Mathematical model as a management tool to analyze organic matter self-purification in reservoirs

Modelo matemático como herramienta de gestión para analizar la autodepuración de materia orgánica en embalses

Amanda de Cássia da Cunha[1,3], Fernando Roberto Momo[2], Cassiana Maria Reganhan Coneglian[1] and Elaine Cristina Catapani Poletti[1]

[1] *School of Technology, State University of Campinas UNICAMP, Limeira, São Paulo, Brazil*
[2] *Science Institute, National University of General Sarmiento UNGS, Los Polvorines, Malvinas Argentinas, Buenos Aires, Argentina*
[3] *Department of Basic Sciences, National University of Luján UNLu, Luján, Buenos Aires, Argentina*

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Abstract—A mathematical model to analyze the self-purification potential of organic matter in reservoirs was developed, seeking to constitute a potential water management tool for easy application. Therefore, it was considered the input of organic matter into the watercourse, its sedimentation, decomposition and its output downstream, as well as the oxygen input through the flow and through re-oxygenation, its consumption by microbial activity and its downstream exit. The model was validated using data of Tietê river and applied using data of Salto Grande reservoir, both located at São Paulo State, Brazil, considering different scenarios of biochemical oxygen demand (BOD), dissolved oxygen (DO), water inlet flow and reservoir water volume. The results show that organic matter is decomposed faster in the first 12 hours of water travel; moreover, self-purification efficiency is better with a greater volume of water in the reservoir. The model is quite representative to study different self-purification scenarios in dammed areas, concluding that the developed model, being tested and improved, can already contribute to the management of reservoirs, with the advantage of having a simple application.

Keywords—Biomathematics, Dams, Superficial water quality, Water contamination, Water monitoring, Organic carbon mineralization

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Resumen—Se desarrolló un modelo matemático para analizar el potencial de autodepuración de la materia orgánica en embalses, buscando constituir una potencial herramienta de gestión del agua de fácil aplicación. Para eso, se consideró el ingreso de materia orgánica al curso de agua, su sedimentación, descomposición y su salida aguas abajo, así como el aporte de oxígeno por flujo y por reoxigenación, su consumo por actividad microbiana y su salida aguas abajo. El modelo fue validado con datos del río Tietê y aplicado con datos del embalse de Salto Grande, ambos ubicados en el Estado de São Paulo, Brasil, considerando diferentes escenarios de demanda bioquímica de oxígeno (DBO), oxígeno disuelto (OD), flujo de entrada de agua y volumen de agua del embalse. Los resultados muestran que la materia orgánica se descompone más rápido en las primeras 12 horas de viaje por agua; además, la eficiencia de la autodepuración es mejor con un mayor volumen de agua en el depósito. El modelo es bastante representativo para estudiar diferentes escenarios de autodepuración en áreas embalsadas, concluyendo que el modelo desarrollado, todavia en prueba y mejorías, ya puede contribuir a la gestión de embalses, con la ventaja de tener una aplicación sencilla.

Palabras clave—Biomatemática, Represas, Calidad de agua superficial, Contaminación de agua, Monitoreo de agua, Mineralización de carbono orgánico

INTRODUCTION

Due to the misuse of superficial water, many tributaries of reservoirs end up carrying (and storing in their sediments) contamination loads from the lack of domestic and industrial sewage treatment. Also, they have their flow rates altered due to innumerable anthropogenic interference in river courses (Curbani et al., 2021; Bianchini Junior, 1999; Bianchini Junior and da Cunha-Santino, 2018)

The concentration of contaminant compounds, however, can naturally be reduced by water bodies through the self-purification process. It is the natural ability of an aquatic ecosystem to depurate organic and inorganic compounds through biological, biochemical and physical-chemical processes. Decomposition of compounds by aquatic microorganisms, chemical oxidation of organic matter, and inlet and outlet of gases in surface waters are the main factors that characterize the water self-purification process (de Esteves, 2011).

It is important to understand that self-purification transforms excess organic compounds (which is harmful to the aquatic ecosystem) into inert compounds that are no longer harmful to organisms. This purification does not necessarily bring potability to water, but restores the original characteristics of a water body that has suffered some kind of contamination, returning the equilibrium to the ecosystem (Suslova et al., 2018).

For conceptual purposes, self-purification process can be divided into zones: 1) the degradation zone, where effluent is discharged; 2) active decomposition zone, where dissolved oxygen reaches its lowest concentration and organic matter is mostly decomposed; 3) recovery zone, in which the dissolved oxygen begins to be reintroduced, algae and some species of fish reappear; and 4) clean water zone, where dissolved oxygen is recomposed in the environment and the excess organic material has already been degraded. Also, the presence of species of algae, fungi and bacteria and nutrient concentration are characteristic of balanced environments (Dodds and Whiles, 2020).

The type of watercourse influences the extent and time of each of these zones. In a lentic system with less water movement, purification is more dependent on water residence time; whereas in the lotic system, like a river, with almost continuous movement, purification is related to the space covered by water (Wetzel, 2001). Each water body has its purifying potential, which depends on ecosystem characteristics such as temperature, salinity, biodiversity, length and depth, water velocity and flow. This potential can be affected by climatic variations such as annual temperature, wind and humidity (Delgadillo et al., 2010). Also, the characteristics of wastewater discharged into water sources affect the self-purification potential (Skulovich et al. 2018). The composition of organic material, the presence of inhibitory substances and the disposal of (Skulovich and Ostfeld, 2018).Self-purification capability of a stream has to be known by the monitoring organs. They determine in what quality stage each watercourse belongs to and for what purpose it can be used, among all of the possible uses of a watercourse. This capability is also a necessary information for those who develop and maintain sewage treatment stations. In this sense, the application of mathematical modeling can represent to the state monitoring agencies a viable and low-cost alternative for management understandings and subsidies, favoring the administration of water volume and flow to the downstream river.

Due to the problems related to reservoir constructions (Federice, 2014), developing and applying mathematical models in dammed areas can be strategic in order to: scale the damage caused by damming; impacts caused by the damming ecosystem; changes in river flow downstream of the reservoir construction; growth and death of organisms; purification of organic material; increased area of gas exchange between air and atmosphere; effects of thermocline created by incorporating lacustrine environment into a previously fluvial environment; physical effects of diffusion of water; among other analysis that can be performed for many purposes, using mathematical modeling as a tool.

Several self-decay studies have been performed to evaluate the potential for purification in a watercourse (Blodau et al., 2018; de da Cunha et al., 2018; Ricciardone et al., 2011; LaRowe and Van Cappellen, 2011; de Silva et al., 2007), to analyze the impact of reservoir construction in water self-decay capability (Wei et al., 2009), to evaluate the clearance of organic matter in marine sediment (Arndt et al., 2013), to understand the impact of some effluents in the self-purification capability (Mengistie et al 2016), to analyze the poly-functional role of biota in water self-decay capability (Ostroumov 2017), to evaluate the decay potential in a constructed wetland (Ophithakorn et al., 2013) and to analyze, in addition to self-purification capacity, the deoxygenation and reoxygenation rates of the environment (de Menezes et al., 2015), among others.

Regarding models performed to study reservoir water quality, CE-QUAL-R1 was developed for temperature, chemical species and biological assemblies (Wlosinski and Collins, 1985);the model CE-QUAL-RI is a complement to the previous model and includes vertical oxygen concentration, some algae groups, particulate organic matter and dissolved organic matter, among other parameters (MCA Filho et al., 1990),and CE-QUAL-W2 (Cole and Wells, 2006),that is a two-dimensional model. CE-QUAL-RI and CE-QUAL-W2 models are quite complete, but the high number of parameters contained in them restrict their application; Mike models evaluate hydrodynamics processes (MIKE, 2007). For both models, the user needs to purchase a license; (Vázquez and Mokrova, 2019) present the functionalities integrating mathematical models to the Geographic Information System (GIS) for studies of only hydrological and hydraulic processes; (Jiang et al., 2016) developed a model to assess the effect of reservoir regulation on water quality; and (Reartes et al., 2016) developed a model including as parameters the main taxonomic groups of phytoplankton in reservoirs, some nutrients, dissolved oxygen, biochemical oxygen demand and cyanobacteria. However, it was developed to be used only in stratified reservoirs and therefore not in all of the reservoirs. All of these models have the common property of not having such an intuitive implementation and are not focused on the analysis of water self-purification.

In this work, it was developed a mathematical model to evaluate the self-purification capacity in water reservoirs and other flooded areas with intermediate system profiles. It has the advantage to be composed by simple parameters and is easy to be implemented, assuming as hypothesis that this is an innovative model compared to the works presented in the literature. Thinking the mathematical modeling as an object representation tool, in order to study the interaction between its variables under different situations, a system of mathematical equations was developed. These equations represent the behavior of organic material and dissolved oxygen in a reservoir since its input with upstream river water flow, to its output through the dam, and has the purpose to be a simple and easy model to apply.

THE MODEL

For the composition of this model, it was considered the purification process of organic matter present in the reservoir: by the dilution of compounds that occurs in the transition space between lotic (riverine region, that is, beginning of the reservoir) and lentic (damming water near barrage) zones; by the biodegradation, which is part of the trophic chain existing in both environments; and by the sedimentation that occurred mainly in its lentic region. All of these adopted interactions are performed mainly in the epilymium of the dammed body.

Thus, the developed model proposes to evaluate the amount of oxygen O_2 and carbon C, both as a function of continuous time t, with $t \in [0,T) \subset R$, where $\dfrac{dO_2}{dt}$ and $\dfrac{dC}{dt}$ represent the rates of variation of this amount of oxygen and carbon as a function of time, in the case of reservoirs with a downstream river outlet.

Figure 1 presents a sectional drawing of the dam and the interactions considered in the composition of the model.

In Figure 1, DIC represents dissolved inorganic carbon, DOC represents dissolved organic carbon and POC, particulate organic carbon. The interactions among contributions of effluents, macrophytes, phytoplankton, DOC and POC with heterotrophic organisms represent the mineralization and metabolic consumption of organic carbon. The interactions between DIC and CO_2 represent the gas exchange between air and water.

Table 1 shows what each of the interactions in Figure 1 represents in the developed model:

TABLE 1: INTERACTIONS CONSIDERED IN THE RESERVOIR AND THEIR RESPECTIVE REPRESENTATIONS IN THE DEVELOPED MATHEMATICAL MODEL

Reservoir	Model
Contributions of effluents and macrophytes	Input of carbon: $\frac{Q_i}{V}C_0$
Water flow of the river(s) upstream	Inlet flow: $\frac{Q_i}{V}$ Input of oxygen: $\frac{Q_i}{V}C_0$
Gas exchange and air-water interactions	Reoxygenation constant: k_r Input of oxygen: $k_r[O_{sat} - O_2]$
Mineralization and metabolic consumption of C	Deoxygenation constant: k_d Proportionality between C and O_2: β
Dissolved oxygen	Oxygen consumption and production in epilymium: $k_r[O_{sat} - O_2]$ and $\beta k_d C$ Reoxygenation constant: k_r
Sediment-water interactions	Non-linearity between load and sedimentation: γ Sedimentation constant: μ
Downstream water discharges	Outlet flow: $\frac{Q_{s_1}}{V}$

For the oxygen variation rate as a function of time, Equation (1), we considered: “ *the reoxygenated oxygen portion, plus the portion of oxygen that enters the epilymium, minus the portions of oxygen that flows out to the downstream river, less a portion of carbon that deoxygenates*”.

Mathematically, this is:

$$\frac{dO_2}{dt} = \frac{Q_i}{V}O_{2_0} + k_r[O_{sat} - O_2] - \beta k_d C - \frac{Q_{s_1}}{V}O_2 \qquad (1)$$

Where

$$C = \frac{BOD}{\beta} \qquad (2)$$

Regarding the carbon variation rate as a function of time, Equation (3), we considered: “ *the portion of carbon that enters the epilymium, minus the portion of carbon that decarboxylates, minus the portion of carbon that sediment, minus what goes out with the flow downstream*”.

Mathematically, this is:

$$\frac{dC}{dt} = \frac{Q_i}{V}C_0 - k_d C - \mu C^{\gamma} - \frac{Q_{s_1}}{V}C \qquad (3)$$

With $O_2(0) = O_{2_0}$ and $C(0) = C_0$, where:

- $O_2 = O_2(t)$ indicates the oxygen of the epilymium (mg/m^3);
- Q_i indicates the inlet flow (m^3/d);
- V represents the water volume of the reservoir (m^3);
- O_{2_0} indicates the input of oxygen (mg/m^3);
- k_r represents the reoxygenation constant (d^{-1});
- O_{sat} represents the saturation oxygen in the epilymium (mg/m^3);
- β indicates the proportionality constant between C and O_2 (d^{-1});
- k_d indicates the deoxygenation constant in the epilymium (d^{-1});
- Q_{s_1} indicates the outlet flow (mg/m^3);
- $C = C(t)$ represents the carbon in the epilymium (mg/m^3);
- BOD represents the biochemical oxygen demand (mg/m^3);
- C_0 represents the input of carbon (mg/m^3);
- μ indicates the sedimentation constant (d^{-1});
- γ represents the non-linearity between load and sedimentation.

The model was solved numerically using one 4^{th} order Runge-Kutta Method (RK4), widely used to solve initial value problems, given its simplicity of implementation and high precision (Carnahan and Wilkes, 1973; Cunha, 2001), with local truncation error on the order of $O(h^5)$. To implement the problem, Matlab®was used.

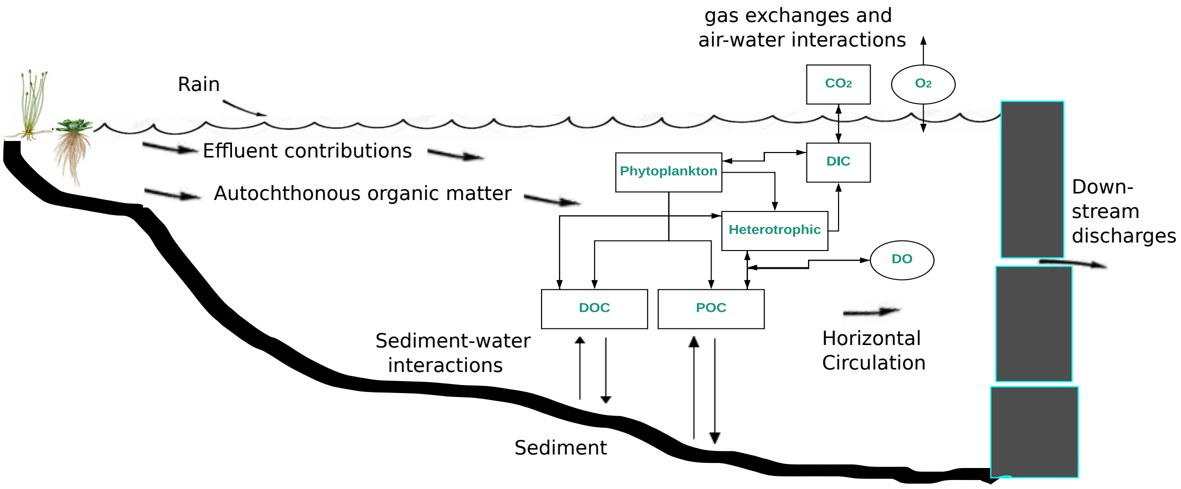

Figure 1: Interactions considered in the reservoir to develop the model. Source: adapted from (de Esteves, 2011) and (Tundisi, 2013).

Model Validation

The validation of the developed model (Equations 1 and 3) was performed using data from collections by Tercini and Méllo Junior (2016) and Tercini (2014) The authors evaluated the self-purification of the Tietê River from the municipality of Pirapora to Salto, in São Paulo State, Brazil, through an adaptation of the Streeter & Phelps model. The Tietê river stretch considered has small reservoirs. The field work carried out by the authors consisted of monthly water sample collections and analysis, in 2012, of biochemical oxygen demand (BOD), dissolved oxygen (DO) and temperature in some points of the river and reservoirs. They also stipulated the reaeration and deoxygenation constants for the lentic and lotic stretches.

Considering the model proposed in this study, the self-purification of the Tietê River stretch is evaluated, adopting the input data from BOD (which represents the input of carbon) and DO downstream and upstream of the Rasgão reservoir studied by Tercini (2014). Thus, we were able to analyze whether what was depurated at the outlet of the reservoir coincides with the result predicted by the model.

Figure 2 presents Tietê sub basin chosen by Tercini and Méllo Junior (2016) to perform the study:

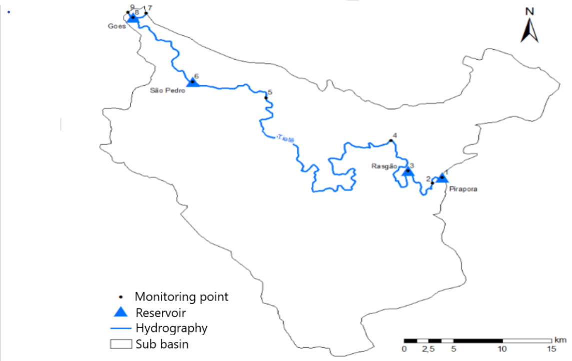

Figure 2: All the collections points chosen by Tercini and Méllo Junior (2016) through the Tietê sub basin between Pirapora and Salto cities. Source: Tercini (2014).

Figure 3 shows the collection points performed by Tercini and Méllo Junior (2016). selected to validate the developed model (Equations 1 and 3) (which we call Points 1, 2 and 3):

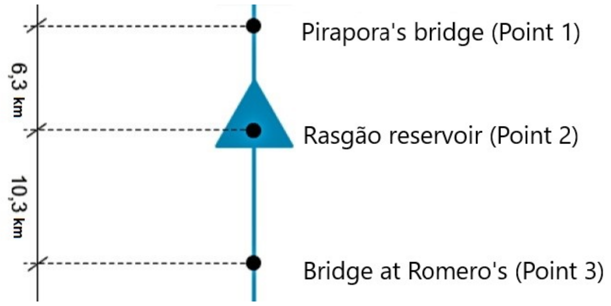

Figure 3: Point 1, Point 2 and Point 3 of the collections carried out by Tercini and Méllo Junior (2016). in the Tietê river that were used to validate the developed model. Source: adapted from Tercini (2014).

Point 1 (Pirapora's bridge) provides input data for the validation of the developed model. Considering 6.3 km of river stretch until the arrival at the reservoir at Point 2 (Rasgão Reservoir), the self-purification of this river stretch was determined using the Streeter & Phelps model, which is more appropriate for river sections. Equation 4 presents the model:

$$\frac{dO}{dt} = -k_d L + k_r (O_{sat} - O_2) \tag{4}$$

Thus, for the simulations in this section, we applied the Streeter & Phelps model and used the values of BOD, OD, k_d, k_r, average velocity and distance between sections shown by Tercini et al. (2016), according to Table 2. The BOD and DO results used were from May 2012 analysis accomplished by Tercini et al. (2016).

Figure 4 expresses the simulation between Point 1 and Point 2 using the Streeter & Phelps model:

The final BOD after 6.3 km of the route, or 5.1h, was 2.786×10^4 mg/m^3 and the final DO was 3.907×10^3 mg/m ^{3}. These results were used as initial BOD and DO to simulate the next section, which is the reservoir.

In the reservoir, the developed model was applied using the parameters: k_d of 0.183/day, k_r of 0.009/day, inflow of 11230000 m^3 /day, outflow flow of 10329984 m^3/day, reservoir volume of 6677000 m^3 and water residence time in the reservoir of 15.51h (0.65day) (Tercini et al. 2016). We

TABLE 2: VALUES OF BOD AND OD FROM MAY 2012, k_d, k_r AND AVERAGE VELOCITY EXTRACTED FROM TERCINI AND MÉLLO JUNIOR (2016). FOR MODEL VALIDATION. SOURCE: TERCINI AND MÉLLO JUNIOR (2016)

Parameters	Value
BOD	$2.9\text{x}10^4$ mg/m^3
DO	$4.15\text{x}10^3$ mg/m^3
k_d	0.188/d
k_r	1.12/d
Average velocity	29,635.2 m/d

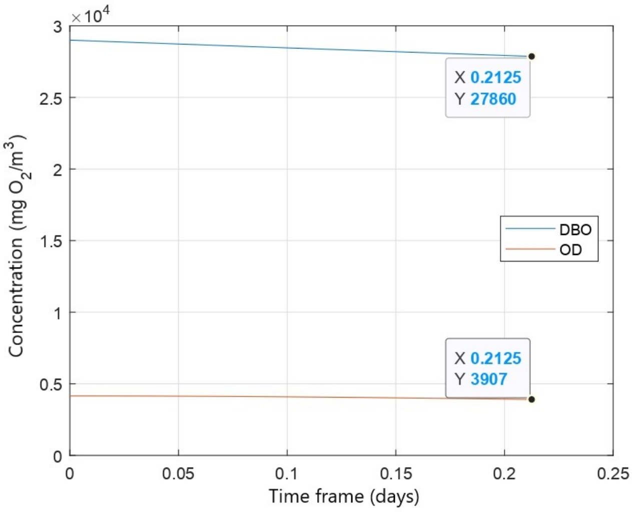

Figure 4: Simulation of the behavior of BOD and DO between Points 1 and 2 of the validation, that is, in the first section.

adopted, following (Margalef, 1983), proportionality constant between C and O_2 (β) of 2.6/day and nonlinear relation between load and sedimentation (γ) of 0.8/day, and sedimentation constant (μ) of 1.0/day (tabulated by (Mizael, 2019)). The generated simulation is shown in Figure 5:

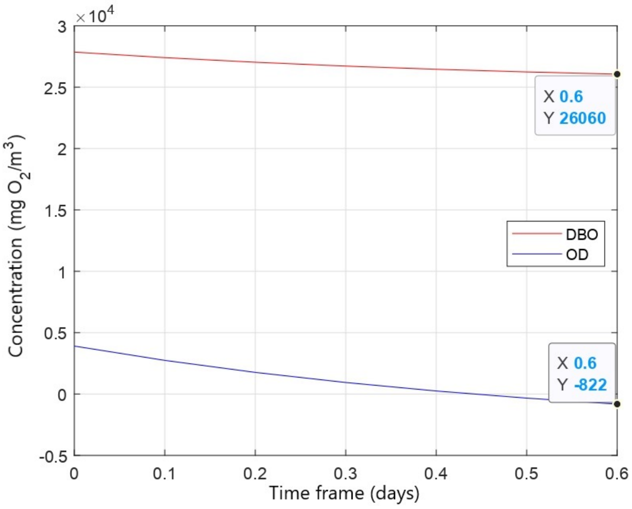

Figure 5: Simulation of the behavior of BOD and DO in the Rasgão reservoir, that is, in the second section.

The endpoint of the simulated curve for BOD is $2.606\text{x}10^4$ mg/m^3 and for DO is $-8.22\text{x}10^{-1}$ mg/m^3. It is noteworthy that, as it is not possible for a negative oxygen concentration to exist, this negative moment of the oxygen curve is attributed to anaerobiosis, that is, to the decomposition carried out by anaerobic microorganisms. Considering the next collection point by Tercini and Méllo Junior (2016)(Point 3) at 10.3 km after the reservoir (or 0.35 days of travel), the Streeter & Phelps model was again applied between Point 2 and Point 3 (bridge on the Romeiros road) to estimate the organic decomposition in the stretch of the river.

Using the end points of the curves in Figure 5 as the initial condition for the simulation, the constants used were the same applied in the simulation of the section between Point 2 and Point 3 (k_d of 0.188/d k_r1.12/d). The simulation is shown in Figure 6:

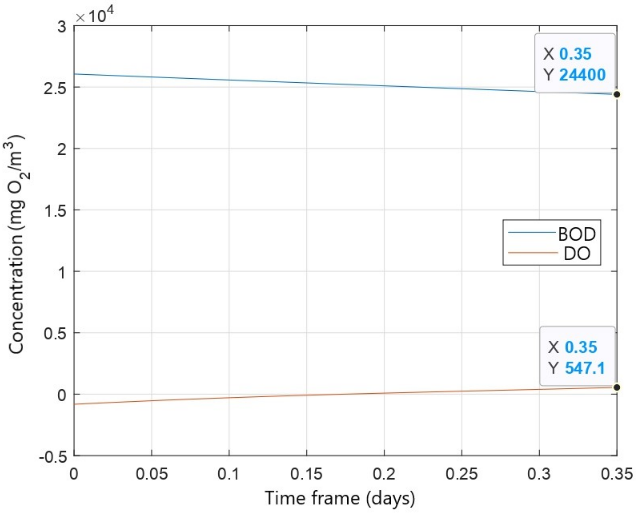

Figure 6: Simulation of the behavior of BOD and DO between the output of the Rasgão reservoir and Point 3, that is, in the third section.

The analysis by Tercini et al. (2016) showed, for Point 3, BOD of 25000 mg/m^3 and DO of 480 mg/m^3. The values obtained using the mathematical modeling were: BOD of 24400 mg/m^3 and DO of 547 mg/m^3. The difference between the empirical results found by the authors and those predicted by the proposed model are 600 mg/m^3 for BOD and 67 mg/m^3 for DO. This is qualitatively extremely similar, considering the dynamism of aquatic environments and the margins of error applied to empirical analysis of Physical-Chemical parameters (APHA 2017). Thus, it is concluded that the model is valid for the study of self-purification in reservoirs.

SALTO GRANDE RESERVOIR, AMERICANA, SÃO PAULO, BRAZIL.

The model developed was applied in a case study performed in Salto Grande Reservoir, located at the city of Americana, 120 km far from São Paulo city, Brazil. This reservoir is at a populated macro zone, with around 3 million people and very important economically to the country due to its industrial and agricultural development (IBGE 2019).

The dam was constructed in the 40's and started to work in 1950, producing electrical energy in its small hydroelectric plant (Bottura, 1998). The dammed river for its construction is called Atibaia and it is an important river for São Paulo State, providing water for Cantareira System and supplying large cities like Campinas, with almost 1.2 million inhabitants (Montagner and Jardim, 2011).

Salto Grande Reservoir has a contribution area of 2724 km^2 and residence time from 10 days (summer) to 4 months (winter) (Mizael, 2019), the reservoir is eutrophic, since Atibaia river receives disposal of liquid effluents from many of the cities it crosses, taking to the dam large concentrations of organic matter, nutrients and several compounds that lower the quality of the water body (Rodrigues et al., 2019).

Surface water collection and BOD and DO analysis of Salto Grande reservoir samples were performed in five different points along the reservoir (P1, P2, P3, P4 and P5) and one point downstream (P6) with the intention to pursue a self-decay evaluation using the model presented at this study, that could after be applied at any reservoir. The distance between the points within the reservoir varies from 2 to 2.7km. The distance between the dam and P6 is 600m, since P6 collection happened from a bridge that is the closest access to water downstream from the dam. This spacial variation is not considered within the model. The collection points can be seen in Figure 7.

Each collection point presents coordinates and some characteristics are exposed in Table 3:

TABLE 3: CHARACTERISTICS OF EACH OF THE COLLECTION POINTS.

Point	Coordinates	Depth (m)[1]
P1	$22^{o}43'47,68$”S and $47^{o}13'18,44$”O	
Characteristics	Entry point of the Atibaia river; presence of aquatic plants; some crops on the nearby banks.	2.62
P2	$22^{o}43'18,10$”S and $47^{o}14'5,24$”O	
Characteristics	Reduced distance between margins; presence of algae (in most of the time).	11.59
P3	$22^{o}42'58,58$”S and $47^{o}15'5,94$”O	
Characteristics	Area with small farms on the banks.	8.56
P4	$22^{o}42'57,05$”S and $47^{o}16'5,85$”O	
Characteristics	Small farms on one of the banks; native vegetation and crops on the other bank.	9.95
P5	$22^{o}42'2,43$”S and $47^{o}16'18,13$”O	
Characteristics	Presence of aquatic plants; small farms on one of the banks; small native vegetation area and crops on the other bank.	13.79
P6	$22^{o}41'46,02$”S and $47^{o}17'20,73$”O	
Characteristics	River point; water with little turbidity and high velocity	-

The samples were collected and stored in glass bottles under refrigeration in a polystyrene box. All analysis were performed in the Physical-Chemical Laboratory of the Faculty of Technology, State University of Campinas, with certified technical assistants and following the standard methods for each of the analysis (APHA, 2017), within 2 hours after collection.

The result of the first water collection point was used as the BOD and DO intake at one simulation with the model. All of the other points at this simulation, each of them 2 days far from the others in summer season, were compared to the empirical results of Salto Grande reservoir.

Besides, some analysis were accomplished considering hypothetical scenarios in the reservoir. The main objective of this is evaluating changes in the purification disposition of organic matter under the occurrence of some phenomena, such as effect of effluent disposal, changes in inlet flow and volume. Thus, the following hypothetical cases were evaluated:

- Case 1: there happens the occurrence of average income of organic material and average volume of the reservoir, so a normalized average of BOD concentration input, inlet flow and volume of the reservoir was also maintained;
- Case 2: there happens the occurrence of high inflow of organic material from the Atibaia River, with normalized average of inlet flow and volume of the reservoir, that is, organic matter intake was increased and dissolved oxygen was reduced;
- Case 3: there happens the occurrence of average organic matter concentration, with high inlet flow and average volume of the reservoir, so there is a substantial increase in the flow of the Atibaia River and, therefore, an inflow increase;
- Case 4: there happens the occurrence of high inflow of organic material from the Atibaia River, with low water inlet flow and average volume of the reservoir;
- Case 5: it was compared the self-purification process in the reservoir from two perspectives: the first (a) with low water volume, average inlet flow and high organic matter inlet flow concentration and the second (b) with low water volume, average inflow and low organic matter inflow concentration.

All the analysis were carried out considering 10 days of total water travel time inside the reservoir. Table **??** shows the values used in the simulations.

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[1] The average depth of each point was calculated based on the depth analysis performed in Cunha (2020)

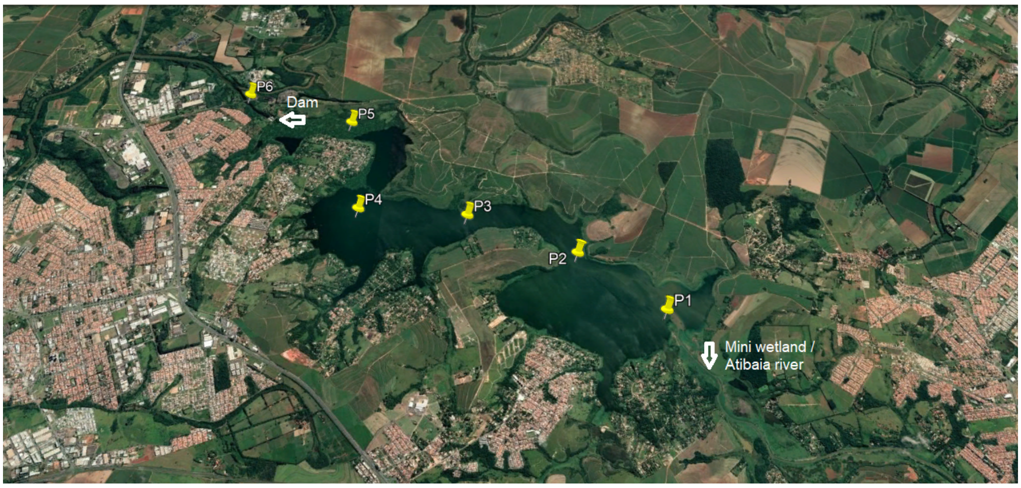

Figure 7: Water collection points from Salto Grande reservoir for BOD and DO analysis. Source: adapted from Google Earth®.

	Input flow (m^3/s)	Volume (m^3)	BOD (mg/m^3)	DO (mg/m^3)	Output flow (m^3/s)
Case 1	60.2	1.06×10^8	12000	5000	54.2
Case 2	60.2	1.06×10^8	20000	5000	54.2
Case 3	106.5	1.06×10^8	12000	5000	95.9
Case 4	12.8	1.06×10^6	20000	5000	11.5
Case 5 (a)	60.2	1.06×10^6	20000	5000	54.2
Case 5 (b)	60.2	1.06×10^8	8000	6000	54.2

Table 4: Flow, volume, organic concentration and dissolved oxygen used in the simulations.

The inflow of 60.2 m^3/s was assumed based on the average flow of the Atibaia River in the rainy season (DAEE, 2019). High and low flow rates were assumed. All outlet flows were assumed to be 10% less than inlet flows, as presented by (Tercini, 2014). The normal volume of the reservoir, 1.06×10^8, is presented by Espíndola et al. (2004) and the reduced volume was stipulated, as well as the concentrations of dissolved oxygen and organic matter. Volume was assumed to be constant along the reservoir. The following constant values were used in all simulations: k_r=0.12 and k_d=0.19 (according to the table presented by Von Sperling (2014), regarding constants used for reservoir ecosystems), μ=1.03 (tabulated by Mizael (2019)), γ=0.8 and β=2.6 (Margalef, 1983).

RESULTS

Salto Grande Reservoir surface water analysis and simulation

Table 5 presents the results of BOD and DO analysis of surface water samples collected in Salto Grande reservoir on April 29, 2019.

Table 5: Results of BOD and DO analysis of surface water samples collected in Salto Grande reservoir.

Date	Analysis	P1	P2	P3	P4	P5	P6
04/29/2019	BOD (mg/m^3)	5040	3460	1490	1190	1220	980
	DO (mg/m^3)	6950	6440	6310	4880	3630	6030

Figure 8 shows the simulation of the self-purification curves for BOD and DO on April 29, 2019 using the results presented in Table 5 and using the model developed.

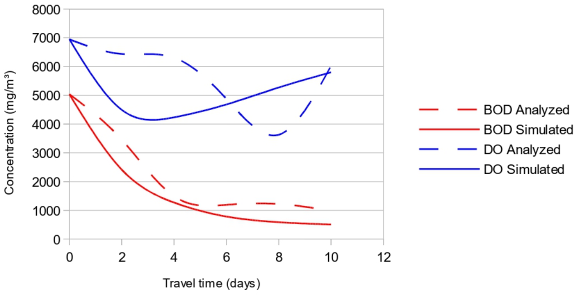

Figure 8: Simulation of the self-purification curves for BOD and DO on April 29, 2019 using the model developed.

Both BOD and DO curves start with the same concentration, since the initial concentration for the simulation curves are the concentrations analyzed in the collection whose results are in Table 5.

In the case of DO, it is observed that the simulated curve shows a notable decay in the first two days of travel. This is due to DO consumption in the system by the decomposition of organic matter, and subsequent growth from the third day of travel. However, the DO decay observed in the field assessment starts at P4 and intensifies at P5, reaching about 6000 mg/m³ at P6, a value very close to the tenth day of simulated travel.

The DO values diverge between day 0 and 10 because the collections were carried out on the same day. Therefore, the analyzed DO curve contains information that the simulations cannot give us from the path, such as: punctual changes in organic load in the reservoirs from aquatic plant banks or algae blooms; punctual changes caused by punctual contamination, such as runoff, not considered in the model; resuspension of organic matter from the deep zone.

Nevertheless, the graph is relevant for the study of the DO concentration after 10 days, presenting the same result for the final DO with the same initial DO, considering statistical error margins.

Also, for DO, the greatest variation between measured and simulated concentration was 2075 mg/m^3 at P2. The average variation between all points was 1217 mg/m^3. The empirical result of the DO concentration in the fifth point, that is the closest point to the dam that was analyzed was lower than the expected for the self-purification curve at this point. This is possibly because of the presence of macrophytes in this area of the reservoir, which reduce the gas exchange between air and water. In addition, the increase in the concentration of particulate organic matter causes a reduction in dissolved oxygen consumed by decomposing microorganisms.

In the case of BOD, both curves (analyzed and simulated BOD) evolve very similarly in relation to the travel days, ending very close to 1000 mg/m³ on the tenth travel day / P6.

The greatest variation between the measured and simulated BOD concentration was 1044 mg/m^3 at P1 and the average range of variation for all points was 556 mg/m^3, which is quite low.

Although this simulation was not performed in order to validate the model, it is possible to observe that the results achieved with this simulation are qualitatively similar to the results obtained at the same points through empirical analysis.

Case 1

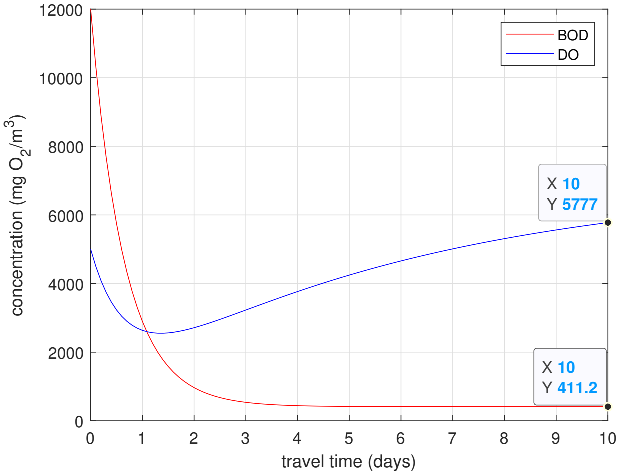

Figure 9: Case 1: normal flow, volume and organic concentration in 10 days of travel time

It is possible to observe in Figure 9 that in cases of average inlet and outlet flows, as well as the volume and concentration of organic matter and dissolved oxygen input, BOD would be reduced to less than half of its original concentration within the first 12 hours of travel. In the case of the analyzed scenario, BOD reduced from 12000 mg/m^3 to approximately 5700 mg/m^3 in the first half part of the day.

Dissolved oxygen, on the other hand, was reduced from 5000 mg/m^3 to about 3200 mg/m^3, since it is consumed by the organic material mineralization and also through oxidation.

In the 24 hours of travel, BOD decay is intensified, reaching approximately 2900 mg/m^3, and dissolved oxygen reaches 2600 mg/m^3.

It is also possible to observe that the dissolved oxygen concentration, in this analyzed scenario, would increase again on the second day of the journey, while the BOD concentration would reach stability, that is, would stop concentration decrease on the third day of the journey.

Case 2

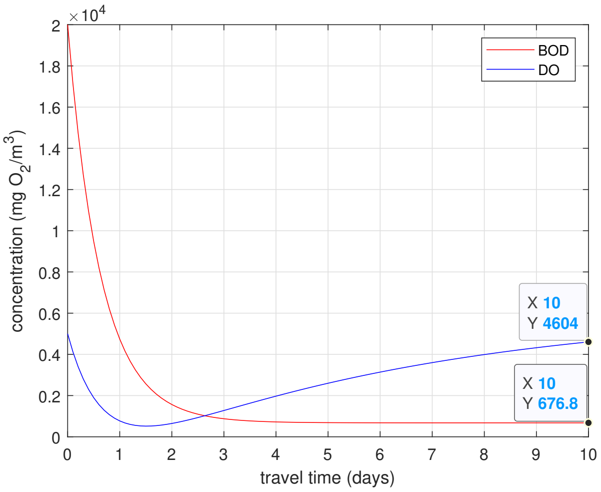

Figure 10: Case 2: Normal flow and volume and high organic concentration in 10 days of travel time

Regarding the second case analyzed, BOD is also reduced in the period of 12 hours of travel, but less than in the first case. This is attributed to the fact that the initial BOD concentration was 20000 mg/m^3. In Figure 10 it is possible to observe that BOD reaches, after half day of travel, approximately 9500 mg/m^3, while the DO reaches approximately 1900 mg/m^3. That is, it is drastically reduced by organic material decomposition. After 24 hours of travel, BOD and DO continue to decline, reaching a concentration of 4700 mg/m^3 of BOD and 770 mg/m^3 of DO, very close to anaerobiosis.

Dissolved oxygen concentration increases again on the second day of the journey, and BOD stabilizes on the third day. The reduction rates of organic matter are similar in this second case and in the first one, with the difference that in the first case, the dissolved oxygen reaches a greater value and the organic concentration a lower value in the same travel time as the second case.

Case 3

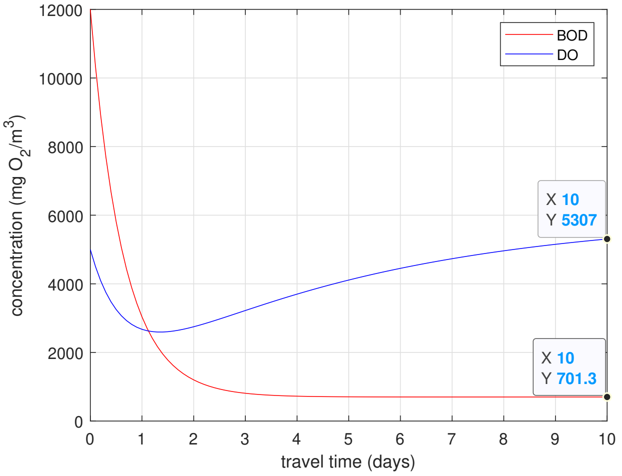

Figure 11: Case 3: High flow, normal volume and organic concentration in 10 days of travel time

According to Figure 11, the flow increase also causes a greater inflow of organic concentration and dissolved oxygen. That is, the concentration of BOD and DO in mg/m^3 increases mathematically when there is a greater flow in m^3. So, even if BOD and DO concentrations are the same simulated in the first case (12000 mg/m^3 of BOD and 5000 mg/m^3 of DO), there are more liters of water entering the reservoir, then more BOD and DO. Therefore, it is possible to observe that BOD and DO concentration after 12 or 24 hours of travel is slightly greater than the concentrations found in the first case: BOD ranges from 12000 mg/m^3 to 5800 mg/m^3 after 12 hours and to 3070 mg/m^3 after 24 hours; dissolved oxygen, from 5000 mg/m^3 to 3200 mg/m^3 after 12 hours and to 2670 mg/m^3 after 24 hours.

It was observed that, although the oxygen concentration also starts to increase on the second day of the journey, as in the previous cases, it stops being reduced before the other analyzed cases. In other words, the inflection of the DO curve occurs before what happened in the previous cases, which demonstrates that the degradation and active decomposition zones (which are the zones of greatest oxygen consumption in the self-purification process) are smaller in this case. This is because the entry of dissolved oxygen was initially greater and, therefore, the organic decomposition is faster.

Case 4

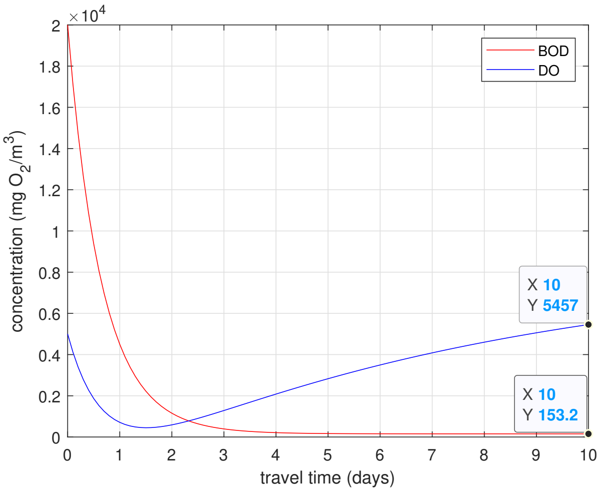

Figure 12: Case 4: low flow, normal volume and high organic concentration in 10 days of travel time

Figure 12 show that, even with low flow and high organic concentration entered in the reservoir (20000 mg/m^3 BOD), the organic matter is strongly depurated in the first 12 hours, reaching half of its initial concentration in this travel time.

Dissolved oxygen, in turn, reduces to a fifth part after 24 hours of travel, close to anaerobiosis. It is observed that it is only at the end of the second day of the journey that the DO concentration begins to increase in the reservoir, indicating that the recovery zone in the self-purification process happened later than in the previous cases analyzed .

Case 5

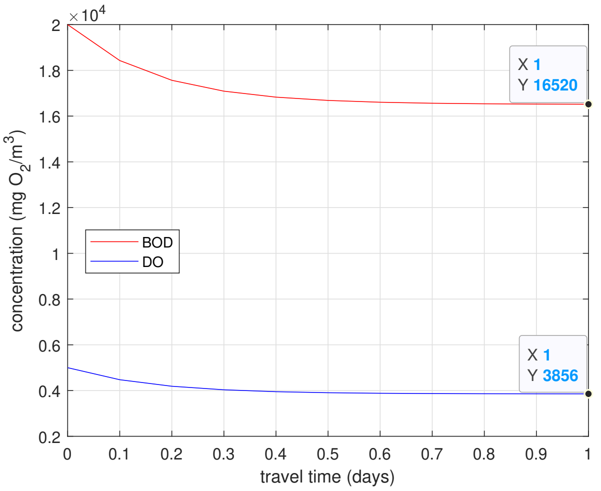

Figure 13: Case 5 (a): normal flow, low volume and high organic concentration in 24 hours of travel time

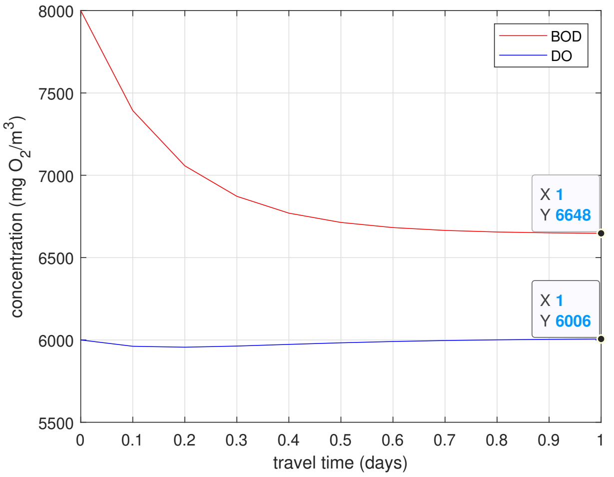

Figure 14: Case 5 (b): normal flow, low volume and low organic concentration in 24 hours of travel time

In the fifth case, it was analyzed how self-purification in the reservoir with low water volume and average flow rate occurs if there is a high input of organic matter and if there is a reduced input.

In Figure 13 it is observed that, with the entry of 20000 mg/m^3 of BOD under low volume of water, in 12 hours of travel this concentration is reduced to approximately $\frac{3}{4}$ than initially. In the case of DO, it is reduced to $\frac{4}{5}$ from the initial concentration in the same period. On the other hand, with low input of organic matter, as shown in Figure 14, the BOD has a 13 % reduction in the 12-hour period, and the DO has only 4 % of its concentration reduced in the same period.

The percentage of reduction in organic concentration, in both cases, was the same: 17 % of BOD. The difference, however, was in the dissolved oxygen consumed in the aquatic environment to perform the purification: in the first case, with high organic concentration, 22 % of the oxygen in the medium was consumed to depurate the organic matter; in the second case, less than 1 % of oxygen was consumed.

The decomposition of organic material happens more slowly in the last 12 hours of the day. Figure 13 shows that BOD ranges from 20000 mg/m^3 to 16500 mg/m^3 in one day, and the oxygen goes from 5000 mg/m^3 to approximately 3900 mg/m^3. In the scenario with low organic concentration (Figure 14), BOD drops from 8000 mg/m^3 to 6600 mg/m^3, while the DO goes from 6000 mg/m^3 to 6006 mg/m^3, or technically remains at 6000 mg/m^3. That is, after 24 hours BOD still decays at the same rate in both cases, but the dissolved oxygen is presented in a scenario more favorable to a reservoir facing a low volume if it receives less organic discharge.

It was found that the efficiency of self-cleaning is greater when there is a greater volume of water in the reservoir. In the second case analyzed (Figure 10), whose BOD input was 20000 mg/m^3, the removal efficiency of organic matter was 52.6 % for 12 hours of travel and 76.3 % for 24 hours. In the fifth case (a) (Figure 13), whose BOD input was also 20000 mg/m^3 however the volume of the reservoir was quite reduced, the organic matter efficiency of removal was 16.55 % in the first 12 hours of travel and 17.4 % for 24 hours.

DISCUSSION

The model developed (Equations 1 and 3) has shown to be applicable to different reservoirs, since it was validated having as parameters a reservoir present in a large river and which contains several other reservoirs. Also, it was applied in a reservoir dammed in a medium-sized river and with another water residence time.

The one-dimensional model CE-QUAL-R1 is, as well as the model proposed by this study, a model based on the conservation of mass and energy. There is, both models consider mass/energy input - output, ± reactions. CE-QUAL-R1, however, divides a reservoir in horizontal layers, and so it presents a set of differential equations that makes the computational implementation less simple (Wlosinski 1985). On the other hand, the model presented at this study is quite simple to be implemented.

The model CE-QUAL-RI, although more complete than CE-QUAL-R1, presents similar restrictions to CE-QUAL-R1, that is the difficult computational implementation and a high number of parameters, which requires a greater number of laboratory analysis.

Mike models are not analyzed in this discussion because the access to their model equations and parameters require the purchase of a license, which makes their application deprecated when compared to other existing models.

Vázquez and Mokrova (2019) suggest the use of the models through GIS-MM integration. The study presents the advantages and disadvantages of using two models that could fulfill this integration function: SWAT model (Arnold et al., 2012), a model widely used for the analysis of hydrological processes. That is also based on the equation of the water balance and has, as initial parameters, the inflow and outflow of water by flow, water input by rain and water out by evaporation; and the IBER Bi-dimensional Model, used for river hydrodynamics, flood areas studies, evaluation of sediment transport, among other tools for hydrodynamic studies, also based on the equations of conservation of mass and momentum, in this case in two horizontal directions, since the model is two-dimensional.

The model is quite complete in terms of physical phenomena in the reservoir, including parameters such as friction caused by wind. However, it is a model whose application requires more advanced computational implementation, since it is a two-dimensional model, and does not consider physical-chemical and biological phenomena whose studies allow the evaluation of water self-purification, such as mineralization of organic compounds.

The model proposed by Vázquez and Mokrova (2019) proposes an easy daily application of the tool by operators and managers (once implemented), as some of the data that feeds the model could be obtained through GIS. However, the study lacks validation and, as it has been presented so far, it would not be useful to specifically study the self-purification capacity in reservoirs.

Jiang et al. (2016) use the combination of the Hydrodynamic Model of MIKE 21 coupled with the transport module (TR). They propose the use of a 2-D model to simulate the flow behavior and the contaminant convection transport in the tidal river, using the two-dimensional advection-dispersion equation. Although it is a very complete model, it is two-dimensional, which makes its computational implementation more elaborated. Besides, it presents quite many parameters to fill, which diverges from the proposal of this study, that is to present a model with few parameters and easy to apply.

The model proposed by Reartes et al. (2016) differs from the model presented in this study in terms of practicality of application due to the number of parameters it considers. The model exposed in Reartes et al. (2016) was developed by dividing the reservoir into two layers: upper and lower. The first aspect to highlight is that the Reartes et al. (2016) model has an output for water treatment in the lower layer, so it is interpreted as a model for a reservoir that has an outlet for public supply; the second point is that it has many parameters for estimating the problem, many of them specific and that require a detailed empirical study before applying the model. The model presented in this study through the Equations 1 and 3, on the other hand, requires only empirical data of flow, volume, BOD and DO.

Regarding the model applied by Tercini and Méllo Junior (2016)study used at this work to validate the model, it is an adaptation of Street & Phelps model, a model initially developed to study self-decay capability in lotic watercourses. Though, in the case of Tercini and Méllo Junior (2016), it was used residence time as a parameter to analyze self-decay rates in dammed environments. Although it is also a simple model to apply in lentic aquatic environments, it does not consider the organic matter sedimentation effect in the water quality of the reservoir's epilimnium.

Thus, when compared to other models, the model presented in this study has advantages due to its easy application, and can be used with simplicity by sectors that carry out water management, accepting the hypothesis initially posed in this study. It has, however, limitations that could be evaluated in future works. Temperature was not included as a parameter to analyze water clearance and this can lead to a less accurate analysis in months of thermal stratification. Furthermore, the *in loco* contributions of organic matter, which could provide a more detailed analysis of organic load by study point, as discussed in Figure 8, Section Results, might also be considered in future researches.

Furthermore, it is suggested the insertion of parameters that represent the decomposition in the hypolimnion and the interactions between water and sediment that result, for example, in the resuspension of organic material in the deep zone of the reservoirs. A more punctual study of the hypolimnion is extremely important to, in addition to understanding organic purification in deep areas, understand the real situation of reservoirs that receive large loads of organic material from untreated sewage; this is because the study of the epilimnion can result in the false idea that a reservoir that receives certain organic loads happens to have these organic loads mostly mineralized. Though, part of this organic load ends up being sedimented and, in the hypolimnion, faces a slower mineralization time, as the decomposition there is mostly carried out by anaerobic organisms (Wetzel, 2001).

CONCLUSIONS

Self-purification has an essential function improving the water sources quality, as observed in the simulations. In all cases analyzed, the reservoir would begin to recover its balance within the first two days of the journey, and with higher efficiency when the volume of water in the reservoir is greater.

The mathematical model developed is a suitable tool to study and evaluate the self-purification process and run-time in any reservoir. It was possible to make analysis and predictions of the organic matter and dissolved oxygen concentrations at the reservoir studied using the developed model and considering possible scenario changes.

It is shown as an innovative and relevant model to be used both in private enterprises and in the public management of watercourses to evaluate self-purification capability of any reservoir. That confirms the hypothesis initially assumed to develop this work. The effective monitoring and control carried out by the competent organizations can result in actions to improve the water bodies quality, such as incentives to increase the rates of domestic and industrial sewage treatment that are discharged in reservoirs and restoration of riparian forests.

It is pointed out the possibility of adding, for future works - since the model is passive of upgrading - the study of hypolimnium in the mathematical model, in addition to the alternative of complementing the model considering other physical-chemical and biological phenomena.

Also, for future works, it is recommended the validation and application of the developed model using interconnected reservoirs, adding model output parameters without major complications in the computational implementation.

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