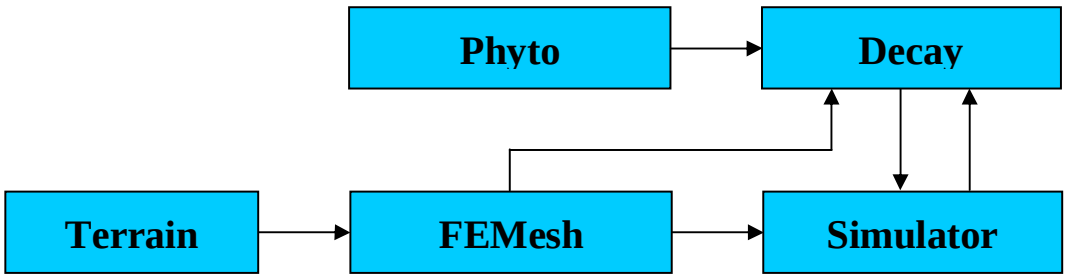

Figure 1. Data flux between the system's modules.

The FEMesh generator module is closely related to the terrain modeling module. In fact, the triangular mesh is built using topological data provided by the Terrain module. The terrain can be represented by a set of points (named CloudTerrain), a cartesian mesh of points (RasterTerrain), a set of level-curves (ShapeTerrain), or a triangular mesh (MeshTerrain). The mesh triangulation is made from the CloudTerrain representation, using Delaunay triangulation. After this stage, the mesh can be improved employing a refining algorithm, and information regarding boundary conditions is included in the data structure, to prepare for the application of the mesh in the Finite Elements Method, in the Numerical Simulations Module.

3. CONCEPTUAL MODEL:

The biomass present in the reservoir is classified in four basic mass types – barks, thin branches, leaves and litter – and each one have slow labile and fast labile mass percentages. The model utilizes data from several sources, mainly based on topologic and phytophysiognomic information about the terrain. The phytophysiognomic data are contained in

a vegetation map (ShapePhyto) and complemented by phytophysiognomy data files. In a first step, the initial calculation of the organic mass is performed separately for each element of the mesh, combining the region occupied by the triangle with the corresponding ShapePhyto area, and applying the superficial densities for each phytophysiognomy and mass type. The second step consists of updating the mass quantities in specified time steps, according to the solution of decay differential equations system. The independent computation of the biomass for each element of the mesh provides a spatial distribution of the densities, in the area covered by the reservoir, which allows the identification of regions where the impacts are more critical and the oxygen consumption by the decomposition is more accentuated. The oxygen rates present in the water are also function of oxygen intake through the lake surface, by reareation.

4. MATHEMATICAL MODEL

4.1. 2DH Navier-Stokes equations

The governing equations for the hydrodynamic circulation were described by "Rosman (2001)", in which the 2DH technique is employed to solve the kind of problem this work is focused on. More details about 2DH hydrodynamic modeling can be found in this reference. Here, the main results will be briefly presented.

For each time step the 2DH simulator determines the vertically averaged velocity, components in the *x* and *y* directions, *U(x,y,t)* and *V(x,y,t)* respectively, and the elevations on the free surface, *z=ζ(x,y,t)*. The three necessary equations to determine three unknowns of hydrodynamic circulation in 2DH flow, integrated on the vertical direction, ζ, U and V, are represented below:

2DH equation of momentum conservation for a flow integrated on the vertical, in the x direction:

$$\frac{\partial U}{\partial t}+U\frac{\partial U}{\partial x}+V\frac{\partial U}{\partial y}=-g\frac{\partial \zeta}{\partial x}+\frac{1}{\rho_0 H}\left(\frac{\partial(H\,\bar{\tau}_{xx})}{\partial x}+\frac{\partial(H\,\bar{\tau}_{xy})}{\partial y}\right)+\frac{1}{\rho_0 H}\left(\tau_x^s-\tau_x^B\right)+2\phi sen\theta V \tag{1}$$

Where *H* is the distance from the bottom to the surface at each point, and ρ_0 is the water density.
2DH equation of momentum conservation for a flow integrated on the vertical, in the y direction:

$$\frac{\partial V}{\partial t}+U\frac{\partial V}{\partial x}+V\frac{\partial V}{\partial y}=-g\frac{\partial \zeta}{\partial x}+\frac{1}{\rho_0 H}\left(\frac{\partial(H\,\bar{\tau}_{xy})}{\partial x}+\frac{\partial(H\,\bar{\tau}_{yy})}{\partial y}\right)+\frac{1}{\rho_0 H}\left(\tau_y^s-\tau_y^B\right)-2\phi sen\theta U \tag{2}$$

Continuity equation integrated along the vertical direction:

$$\frac{\partial \zeta}{\partial t}+\frac{\partial UH}{\partial x}+\frac{\partial VH}{\partial y}=0 \tag{3}$$

The terms of equation (1) can be explained as follows:

$\frac{\partial U}{\partial t}\rightarrow$ represents the local acceleration of the flow, at a given position, or, in other words, the temporal variation rate of the 2DH momentum flux per mass unit. In permanent flows, this term is zero.

$U\frac{\partial U}{\partial x}+V\frac{\partial U}{\partial y}\rightarrow$ represents the advective acceleration of the flow, on a given instant. These terms represents the spatial variation rate of the 2DH momentum flux on the x direction per mass unit. In uniform flows, these terms are zero.

$-g\frac{\partial \zeta}{\partial x}\rightarrow$ represents the resultant hydrostatic pressure on the x direction (pressure gradient). Due to the water surface declivity on the x direction, as indicated by the negative sign, the flow tends to move from places where the water level is higher to places where the water level is lower.

$\frac{1}{\rho_0 H}\left(\frac{\partial(H\,\bar{\tau}_{xx})}{\partial x}+\frac{\partial(H\,\bar{\tau}_{xy})}{\partial y}\right)\rightarrow$ represents the resultant of the 2DH turbulent dynamic tensions in the flow. For example, these terms are caused by horizontal vortices in recirculation zones.

$2\phi sen\theta V\rightarrow$ represents the Coriolis force. This term is present because the referential is moving with the Earth surface.

$\frac{1}{\rho_0 H}\left(\tau_x^s\right)\rightarrow$ represents the wind tension on the free surface per mass unit. If the wind is on the same direction of the flow, this term will speed up the flow; otherwise, if the wind is on the opposite direction, it will slow down the flow.

$\frac{1}{\rho_0 H}\left(-\tau_x^B\right)\rightarrow$ represents the friction tension on the bottom of the flow per mass unit. As indicated by the negative sign, this term always tends to decelerate the flow. It is always opposite to the flow.

Evidently, the meaning of the similar terms in the equation (2), of the momentum conservation on the y direction is analogous.

For the 2DH continuity equation (3), we have:

$\frac{\partial(\zeta+h)}{\partial t}=-\frac{\partial HU}{\partial x}-\frac{\partial HV}{\partial y}\rightarrow$ represents the variation of the water column height (ζ+h) in time as result of the effective fluxes through the water column on the x and y directions, respectively $\frac{\partial HU}{\partial x}$ and $\frac{\partial HV}{\partial y}$.

The water source is given only by tributary rivers, where the boundary conditions are prescribed velocity. The points of outflow are treated with prescribed height ζ boundary conditions, and on the reservoir margins the velocity is equal to zero. The water source due to precipitations is accounted for in the inflow velocities.

The solution technique chosen is the Finite Element Method with Galerkin variational formulation. The method is applied on a mesh of Delaunay triangles, with the domain represented by mini-elements – pressure on the vertices and velocity on the vertices and centroid. For the convective term, the semi-lagrangian formulation was used, and the projection method was chosen to decouple the velocity and pressure calculations.

The discretization produces two algebraic linear equation systems in each time iteration. To solve these systems, the preconditioned conjugated gradient method is employed, using an incomplete Cholesky preconditioner.

4.2. Transport Equations

If ϕ_1 and ϕ_2 represents the DO and BOD concentrations, respectively, the transport equations can be written as follows:

$$\frac{D\phi_1}{Dt}-div(Dgrad\,\phi_1)=-k\phi_1\phi_2+(\phi_{SAT}-\phi_1)h_{reaer} \tag{4}$$

$$\frac{D\phi_2}{Dt}-div(Dgrad\,\phi_2)=-k\phi_1\phi_2+k_{dec}\dot{\phi}_2 \tag{5}$$

where D is a diffusion coefficient, k is a constant related to the DO-BOD chemical interaction, h_{reaer} and k_{dec} are coefficients for the source terms of oxygen transport and BOD transport, respectively, ϕ_{SAT} is a saturation O_2 concentration and $\dot{\phi}_2$ is a BOD source (it is equivalent to the biomass transferred to the water in a time step).

4.3. Decay modeling

An initial mass is calculated, from which the variation of organic matter quantity will be obtained (*M*). This initial mass is determined, in each element of the mesh, from the relation of the areas covered by the different phytophysiognomy types, provided by the ShapePhyto module, with its respective superficial density.

$$M_{tm} = \alpha_{tm} \times \rho_{ff} \times A_{ff} \tag{6}$$

where M_{tm} is the mass of type *tm* (which can be leaf, litter, thin branch or bark), α_{tm} is the mass type percentage *tm* related to the specified phytophysiognomy, ρ_{ff} is the superficial density of organic matter respect to the phytophysiognomy *ff* and A_{ff} is the area covered by it.

The result is stored in a matrix M_{mn}, where *m* is the number of elements in the mesh and *n* represents the number of mass types, constituting a matrix whose lines carry the quantity of each mass type in a certain element. Every calculated organic mass holds a percentage of slow labile biomass and another of fast labile biomass, in such a way that the obtained matrix of initial masses can be decomposed in a sum of two others: one of slow labile mass and another of fast labile mass. It can be represented as follows:

$$[F \quad G \quad C \quad S] = [F_L \quad G_L \quad C_L \quad S_L] + [F_R \quad G_R \quad C_R \quad S_R] \tag{7}$$

where *F*, *G*, *C* and *S* represents the leaves, thin branches, barks and litter masses, respectively; *L* and *R* represents slow and fast labile masses.

Mass update:
The organic matter decay is given by the equation "(Bianchini, 2005)":

$$\frac{dm}{dt} = -km \tag{8}$$

where *m* is the mass, $\frac{dm}{dt}$ the temporal variation of *m*, and *k* is a decay coefficient, considered constant at each time step. It allows us to write:

$$m = Ce^{-kt} \tag{9}$$

where *C* is an integration constant. From the initial condition $m = m_0$ we have:

$$m = m_0 e^{-kt} \tag{10}$$

During the iterative process the initial mass will be obtained from the previous time step, resulting in the following exponential equation:

$$M^p = M^{p-1} e^{-k\Delta t} \tag{11}$$

where p is the iteration index and Δt is the time increment.

The transport equations as well as the Navier-Stokes equations are taken into account in its non-dimensional form.

5. SIMULATIONS

First, we select a terrain region and call the 2-d mesh generator. After some refining routines, the boundary conditions are inserted and the corresponding terrain vegetation map is loaded, carrying out the phytophysiognomy data. The organic matter decay and reareation coefficients also must be set.

The next two figures show the selected terrain area in a ShapeTerrain representation and the bi-dimensional mesh, which gives us a good perspective on the reservoir topology.

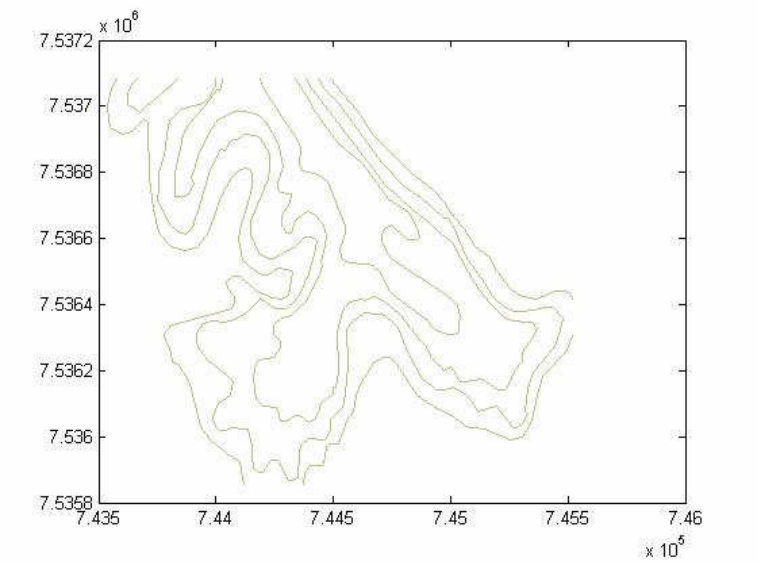

Figure 2. ShapeTerrain model

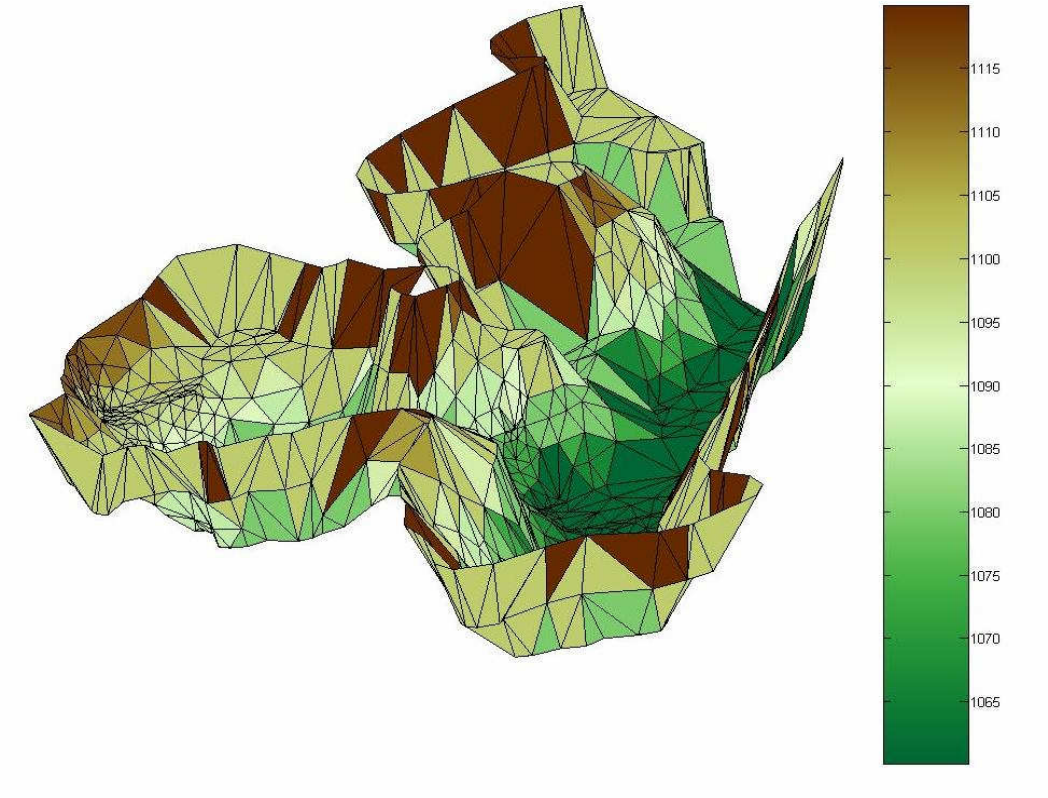

Figure 3. perspective of the two-dimensional mesh

After refining the mesh, which is an optional task, the outflow boundary must be indicated. The next stage is boundary conditions insertion and consists of informing the two velocity components *u* and *v*, the DO and BOD inflow concentrations and an artificial height *H*.

In figure 4 we can see the vegetation map (ShapePhyto) representing the regions of different phytophysiognomy. Traducing it in biomass density, the Decay module provides a first notion of the locations of more potential organic matter decomposition. This is graphically represented by figure 5.

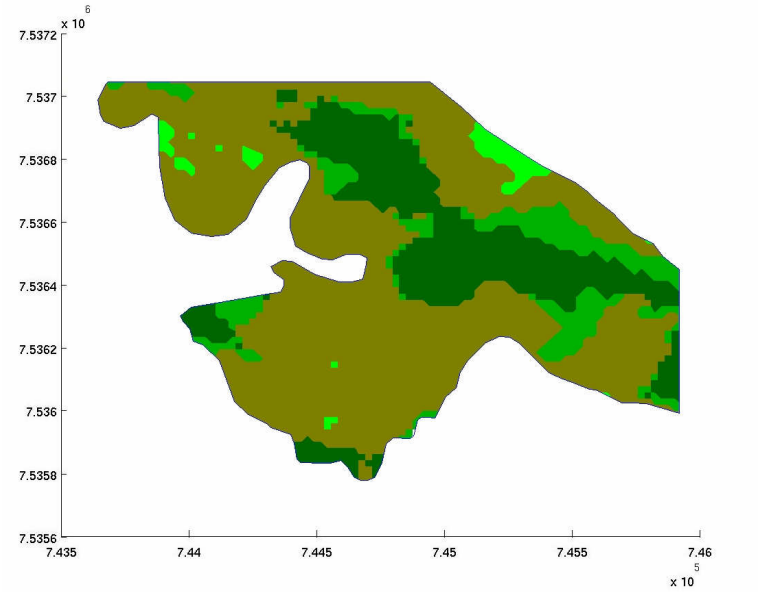

figure 4. ShapePhyto vegetation map (phytophysiognomy distribution)

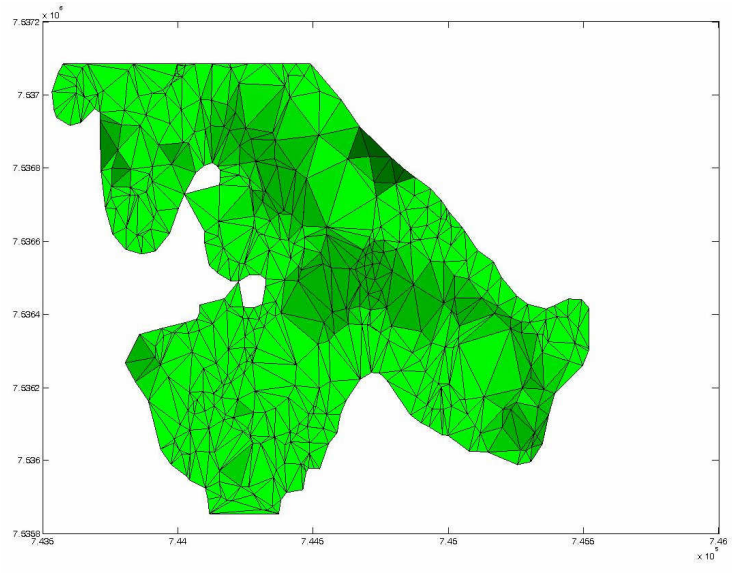

figure 5. biomass density distribution

The following figures show the time evolution of DO/BOD concentrations. Note that the expected areas of major BOD concentrations are pretty visible in the first figures, before the chemical reaction with dissolved oxygen.

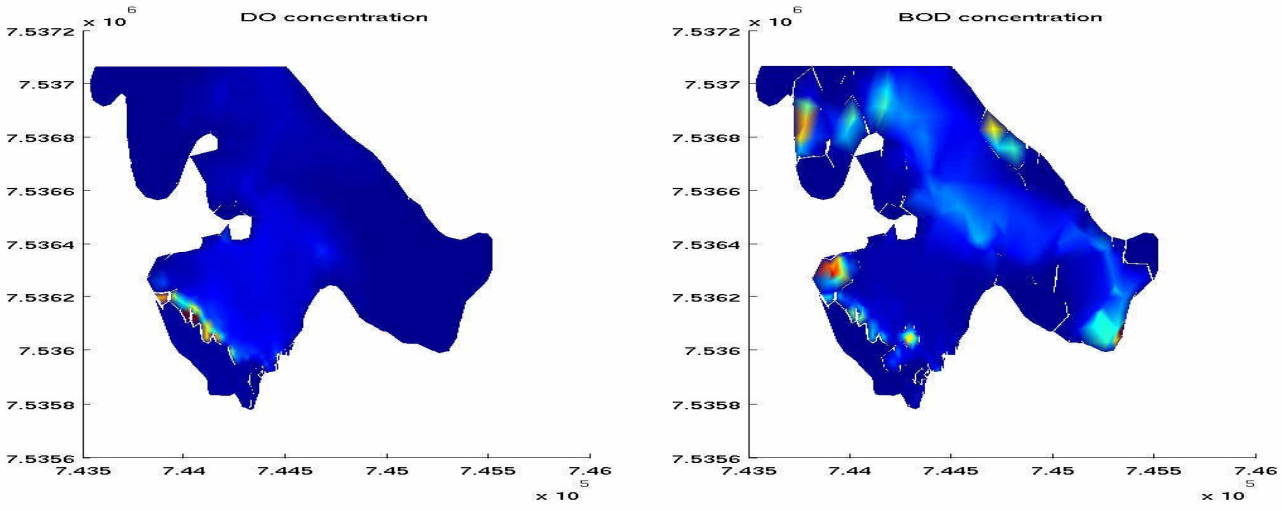

Figure 6. time step 0

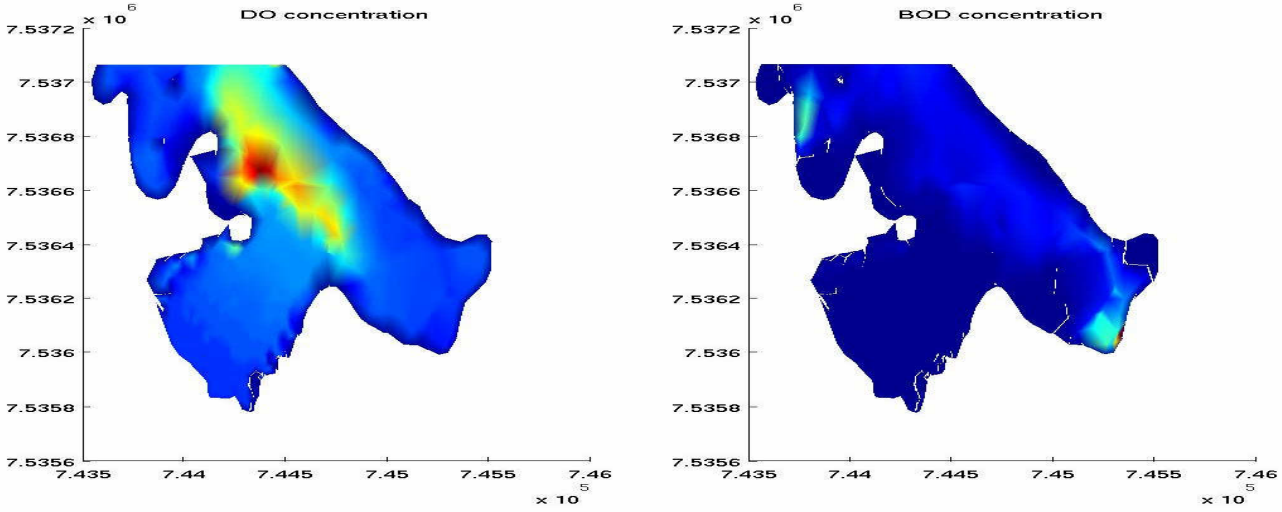

Figure 7. time step 7

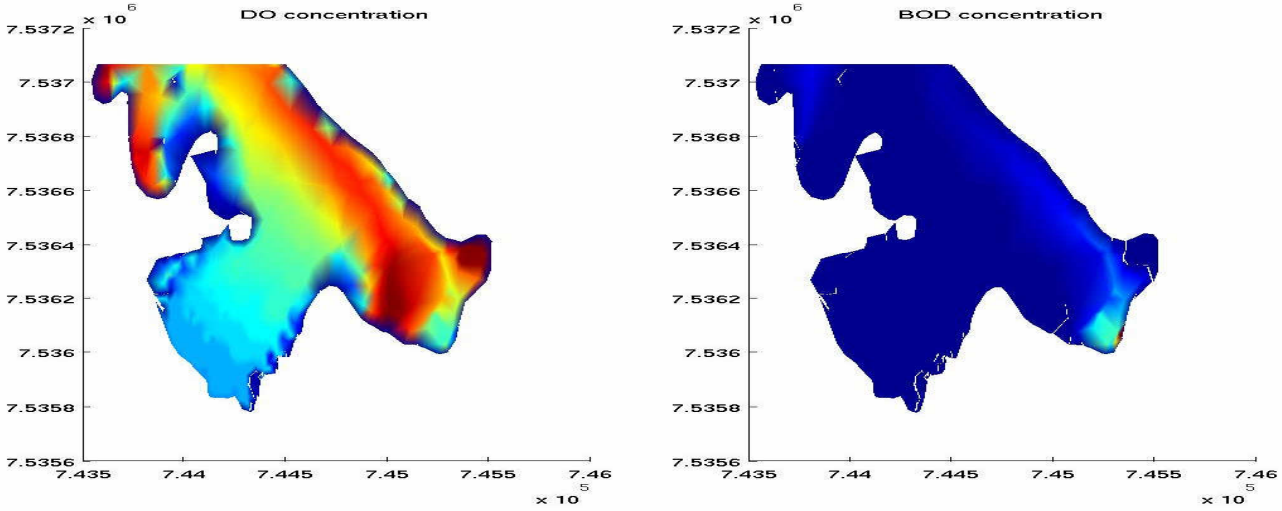

Figure 8. time step 28

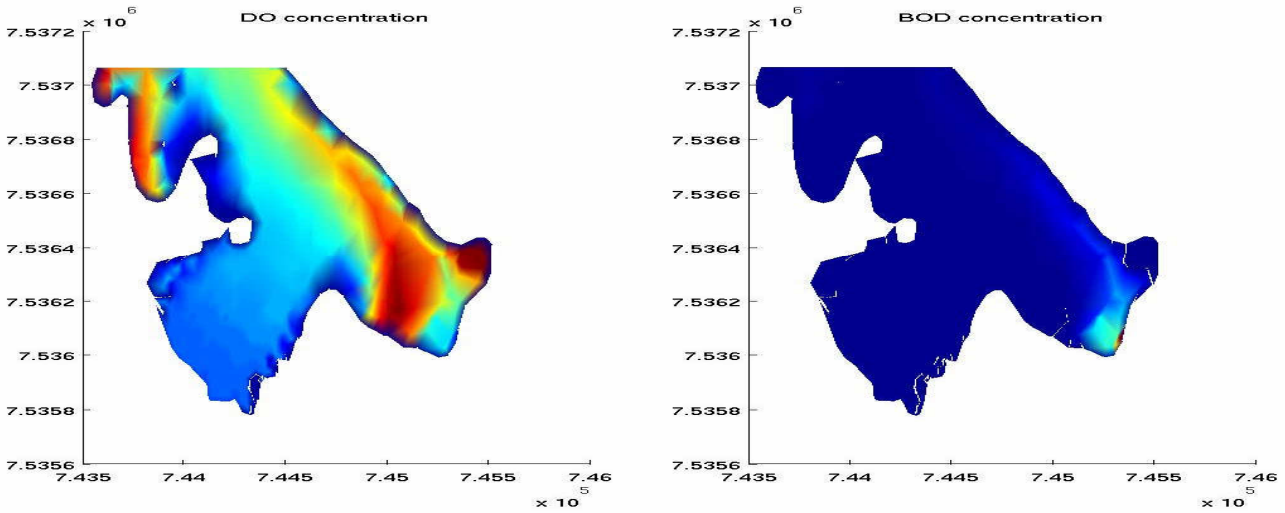

Figure 9. time step 35

6. CONCLUSION

The presented resources of terrain data manipulation and mesh generation, which allows a large flexibility on the discretization of the simulation domain, allied to the adopted numerical methodology, constitute an efficient prediction tool about the possible impacts on water quality in reservoir environments. As the computational structure, the presented model proved to be of fast and flexible development, providing the possibility of incorporating other parameter to the biochemical model, in the research continuation, such as phosphorus and oxygen production and consumption due to algae populations.

7. ACKNOWLEDGEMENT

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