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A transport modeling of the carbon-nitrogen cycle at Igapó I Lake - Londrina, Paraná State, Brazil

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ABSTRACT. This work is a contribution to a better understanding of the effect that domestic sewage discharges may cause in a water body, specifically at Igapó I Lake, in Londrina, Paraná State, Brazil. The simulation of the dynamics of pollutant concentrations throughout the water body was conducted by means of structured discretization of the geometry of Igapó I Lake, together with the finite differences and the finite elements methods. Firstly, the hydrodynamic flow (without the pollutants), modeled by Navier-Stokes and pressure equations, was numerically resolved by the finite differences method, and associated with the fourth order Runge-Kutta procedure. After that, by using the hydrodynamic field velocity, the flow of the reactive species (pollutants) was described through a reaction transport model, restricted to the carbon-nitrogen cycle. The reaction transport model was numerically resolved by the stabilized finite elements method, by means of a semi-discrete formulation. A qualitative analysis of the numerical simulations provided a better understanding of the dynamics of the processes involved in the flow of the reactive species, such as the dynamics of the nitrification process, of the biochemical demand of oxygen and of the level of oxygen dissolved in the water body at Igapó I Lake.

Keywords: water quality model, pollutants, numerical simulation, finite differences method, finite elements method.

Uma modelagem do transporte do ciclo carbono-nitrogênio no Lago Igapó I - Londrina, Estado do Paraná, Brasil

RESUMO. Este artigo é uma contribuição para um melhor entendimento do efeito que uma descarga de esgoto doméstico pode causar num corpo d'água, em particular, no lago Igapó I, Londrina, Paraná, Brasil. A simulação da dinâmica das concentrações dos poluentes em todo o corpo d'água é realizada por meio de uma discretização estruturada da geometria do lago Igapó I, juntamente com os métodos de diferenças finitas e de elementos finitos. Primeiramente, o escoamento hidrodinâmico (sem os poluentes), modelado pelas equações de Navier-Stokes e de pressão, é resolvido numericamente pelo método de diferenças finitas, associado ao procedimento de Runge-Kutta de quarta ordem. Em seguida, utilizando o campo de velocidades fornecido pelo modelo hidrodinâmico, descreve-se o escoamento de espécies reativas (restrito ao ciclo carbono-nitrogênio), por meio de um modelo de transporte de poluentes com reações. O modelo de transporte de poluentes com reações é resolvido numericamente pelo método de elementos finitos estabilizados, através de uma formulação semi-discreta. Uma análise qualitativa das simulações numéricas proporcionou uma melhor compreensão da dinâmica dos processos envolvidos no escoamento de espécies reativas, tais como a dinâmica do processo de nitrificação, da demanda bioquímica de oxigênio e do nível de oxigênio dissolvido no corpo d'água do lago Igapó I.

Palavras-chave: modelo de qualidade de água, poluentes, simulação numérica, método de diferenças finitas, método de elementos finitos.

Introduction

The growing demographic and industrial expansion that has been observed in recent decades brought about, as a consequence, water pollution caused, among other factors, by the discharge of industrial and domestic sewage. With waters from rivers, lakes and reservoirs compromised, sophistication in the treatment of such a resource is increasingly required. Therefore, to understand this issue and search for solutions is a highly important current problem, and one way to solve it is to analyze the relationship between the polluting sources and their degradation mechanisms by using water quality models.

According to Chapra (1997), the history of water quality modeling can be presented in four phases.

The first phase had as its landmark the model proposed by Streeter and Phelps (1925). This model described the consumption process of oxygen and the reaeration capacity of the water body by means of two first order ordinary differential equations, considering permanent and uniform flow. Due to lack of computer tools, the models from the 1920's to the 1960's were one-dimensional and limited to the primary treatment of effluents in streams or estuaries with linear kinetics and simple geometries. Such models presented analytical solutions.

In the second phase, during the 1960's, technological advances allowed numerical approaches in more complex geometries. The focus started to be the primary and secondary treatment of effluents and the transport of pollutants in streams and estuaries, modeled in two dimensions. In this period, based on O'Connor and Dobbins's (1958) proposal, models were proposed and consisted of second order differential equations, which added the benthonic and photosynthesis demand treatment to the models from the first period.

In the third phase, in the 1970's, the water body started to be observed as a whole. The eutrophication process, excessive proliferation of algae caused by nutrients in excess, was the focus of the models. Therefore, representations of the biological processes started to be studied in streams, lakes and estuaries. Simultaneously, non-linear kinetics and three-dimensional models also started to be studied by means of numerical simulations. At that time, concern with the environment and ecological movements increased in some sectors of the society. In this context, in 1971, the Texas Water Development Board (TWDB) created a one-dimensional Water Quality Model (QUAL-I), which allowed the description of advective and diffusive/dispersive transport of pollutants in water bodies (TWDB, 1971). Lately, the United States Environmental Protection Agency (USEPA) improved QUAL-I model, which started to be called QUAL-II, simulating up to 13 species of parameters indicative of water quality in deeper rivers (ROESNER et al., 1981).

The fourth phase ranges from the 1980's to the present. In the beginning of the 1980's there was the emergence of the Task Group on River Water Quality (TGRWQ), a group of scientists and technicians organized by the International Association on Water Quality (IAWQ), which standardized the existing models and manuals. In 1987, due to the several modifications in the QUAL-II model, it was renamed QUAL2E, simulating up to 15 species, accepting punctual and non-punctual sources and fluids both in permanent and non-permanent regime (BROWN; BARNWELL JR., 1987). The QUAL2K model (CHAPRA et al., 2007) is the current improved version of the QUAL2E model. Parallel to that, in 1985, the USEPA developed the Water Analysis Simulation Program (WASP), which simulated one-dimensional, two-dimensional and three-dimensional processes of conventional and toxic pollutants. This model was also modified several times and its current version is the WASP7 (AMBROSE et al., 2006). Other numerous water quality models can be found in the literature, such as the Activated Sludge Models (ASM1, ASM2 and ASM3), developed by IAWQ (HENZE et al., 2000); the River Water Quality Models (RWQM), also developed by IAWQ (SHANAHAN et al., 2001), the Hydrological Simulation Program-Fortran models (HSPF), developed by USEPA, (BICKNELL et al., 2001), among others.

In this context, this paper is a contribution to better understand the effect that domestic sewage discharge may cause in the water body of Igapó I Lake, located in Londrina, Paraná, Brazil. In order to simulate the effects of such a discharge, a horizontal two-dimensional model (2DH model) is used, in which water flow in the discretized geometry of the lake is described by Navier-Stokes and pressure equations, whereas the transport of the reactive species is described by an advective-diffusive model. Finally, the model WASP6 (AMBROSE et al., 2001) is used in its linear version to describe the reactions of the carbon-nitrogen cycle that occur in the transport of reactive species by the hydrodynamic flow.

This paper is organized as follows. In section 2 the structured discretization that generates the geometry grid of Igapó I Lake is described. The water quality model of our study consisted of the hydrodynamic model and of the reaction transport model is presented in section 3. In section 4 the numerical simulations that provide the local concentrations of the carbon-nitrogen cycle are presented. At last, in section 5, a qualitative analysis of the numerical results is conducted.

Material and methods

Modeling of the geometry at Igapó I Lake

Igapó Lake, located in Londrina, Paraná State, Brazil, is situated in the microbasin of Cambé Stream, whose spring is in the town of Cambé, approximately 10 km from the city of Londrina, in the State of Paraná. After the spring, it flows to the west crossing all the southern area of Londrina, gathering many streams along its way. The Lake is

subdivided into: Igapó I, II, III and IV. They were designed in 1957 as a solution for the Cambé Stream drainage problem.

Because it is located near the central area of the city of Londrina, Paraná State, Igapó I Lake receives the discharge of untreated pollutants in its waters, besides the discharge of pollutants from Lakes IV, III and II, which pollute Lake I. As observed in Figure 1, the water flows from Igapó II Lake into Igapó I Lake when crossing Higienópolis Avenue, which characterizes its entrance. In the left bank there is undergrowth, as well as an input channel. The right bank is split in private properties and contains another input channel. The exit is a physical dam and the water flow is controlled by water pipes and ramps.

The longitudinal length of the Lake is approximately 1.8 kilometers, while its average width is 200 meters and its average depth is 2 meters (ROCHA, 1995). The reservoir of the Igapó I Lake was constructed so that the draining of water presents low speed due to low declivity and the small volume of input water compared with water volume of the Lake. These characteristics allow modeling the water flow at Igapó I Lake through a laminar model type 2DH (HORITA; ROSMAN, 2006).

In order to generate the interior grid of Igapó I Lake geometry, a system of elliptic partial differential equations was used. The margins were obtained by parametric cubic spline polynomial interpolation (CIRILO; DE BORTOLI, 2006; ROMEIRO et al., 2007a). Such procedures were adopted due to their computer performance and due to the similarity obtained between the Lake's physical geometry (Figure 1) and the computer grid (Figure 2). Notice that in the computer grid in Figure 2, the input channels have been deleted.

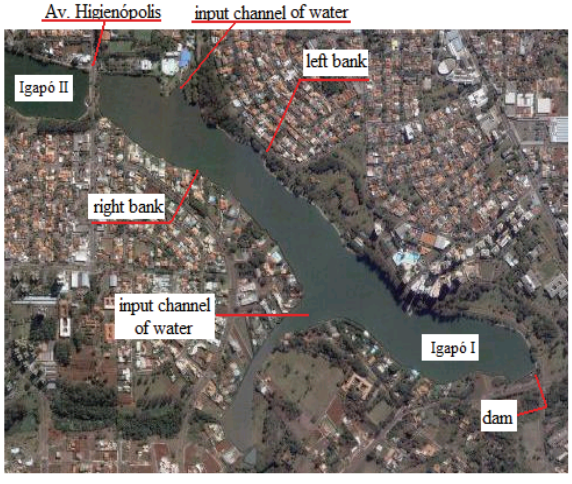

Figure 1. Physical domain of Igapó I Lake.

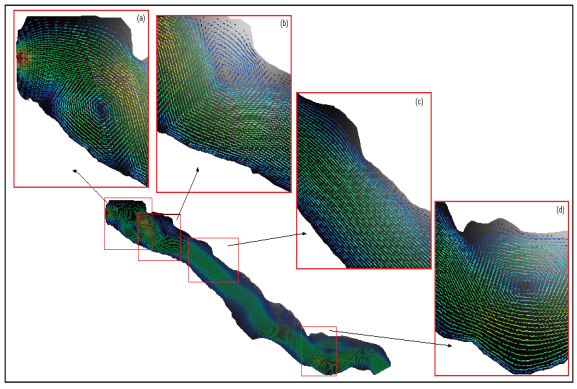

Figure 2. Computational grid of the Igapó I Lake. In (a) - (b) two vortices are observed at entrance of lake. In (c) a central area of the lake is observed, without vortex. In (d) one vortex is observed at exit of the lake.

Water quality model

The bases for the water quality models are the conservation equations of linear momentum for hydrodynamic model, and the equations of mass conservation for transport model, and the equations of reactive processes for reaction model. By means of such equations it is possible to represent the flow dynamics of a water body and study the behavior of the reactive species (pollutants or substances) at Igapó I Lake.

Hydrodynamic model

The water flow of Igapó I Lake is laminar (low declivity and the small volume of input water compared with water volume of the Lake), so that a 2DH hydrodynamic model represents it appropriately (HORITA; ROSMAN, 2006). Considering that the fluid (water body) is incompressible, of the Newtonian type and in hydrostatic equilibrium, so the variations of density ρ are not significant (SHAKIB et al., 1991). Assuming as well that the forces of the external field (actions of wind, heat, ...) are not expressive, that there are no variations in the Lake's boundary and using the Stokes' hypothesis for Newtonian fluids (SCHLICHTING; GERTEN, 2000), the equations of the 2DH hydrodynamic model are given by

$$\frac{\partial u_1}{\partial t} + u_1 \frac{\partial u_1}{\partial x_1} + u_2 \frac{\partial u_1}{\partial x_2} = -\frac{\partial p}{\partial x_1} + \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 u_1}{\partial x_1^2} + \frac{\partial^2 u_1}{\partial x_2^2}\right) \quad (1)$$

$$\frac{\partial u_2}{\partial t} + u_1 \frac{\partial u_2}{\partial x_1} + u_2 \frac{\partial u_2}{\partial x_2} = -\frac{\partial p}{\partial x_2} + \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 u_2}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_2^2}\right) \quad (2)$$

$$\nabla^2 p = -\frac{\partial^2 u_1^2}{\partial x_1^2} - 2\frac{\partial^2 u_1 u_2}{\partial x_1 x_2} - \frac{\partial^2 u_2^2}{\partial x_2^2} + \frac{\partial d}{\partial t} + \frac{1}{\mathrm{Re}}\left(\frac{\partial^2 d}{\partial x_1^2} + \frac{\partial^2 d}{\partial x_2^2}\right) \quad (3)$$

Navier-Stokes equations (1) - (2) and pressure equation (3) are in their dimensionless forms (GRESHO; SANI, 1987; HIRSCH, 1990). They describe the horizontal two-dimensional movement of incompressible Newtonian fluids, establishing the changes in the moments and in the acceleration of the fluid as result of changes in pressure and in dissipative viscous forces (shear stress), acting in the interior of the fluid.

In equations (1)-(3) the independent variable t is time, u_1 and u_2 are the components of the velocity vector in longitudinal direction x_1 and transversal direction x_2, respectively, p is pressure, d is the divergent defined by $d = \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2}$ and Re is the Reynolds number.

Reaction transport model

In lakes without a high concentration of suspended sediments, the reactive species, dissolved in the water body, flow with the hydrodynamic velocity field of the lake. In these situations, the reactive species are in passive regime, and the study of their transport can be carried out independently of the hydrodynamic modeling.

Considering the mass conservation principle to the concentrations of reactive species, the flow variation is almost linear and the total velocity of the reactive species may be split into advective velocity u_i, for i = 1.2 (given by the hydrodynamic model) and into diffusive velocity, which may be modeled by means of Fick's Law, so that the reaction transport model is given by (ROSMAN, 1997)

$$\frac{\partial C}{\partial t} = -u_i \frac{\partial C}{\partial x_i} + D\frac{\partial^2 C}{\partial x_i^2} + \sum R_C, \quad (4)$$

where it is supposed that the molecular diffusion D of all the reactive species are equal and constant.

In (4), the reactions term $\sum R_C$ can be modeled by means of numerous water quality models, some of them mentioned in the introduction. In this work the model WASP6 (AMBROSE et al., 2001) was used in its linearized version (ROMEIRO et al., 2007b), limited to carbon (C) and nitrogen (N) cycles. In this model the reactions scheme of the carbon (C) and nitrogen (N) cycles is described in Figure 3, by clear gray and dark gray arrows, respectively.

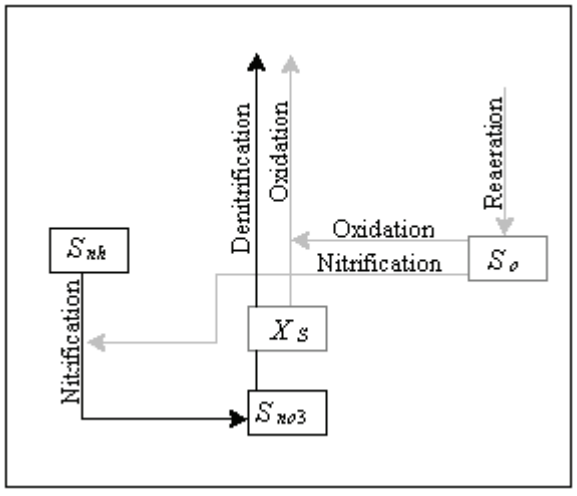

Figure 3. Reactions scheme of carbon (C) and nitrogen (N) cycles, in clear gray and dark gray arrows, respectively.

In the scheme in Figure 3, the concentrations of the four reactive species, namely, the concentration of ammonium S_{nh}, the concentration of nitrite+nitrate S_{no3}, the concentration of the biochemical oxygen demand (BOD) X_S and the concentration of dissolved oxygen (DO) S_o, are affected by the C-N cycle processes of the WASP6 model. In the linearized version of the WASP6 model, for carbon and nitrogen cycles (ROMEIRO et al., 2007b), the concentrations of the reactive species are described by the coupled linear EDOs system below:

$$\begin{aligned}
\frac{dS_{nh}}{dt} &= -K_1 S_{nh} - K_7 S_o + \tau_{S_{nh}} \\
\frac{dS_{no3}}{dt} &= K_1 S_{nh} - K_2 S_{no3} + K_8 S_o - \tau_{S_{no3}} \\
\frac{dX_S}{dt} &= -\frac{20}{7} K_2 S_{no3} - K_5 X_S - K_4 S_o + \tau_{X_S} \\
\frac{dS_o}{dt} &= -\frac{32}{7} K_1 S_{nh} - K_5 X_S - K_6 S_o + \tau_{S_o}
\end{aligned} \quad (5)$$

where the following constants are defined

$$
\begin{aligned}
K_1 &= k_{12}\Theta_{12}^{T-20}\left(\frac{\overline{S}_o}{k_{nit}+\overline{S}_o}\right)\\
K_2 &= k_{2D}\Theta_{2D}^{T-20}\left(\frac{k_{no3}}{k_{no3}+\overline{S}_o}\right)\\
K_3 &= k_D\Theta_D^{T-20}\frac{\overline{X}_S\,k_{DBO}}{\left(k_{DBO}+\overline{S}_o\right)^2}\\
&\quad+\frac{32}{7}k_{12}\Theta_{12}^{T-20}\frac{\overline{S}_{nh}\,k_{nit}}{\left(k_{nit}+\overline{S}_o\right)^2}\\
K_4 &= k_D\Theta_D^{T-20}\left(\frac{\overline{X}_S\,k_{DBO}}{\left(k_{DBO}+\overline{S}_o\right)^2}\right)\\
&\quad-\frac{20}{7}k_{2D}\Theta_{2D}^{T-20}\left(\frac{k_{no3}\,\overline{S}_{no3}}{\left(k_{no3}+\overline{S}_o\right)^2}\right)\\
K_5 &= k_D\Theta_D^{T-20}\left(\frac{\overline{S}_o}{k_{DBO}+\overline{S}_o}\right)\\
K_6 &= k_2\Theta_D^{T-20}+k_D\Theta_D^{T-20}\left(\frac{\overline{X}_S\,k_{DBO}}{\left(k_{DBO}+\overline{S}_o\right)^2}\right)\\
&\quad+\frac{32}{7}k_{12}\Theta_{12}^{T-20}\left(\frac{\overline{S}_{nh}\,k_{nit}}{\left(k_{nit}+\overline{S}_o\right)^2}\right)\\
K_7 &= k_{12}\Theta_{12}^{T-20}\left(\frac{\overline{S}_{nh}\,k_{nit}}{\left(k_{nit}+\overline{S}_o\right)^2}\right)\\
K_8 &= k_{12}\Theta_{12}^{T-20}\left(\frac{\overline{S}_{nh}\,k_{nit}}{\left(k_{nit}+\overline{S}_o\right)^2}\right)\\
&\quad+k_{2D}\Theta_{2D}^{T-20}\left(\frac{k_{no3}\,\overline{S}_{no3}}{\left(k_{no3}+\overline{S}_o\right)^2}\right),
\end{aligned}
\tag{6}
$$

$$
\begin{aligned}
\tau_{S_{nh}} &= K_7\,\overline{S}_0\\
\tau_{S_{no3}} &= K_8\,\overline{S}_0\\
\tau_{X_S} &= K_4\,\overline{S}_0\\
\tau_{S_0} &= k_2\,\Theta_D^{T-20}\,S_{Sat}+K_3\,\overline{S}_0\,,
\end{aligned}
$$

with $\overline{S}_0$, $\overline{X}_S$, $\overline{S}_{no3}$ and $\overline{S}_{nh}$ the center around which the linearization by Taylor's series was made. The symbols, values and units of the parameters of the linearized reaction model (5-6) are given in Table 1.

Substituting the reaction model (5-6) in (4), for the four reactive species under consideration, we obtain the reaction transport model, that is,

$$
\begin{aligned}
&\frac{\partial S_{nh}}{\partial t}+u_i\frac{\partial S_{nh}}{\partial x_i}-D\frac{\partial^2 S_{nh}}{\partial x_j^2}=\\
&-K_1S_{nh}-K_7S_0+\tau_{S_{nh}}\\
&\frac{\partial S_{no3}}{\partial t}+u_i\frac{\partial S_{no3}}{\partial x_i}-D\frac{\partial^2 S_{no3}}{\partial x_j^2}=\\
&K_1S_{nh}-K_2S_{no3}+K_8S_0-\tau_{S_{no3}}\\
&\frac{\partial X_S}{\partial t}+u_i\frac{\partial X_S}{\partial x_i}-D\frac{\partial^2 X_S}{\partial x_j^2}=\\
&-\frac{20}{7}K_2S_{no3}-K_5X_S-K_4S_0+\tau_{X_S}\\
&\frac{\partial S_0}{\partial t}+u_i\frac{\partial S_0}{\partial x_i}-D\frac{\partial^2 S_0}{\partial x_j^2}=\\
&-\frac{32}{7}K_1S_{nh}-K_5X_S-K_6S_0+\tau_{S_0}
\end{aligned}
\tag{7}
$$

Table 1. Symbols, values and units of the constants of the WASP6 model, at steady temperature of 20ºC (AMBROSE et al., 2001).

Symbol	Value	Unit	Parameter
Θ_{2D}	1.045		Temperature coefficient for denitrification.
Θ_{12}	1.08		Temperature coefficient for nitrification.
Θ_D	1.047		Temperature coefficient for Carbon oxidation.
Θ_2	1.028		Temperature coefficient for reaeration.
k_{2D}	0.09	h^{-1}	Denitrification index.
k_{12}	0.22	h^{-1}	Nitrification index.
k_D	0.38	h^{-1}	Oxidation index.
k_2	1.252	h^{-1}	Reaeration index.
k_{DBO}	0.001	mg L^{-1}	Half saturation constant of the carbonated BOD.
k_{nit}	0.2	mg L^{-1}	Half saturation constant for DO limited to the nitrification process.
k_{no3}	0.1	mg L^{-1}	Half saturation constant for DO limited to the denitrification process.
S_{Sat}	8.3	mg L^{-1}	DO saturation concentration.

where the indexes i = 1.2 represent the longitudinal and transversal directions, respectively, in relation to the computer grid lines, u_i are the components of the vector velocity given by the hydrodynamic model and D is the diffusion coefficient of the reactive species.

Results and discussion

Numerical simulations

For the numerical simulations, it is supposed that Igapó I Lake does not present sources and drains, except for the entrance and exit dams, showed in Figure 2.

To generate the interior of Igapó I Lake geometry, a structured discretization was used, in generalized coordinates, by an elliptic PDEs system, whereas the margins were obtained by a parametric

cubic spline polynomial interpolation (CIRILO; DE BORTOLI, 2006). Such procedures were adopted due to their computer performance as well as by the fast similarity obtained with the physical geometry, from little known points of the domain (MALISKA, 1995). The study considered 839 points located along the left and right margins and 35 points located in the entrance and exit contours. To solve the resulting tridiagonal linear systems, the TDMA (TriDiagonal Matrix Algorithm) procedure was utilized, which reduces the memory time (DE BORTOLI, 2000).

In the numerical resolution of the PDEs systems (1-3), which constitute the horizontal two-dimensional hydrodynamic model, the block technique was used (DE BORTOLI, 2000). In this procedure, firstly, it is necessary to make an analysis of which and how many subgrids (sub-blocks) would constitute the whole grid. After distinguishing the sub-blocks, for each one, it is necessary to define the boundary and their interior. Finally, the sub-blocks are read and recorded in files referring to the whole grid. The connection of the sub-blocks that compose the grid is made from the reading of the extreme points, common to the sub-blocks (CIRILO; DE BORTOLI, 2006). So, the PDEs systems (1-3) were resolved in generalized coordinates, approaching the spatial derivates by central differences. For the discretized velocity field was used the explicit fourth order Runge-Kutta method and for the discretized pressure field was used the Gauss-Seidel method with successive relaxations (SMITH, 1985).

As for the numerical resolution of the transport model (7), the stabilized finite elements method was employed, in its Galerkin's semi-discrete formulation, when the spatial derivate is approached by finite elements and temporal derivate is approached by finite differences. A stabilization procedure of the Streamline Upwind Petrov-Galerkin (SUPG) type, proposed by Brooks and Hughes (1982), was also employed.

Regarding the value of the diffusion coefficient *D*, in (7), it is supposed that it is constant throughout Igapó I Lake geometry and equal for all the reactive species. According to (CHAPRA, 1997), the several reactive species have molecular diffusion values in the interval between $D = 10^{-4} m^2 h^{-1}$ and $D = 10^{-1} m^2 h^{-1}$. However, the turbulent diffusion coefficient in rivers and lakes, which depends on the turbulent phenomenon scale, takes values between $D = 10^{1} m^2 h^{-1}$ and $D = 10^{10} m^2 h^{-1}$. In Romeiro et al. (2011), the calibration of the diffusion coefficient to fecal coliform, in the longitudinal and transverse directions in Lake Igapó, resulted in $D_x = D_y = 10^{-3} m^2 h^{-1}$, respectively, characterizing a diffusion of the molecular type. Based on this discussion, we considered these same values to the diffusion coefficients of carbon-nitrogen cycle.

Therefore, by means of numerical simulations of system (7), the qualitative aspects of transport of the carbon and nitrogen cycles in the water body of Igapó I Lake were studied. It is highlighted that this numerical simulation is not aimed at providing quantitative predictions about the pollution index in a particular time and space of the Lake's physical domain. It is known that the entrance conditions (initial and boundary) of the reactive species vary daily. In fact, measurements that have been conducted since 2007 (TISOLUTION, 2011) by a joint cooperation involving the Environmental Institute of Paraná (IAP), the Municipal Council for the Environment of Londrina (CONSEMMA), the State University of Londrina (UEL) and the Engineering and Architecture Club of Londrina (CEAL), and have provided very discrepant measurements of the Water Quality Index (WQI), according to collection date. Under such conditions, our objective is to provide qualitative information, such as the most polluted sites in the Lake's domain, independently of initial concentrations and of reactive species boundary.

In this context, by using the mathematical model developed, this work describes qualitatively the impact that continuous ammonium discharge at Igapó I Lake entrance has throughout its extension, characterized by the area between Higienópolis Avenue and the dam (Figure 1).

Firstly, there is the numerical calculation, from the hydrodynamic model (1-3), of the components of the velocity field p and of the pressure field p, in all of Igapó I Lake domain.

The lake has little renewal of its waters, due to the small volume of input water when compared to the total volume of the reservoir, and also due to its low slope. This characteristic of this artificial lake explain the low rate of flow, which in turn presents, on average, a low Reynolds number. So, to calibrate the small pressure gradient from the boundary conditions, a low Reynolds number Re=10 was used (ROMEIRO et al., 2011).

The initial and boundary conditions are given below.

- Initial conditions for the hydrodynamic model.

It is considered that at the initial moment $t = 0$,

the dimensionless velocity and pressure fields, in the interior points of Igapó I Lake geometry, are given by

$$\vec{u}(X,0) = (1,0) \text{ and } p(X,0) = 1.0 \ , \tag{8}$$

where:

$X = (x_1, x_2)$ is an interior point of the grid domain at Igapó I Lake, see Figure 2. In equation (8), the velocity field has the direction of the hydrodynamic flow. For $X = \overline{X}$, entrance points of Igapó I Lake, and for $X = \widetilde{X}$, exit points of Igapó I Lake, see Figures 1 and 2, the following values for initial velocities and pressures are taken,

$$\begin{aligned} &\vec{u}(\overline{X},0) = (1,0) \quad \text{and} \quad p(\overline{X},0) = 1.0 \\ &\vec{u}(\widetilde{X},0) = (1,0) \quad \text{and} \quad p(\widetilde{X},0) = 0.9 \end{aligned} \ . \tag{9}$$

Finally, for the other points of Igapó I Lake boundary, the following conditions are considered

$$\vec{u}(X_p,0) = (0,0) \text{ and } p(X_p,0) = 0.0 \tag{10}$$

where:

X_p are points of the Lake's margin, except the entrance and exit ones.

- Boundary conditions for the hydrodynamic model.

For $t > 0$, is considered Neumann's condition boundary to the velocity field at entrance and exit points of Igapó I Lake geometry (FORTUNA, 2000). In the other points of the margin the following conditions are considered

$$\vec{u}(X_p,t) = (0,0) \tag{11}$$

In relation to the pressure field, for $t > 0$, it is considered a gradient of 10% between entrance pressure and exit pressure of Igapó I Lake, as shown in Eq. (12),

$$p(\overline{X},t) = 1.0 \text{ and } p(\widetilde{X},t) = 0.9 \tag{12}$$

and in the others points of the margin, X_p, analogously to Neumann's boundary condition, they are used as well.

In order to simulate the dynamics of the reactive species concentrations in (7), in the modeled geometry of Igapó I Lake, initially the values of the parameters defined in (6) are calculated by using the data in Table 1

$$\begin{aligned} &K_1 = 9.67 \text{ X } 10^{-3} \ h^{-1} \\ &K_2 = 4.67 \text{ X } 10^{-5} \ h^{-1} \\ &K_3 = 4.67 \text{ X } 10^{-5} \ h^{-1} \\ &K_4 = 1.22 \text{ X } 10^{-6} \ h^{-1} \\ &K_5 = 1.66 \text{ X } 10^{-2} \ h^{-1} \\ &K_6 = 5.38 \text{ X } 10^{-2} \ h^{-1} \\ &K_7 = 4.77 \text{ X } 10^{-5} \ h^{-1} \\ &K_8 = 4.77 \text{ X } 10^{-5} \ h^{-1} \\ &\tau_{S_{nh}} = 3.96 \text{ X } 10^{-4} \ mg\,L^{-1}\,h^{-1} \\ &\tau_{S_{no3}} = 3.96 \text{ X } 10^{-4} \ mg\,L^{-1}\,h^{-1} \\ &\tau_{X_S} = 1.01 \text{ X } 10^{-5} \ mg\,L^{-1}\,h^{-1} \\ &\tau_{S_0} = 4.47 \text{ X } 10^{-1} \ mg\,L^{-1}\,h^{-1} \ . \end{aligned} \tag{13}$$

As for the initial and boundary conditions for the reaction transport model (7), the values below are taken.

- Initial conditions for the reaction transport model.

It is considered that at the initial time $t = 0$ the concentrations of ammonium S_{nh}, of nitrite+nitrate S_{no3}, of the biochemical demand of oxygen X_S and of dissolved oxygen S_0 are given by

$$\begin{aligned} &S_{nh}(X_m,0) = 0.00 \ mg\,L^{-1} \\ &S_{no3}(X_m,0) = 0.00 \ mg\,L^{-1} \\ &X_S(X_m,0) = 0.00 \ mg\,L^{-1} \\ &S_0(X_m,0) = 8.30 \ mg\,L^{-1} \end{aligned} \tag{14}$$

where:

$X_m = (x_1, x_2)$ are all the grid points (interior and boundary) of Igapó I Lake.

- Boundary conditions for the reaction transport model.

For $t > 0$ and $X = \overline{X}$, Igapó I Lake entrance points, the following constant boundary concentrations are considered

$$\begin{aligned} &S_{nh}(\overline{X},t) = 1.74 \ mg\,L^{-1} \\ &S_{no3}(\overline{X},t) = 0.00 \ mg\,L^{-1} \\ &X_S(\overline{X},t) = 5.05 \ mg\,L^{-1} \\ &S_0(\overline{X},t) = 8.30 \ mg\,L^{-1} \end{aligned} \tag{15}$$

and for $X = \widetilde{X}$, Igapó I Lake exit points, the Neumann's boundary condition are used.

In the other boundary points, for $t > 0$, due to the hypothesis of absence of other sources and drains, the concentrations are given by

$$\begin{aligned} &S_{nh}(X_p,0) = 0.00 \ mg\,L^{-1} \\ &S_{no3}(X_p,0) = 0.00 \ mg\,L^{-1} \\ &X_S(X_p,0) = 0.00 \ mg\,L^{-1} \\ &S_0(X_p,0) = 8.30 \ mg\,L^{-1} \ . \end{aligned} \tag{16}$$

It should be noticed that the boundary conditions at the entrance of the lake represent a continuous discharge of 1.74 milligrams of ammonium per liter, absence of nitrite+nitrate concentration, which will be generated by means of the nitrification process, a biochemical demand of 5.05 milligrams of oxygen per liter and a saturation concentration of dissolved oxygen of 8.30 milligrams per liter.

From the advective velocity field, given by the hydrodynamic model (1-3) and by conditions (8-12), it is simulated, from the reaction transport model (7) and from conditions (13-16), the transport of the concentrations of ammonium, of nitrite+nitrate, of the biochemical demand of oxygen and of the dissolved oxygen, all over the Lake's domain, at all times, for the diffusion coefficient $D = 10^{-3}\ m^2 h^{-1}$.

The Figure 4 presents the results of the numerical simulations of the four reactive species, in a time interval of 300 hours of continuous discharge, when the flow reaches a stationary situation. These simulations were performed with 500 time steps, with $\Delta t = 0.6$ h.

Some results are listed below, which can be observed in the numerical simulations presented in the Figure 4.

1 - The numerical procedure captured four vortices, two of them located near Igapó I Lake entrance, one on the left margin and the other on the right margin of the Lake, and the other two on the left margin, after the central region of the Lake, see Figures 2 and 4.

2 - It is observed that the concentration of ammonium continuously discharged into the Lake's entrance decreases along the flow, generating higher concentration values of nitrite+nitrate in the Lake's exit. Consistently, a high index of biochemical demand of oxygen is observed in the regions with high concentrations of ammonium.

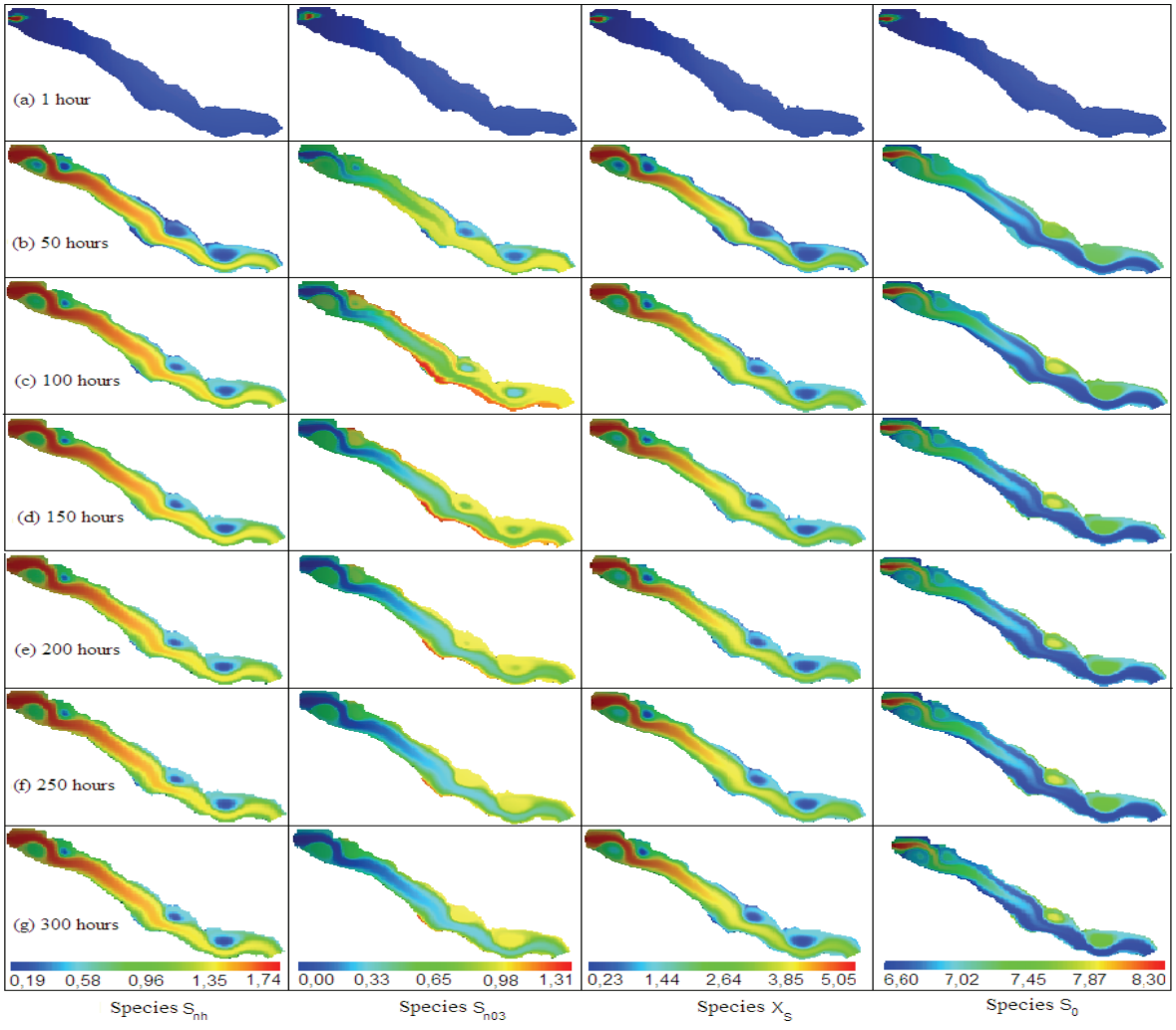

Figure 4. Concentration of the reactive species in Igapó I Lake, in function of time, when $D = 10^{-3} m^2 h^{-1}$.

3 - It is emphasized that the higher concentrations of nitrite+nitrate occur in the Lake's vortices, characterizing them as the most polluted regions by nitrite and nitrate.

Conclusion

The numerical simulations provided a better understanding of the dynamics of the processes involved in the reactive species flow, such as the dynamics of the nitrification process, of the biochemical demand of oxygen and of the level of dissolved oxygen in Igapó I Lake. The Figure 4 presents the transport simulations of these reactive species, throughout the Lake's domain. By analyzing the numerical results presented, it is possible to verify that the most relevant factor is the occurrence of high concentrations of nitrite and nitrate in the Lake's vortices, characterizing them as the most polluted regions in the Lake.

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