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Zero-dimensional modelling as tool for reservoir water quality planning and management

Modelos zero-dimensionais como ferramenta para planejamento e gestão de qualidade da água em reservatórios

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ABSTRACT

Water quality models are often applied to support the definitions for water resources planning and management. This process requires appropriate data to calibrate and make the required verification process for validation analysis. However, in some case studies, there is not enough data to run a complex water quality model whatever is the water system, being river or reservoir. In the context of scarce data, the search for a simple water quality model is an alternative to comprehend the water quality behavior of the water system. In this research, an unsteady zero-dimensional (0D) water quality model was developed and applied using synthetic series of phosphorus concentrations for a Brazilian reservoir. The results of the zero-dimensional models developed in this research were compared to the results of a three-dimensional water quality model, in order to verify if this methodology can be a simpler alternative to a complex three-dimensional model. The compatible results of the zero-dimensional (0D) and three-dimensional (3D) models show the simplified numerical schemes are important potential tools to be considered for initial analysis of water quality dynamics in reservoirs and for management purposes.

Keywords: Reservoir; Unsteady zero-dimensional modelling; Simplified model.

RESUMO

Modelos de qualidade da água são frequentemente aplicados para apoiar as definições de planejamento e gestão de recursos hídricos. Este processo requer dados apropriados para calibrar e fazer o processo de verificação necessário para análise de validação. No entanto, em alguns estudos de caso, não há dados suficientes para executar um modelo complexo de qualidade da água, seja qual for o sistema de água, rio ou reservatório. No contexto de dados escassos, a busca por modelos simples de qualidade da água é uma alternativa para compreender o comportamento da qualidade da água. Nesta pesquisa, um modelo zero-dimensional não-permanente de qualidade de água foi desenvolvido e aplicado utilizando séries sintéticas de concentrações de fósforo para um reservatório brasileiro. Os resultados dos modelos zero-dimensionais desenvolvidos nesta pesquisa foram comparados aos resultados de um modelo tridimensional, a fim de verificar se esta metodologia pode ser uma alternativa mais simples ao modelo tridimensional complexo. Os resultados compatíveis dos modelos zero-dimensional (0D) e tridimensional (3D) mostram que os esquemas numéricos simplificados são importantes ferramentas potenciais a serem consideradas para a análise inicial da dinâmica da qualidade da água em reservatórios e para fins de gestão.

Palavras-chave: Reservatório; Modelo zero-dimensional não permanente; Modelo simplificado.

INTRODUCTION

Reservoirs are built to guarantee distinct water uses, including water and energy supply, recreation activities, fishing and flow regulation. As a consequence, any pollution process can restrict their designated uses. In order to maintain the designated uses of a water body, the governmental agencies around the world provide regulation aiming to guarantee the best strategies for water quality planning and management. In Brazil, for instance, the Brazilian Law nº 9.433/1997 (Brasil, 1997), also known as National Policy of Water Resources, defines five instruments for the water planning and management. One of them is called "Water Quality Classification Framework", that establishes the overall framework considering the future plans for the watershed, main water uses and the overall reference for future scenarios development. These procedures are regulated by National Water Resources Council (CNRH) resolution nº 91/2008 (Brasil, 2008). This instrument defines the class of a waterbody based on the most restrictive designated use. The CONAMA 357/2005 resolution (Brasil, 2005) establishes concentration standards for each class of waterbodies, classified according to the legal Water Quality Classification Framework.

However, there is no specific methodology for reservoirs water quality classification in the framework context considering that, according to the CNRH resolution nº 91/2008, the Water Quality Classification Framework procedure should consider the specificities of the waterbodies, with emphasis on the lentic environments and the stretches with artificial reservoirs, flow seasonality and intermittent regime. Besides, the general overview of waterbodies based on concentration limits does not allow adequate conditions for analysis considering the dynamics of the water system.

Particularly, in order to improve this Water Quality Classification Framework process it is recommended to consider mathematical models that represent physical, chemical and biological processes. Models require appropriate data to guarantee the whole traditional requirements for implementation, such as calibration and validation. However, in some situations, there is not enough data to run a complex three-dimensional water quality model. In the context of scarce data, the search for a simple water quality model is an alternative to comprehend the water quality behavior and to assist in defining the Water Quality Classification Framework management recommendations, particularly, for reservoirs.

In cases where the water quality data is scarce, the tendency highlighted in literature is to simplify the models, using less dimensions and considering less processes. Several applications of models simulate river segmented in reservoir compartments, such as Fan et al. (2009), Cox (2003), Karadurmus & Berber (2004), Berber et al. (2009), Keupers & Willems (2017) and Nguyen et al. (2018).

Complementary, in this strategy for more simplified representation, Slaughter et al. (2017) proposed a water quality model that adopted the strategy of modelling reservoirs as a completely stirred tank reactor (CSTR). The model was able to use the limited observed data to simulate representative frequency distributions of water quality, and the approach used was shown to be suitable for application to data scarce catchments.

Pintilie et al. (2007) also applied a zero-dimensional model considering the mass balance and complementary equations for metals, under several scenarios with steady conditions. Also, Toné (2016) applied and calibrated the CSTR model to 33 reservoirs of Brazil's northeast semiarid region and validates the model with data from 8 reservoirs of the South African semiarid.

Polli (2018) also followed the simplification tendency. The author divided a reservoir in sectors and applied Delft3D model in a simplified configuration. That research showed it was possible to identify periods of mixing and stratification with simple models and low time processing.

A potential use for zero-dimensional modelling is the application of this tool in the context of cascading reservoirs, in a way that integrates with a model suitable for rivers. This application would fulfill a gap noticed in river-reservoir integrated studies: the lack of a specific model that includes both environments and properly considers temporal changes. An example of a study focused on water quality along river-reservoir systems was proposed by Tercini & Méllo Júnior (2016), who applied the one-dimensional Streeter-Phelps equations in order to model Biochemical Oxygen Demand and Dissolved Oxygen concentrations along a Brazilian river. This model indicated the critical location for the dissolved oxygen.

Another example is the system of six cascade reservoirs modeled by Cunha-Santino et al. (2017), applying a zero-dimensional model in order to model 23 limnologic variables. They pointed out that the reservoirs were efficient in retaining elements, which emphasized the role of these reservoirs for the mitigation of eutrophication, turbidity, total solids, color and coliforms of the Juquiá-Guaçu river.

In this work, an unsteady dynamic zero-dimensional (0D) water quality model was developed in order to better assess the system dynamics and the influence from the watershed. The model is capable of consider tendency scenarios for the daily loads that enter the reservoir. Those scenarios that can be helpful to the regulation of the water quality criteria of the watershed. This analysis will be relevant to understanding the limitations of the basin and how such limitations should be reflected in the regulatory legislation. Additionally, the results of zero-dimensional (0D) models developed in this work were compared to the results of a three-dimensional model (3D), in order to verify if this methodology can be a simpler alternative to a complex three-dimensional model in the context of the Brazilian Water Quality Classification Framework process. The model was applied to the phosphorus concentrations of Jurumirim reservoir, at the Paranapanema River, Brazil. Phosphorus was chosen as model variable since its important behavior limiting the primary productivity of the reservoirs (Agência Nacional de Águas e Saneamento Básico, 2019).

MATERIAL AND METHODS

Case study

The Paranapanema basin (Figure 1) is located in Brazilian States of São Paulo (47% of the basin) and Paraná (53%). The Paranapanema River rises in the Serra de Agudos Grandes, in São Paulo State, and has its mouth at Paraná River, after covering about 930 km. In the headspring region it is surrounded by intense native forest. Paranapanema River was considered unsuitable for navigation due to the waterfalls along its course. From the 20th

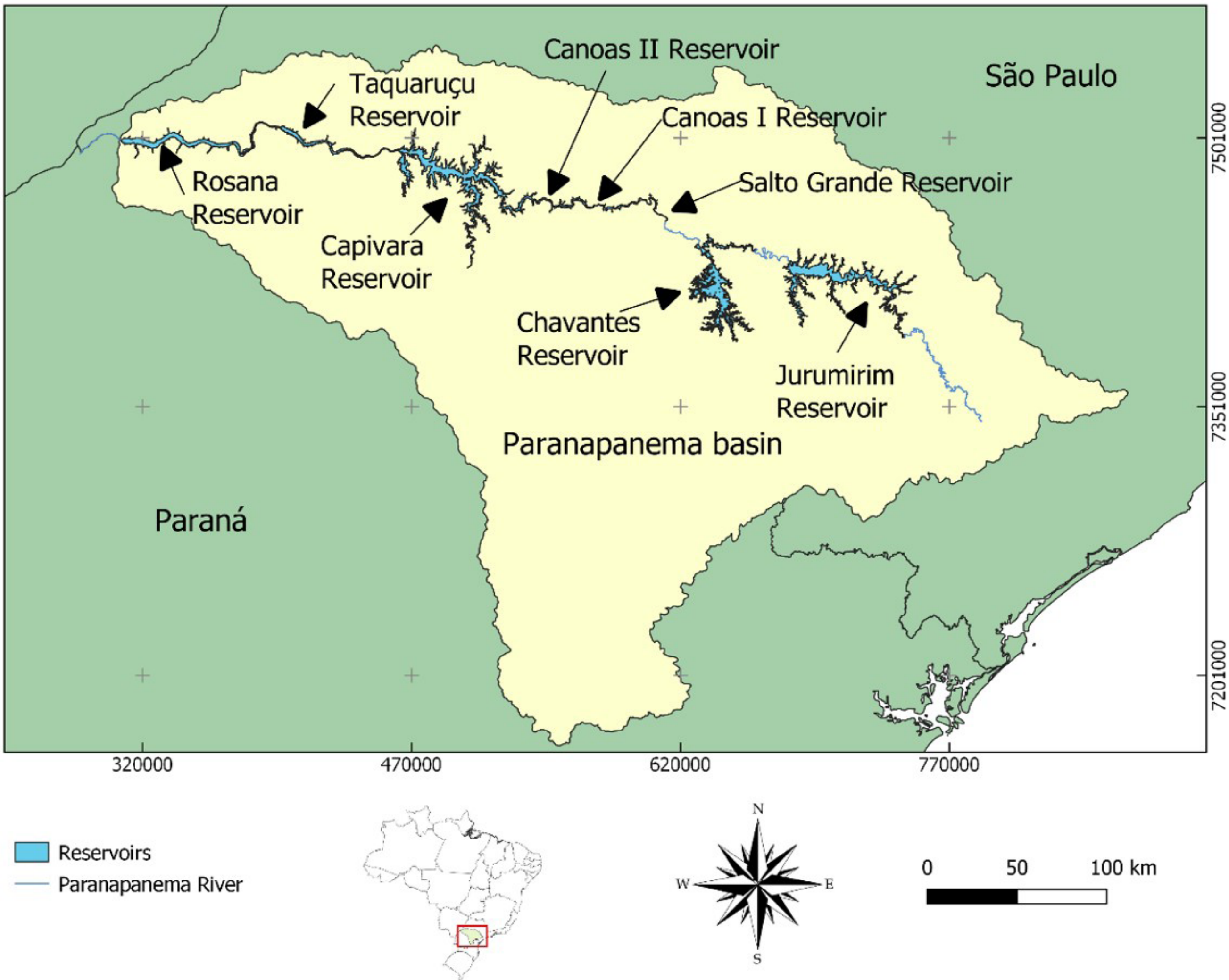

Figure 1. Cascade reservoirs on Paranapanema watershed.

century onwards the energetic potential was discovered. Therefore, the greatest use today is power generation (Grupo Integrado de Aquicultura e Estudos Ambientais, 2013). This work focused on Jurumirim reservoir. It is the first reservoir on the cascade of hydropower plants of the Paranapanema basin. It was the second powerplant built in this river and it generates 101 MW, which represents 2,3% of the total generated in the Paranapanema watershed (Agência Nacional de Águas e Saneamento Básico, 2014). This reservoir has 449 km^2 in a region of great economic development and encourages sports, leisure and tourism practices (Prefeitura de Paranapanema, 2023). The maximum maximorum volume is 7.70109 m^3, which corresponds to the 569.50 m height. In these conditions, the maximum depth is 39.5 m. The length of reservoir flow path is 117 km. The long-term average flow (1940-2012) for Jurumirim reservoir is 263 $m^3.s^{-1}$.

Zero-dimensional model

This work presents a zero-dimensional equation in two different applications. In both situations, the same entry data is applied. However, while in the first one the reservoir is considered as a simple tank reactor (Model A), the second one divides the reactor in four sectors, aiming to create zones with similar water quality characteristics (Model B). Figure 2 shows a schematic illustration of the input and output data of the model.

In this research, the input data are: inflows and outflows, input phosphorus concentrations in daily frequency, which is a synthethic series created based in measured data, and the variation series of volumes and areas. The output result is the concentration time series of the water quality parameter in analysis (phosphorus).

Measured data

The Environmental Company of São Paulo State (CETESB) is responsible for the monitoring of water quality in São Paulo State. CETESB monitors the basin since January/1978 and its data reaches until May/2018.

The HidroWeb Portal is a tool that is part of the National Water Resources Information System (SNIRH) and offers access to the database that contains all the information collected by

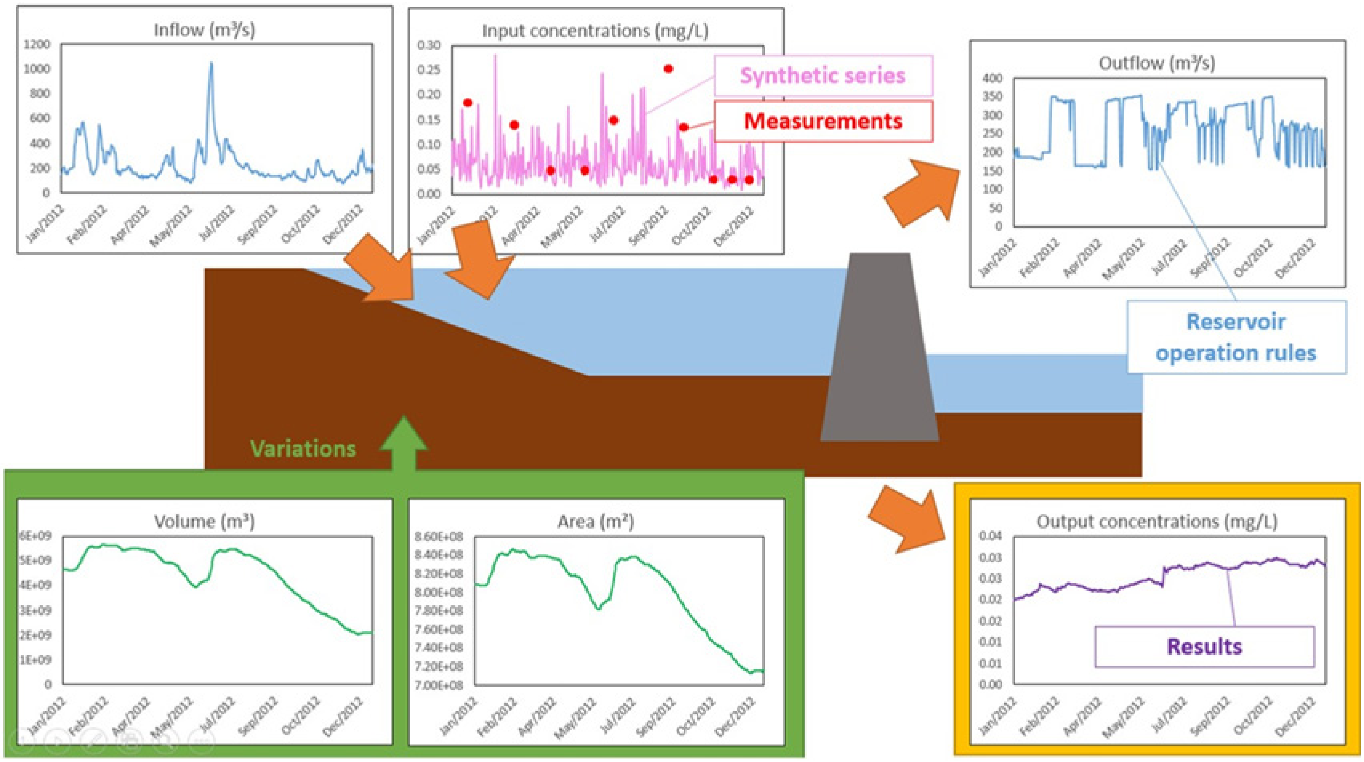

Figure 2. Methodology schematic flowchart.

the National Hydrometeorological Network (RHN), gathering data on river levels, flows, rainfall, climatology, water quality and sediments. The Paranapanema basin water quality data from this portal dates from August/1976 to April/2019.

Grupo Integrado de Aquicultura e Estudos Ambientais (2013) developed a study of areas suitable for aquaculture in the Paranapanema Complex Reservoirs. This study generated water quality data from May/2011 to October/2011.

All of the abovementioned measurements from different sources were joined in the same database and applied in the process of the generation of synthetic series, according to the procedure described in item **Synthetic series**.

Synthetic series

One peculiarity of the water quality monitoring is the scarce time scale, which is different from flow measurement time scales. Ferreira et al. (2019) applied an innovative method to match temporal scales of boundary conditions and generated synthetic pollutographs to convert a historical dataset (monitoring as snapshots during twelve years) into continuous information. The method allow this conversion by integrating the statistical parameters of the historical series and the natural random variability of the environment. The synthetic series generation was based on first order autoregressive process (AR1).

Due to the unavailability of water quality data in the same time scale of the hydrological data, Agência Nacional de Águas e Saneamento Básico (2020), based on the abovementioned study, calculated the synthetic series for the study case reservoir and these results were applied in the present research, as well as in the three-dimensional model whose results were compared.

It is worth mentioning that exploring the challenges of time scales was not the goal of this research. However, this study present an important potential use to that authors' results.

Model A: Continually Stirred Tank Reactor (CSTR): a zero-dimensional model

The Continuously Stirred Tank Reactor (CSTR) is among the simplest ways to model a natural body of water (Chapra, 2008). The equations presented in this research indicate phosphorus concentrations. However, it is worth remembering that this methodology can be adapted to any water quality variable. This model considers the reaction and sedimentation processes represented in Figure 3 as described in Equation 1:

$$\text{Accumulation} = \text{inflow} - \text{outflow} - \text{reaction} - \text{settling} \tag{1}$$

Accumulation represents the change of mass M in the system over time (t), as shown in Equation 2, in which V is the volume (m^3), c is phosphorus concentration ($mg.L^{-1}$) and t is the time (s).

$$\text{Accumulation} = \frac{dcV}{dt} \tag{2}$$

The reaction is represented by the product of the first order reaction coefficient (k), volume (V) and concentration (c), as shown in Equation 3, in which k is the first order decay coefficient (s^{-1}).

$$\text{Reaction} = k\ V\ c \tag{3}$$

The settling is considered as the mass that goes through the water-sediment interface. Therefore, it's calculated by Equation 4, where v is the apparent settling velocity and H is the reservoir depth. Then, the volume (V) divided by the depth (H) are replaced by the corresponding surface area (A_s).

$$\text{Settling} = \frac{v}{H} V\,c = v\,A_s c \tag{4}$$

The equations of each process considered can by replaced in Equation 1, as shown in Equation 5, in which Q_{in} is the inflow ($m^3.s^{-1}$), Q_{out} is the outflow ($m^3.s^{-1}$), c_{in} is the inlet concentration ($mg.L^{-1}$) and c_{out} is the outlet concentrations ($mg.L^{-1}$). The inflows and outflows are the multiplication of the inflow and outflow by the inlet and outlet concentrations, respectively.

$$\frac{dcV}{dt} = Q_{in}c_{in} - Q_{out}c_{out} - kVc - v\,A_s c \tag{5}$$

Using the numerical method of finite difference to approximate the derivative as differences, Equation 5 can be expressed as an algebraic Equation 6.

$$c_{out\ i+1} = \frac{c_{out\ i} + \frac{\Delta t}{V_{i+1}}\left(Q_{in\ i+1}c_{in\ i+1}\right)}{1 + \frac{\Delta t}{V_{i+1}}\left[Q_{out\ i+1} + kV_{i+1} + v\,A_{s\ i+1} + \frac{\Delta V}{\Delta t}\right]} \tag{6}$$

In which $c_{out\ i+1}$ = phosphorus concentration downstream ($mg.L^{-1}$), $c_{out\ i}$ = phosphorus concentration downstream (when i=0, this value is equal to zero, since the initial condition applied in this research is that there was no phosphorus on the reservoir at first), $c_{in\ i+1}$ = phosphorus concentration upstream ($mg.L^{-1}$), Δt = time step (s), V_{i+1} = volume of the corresponding reactor (m^3), ΔV = difference of the volumes (m^3), $Q_{in\ i+1}$ = Inflow ($m^3.s^{-1}$), $Q_{out\ i+1}$ = Outflow ($m^3.s^{-1}$), k = first order decay coefficient (s^{-1}), v = apparent settling velocity ($m.s^{-1}$) and $A_{s\ i+1}$ = surface area of the sediments (m^2). The surface area of the sediment is estimated to be two times the surface area, supposing the reservoir has an equilateral triangle section.

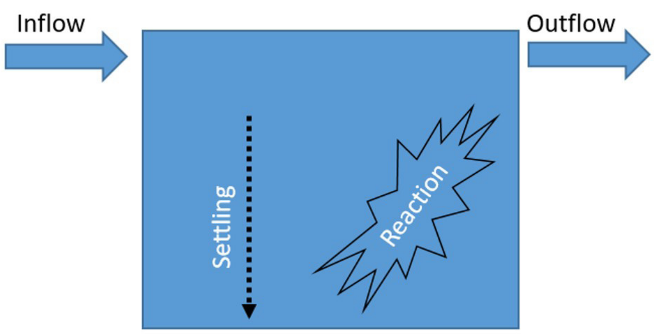

Figure 3. Natural processes represented in CSTR model.
Source: adaptation from Chapra (2008).

Warm up time is the time required for a numerical model to reach a steady state after the initial conditions have been set. Until the warm up period has ended, the results of the model are not reliable. This model was run for a period of two years (2011 and 2012). The first-year results (2011) were discarded in order to guarantee that the warm up time had no influence on the results, since it took some months to reach stable results.

For each day, there was a value of inflow, outflow, volume, area and initial concentration. The flows, areas and volumes came from the Brazilian reservoir tracking system (SAR). The daily initial concentrations are the results from the synthetic series of Agência Nacional de Águas e Saneamento Básico (2020).

The parameters k and v were defined by trial and error, based on the comparison of the simulation median to the observed data median. The selected parameters were selected based on the smallest deviation from observed data. This comparison is presented in item **Model A**.

The simulations were made for a base scenario and four future scenarios: B12, T25, T35, A25 and A35, as described in Table 1. Those scenarios were defined by Agência Nacional de Águas e Saneamento Básico (2020), based in economic scenarios shown in Integrated Water Resources Plan of the Paranapanema Water Resources Management Unit (Agência Nacional de Águas e Saneamento Básico, 2016). In the tendential scenarios, public policies and the cultural socioeconomic arrangement will not differ radically from current ones. Brazil's short-term trend scenario brings stagnation to this basin until 2020, a moderate increasing in the economy until 2025 and a large increase until 2035. The accelerated scenarios represent the hypothesis of a series of positive factors joined, creating favorable conditions to economic growth. In this scenario, the wide increase in the economy starts from the year 2025 and it is maintained until 2035.

Model B: CSTR model with compartments

The CSTR model was applied in the four sectors of the Jurumirim reservoir (Figure 4), which was called Model

Table 1. Future scenarios.

B12	Baseline scenario - 2012	The year 2012 was selected for the reference scenario due to the availability of flow and concentration data.
T25	Tendential scenario - 2025	Brazil's short-term trend economic scenario for the year 2025, considering a moderate increment in the economic situation.
T35	Tendential scenario - 2035	Brazil's long-term trend economic scenario for the year 2035, considering a moderate increment in the economic situation.
A25	Accelerated scenario - 2025	Brazil's short-term trend economic scenario for the year 2025, considering a wide increment in the economic situation.
A35	Accelerated scenario - 2035	Brazil's long-term trend economic scenario for the year 2035, considering a wide increment in the economic situation.

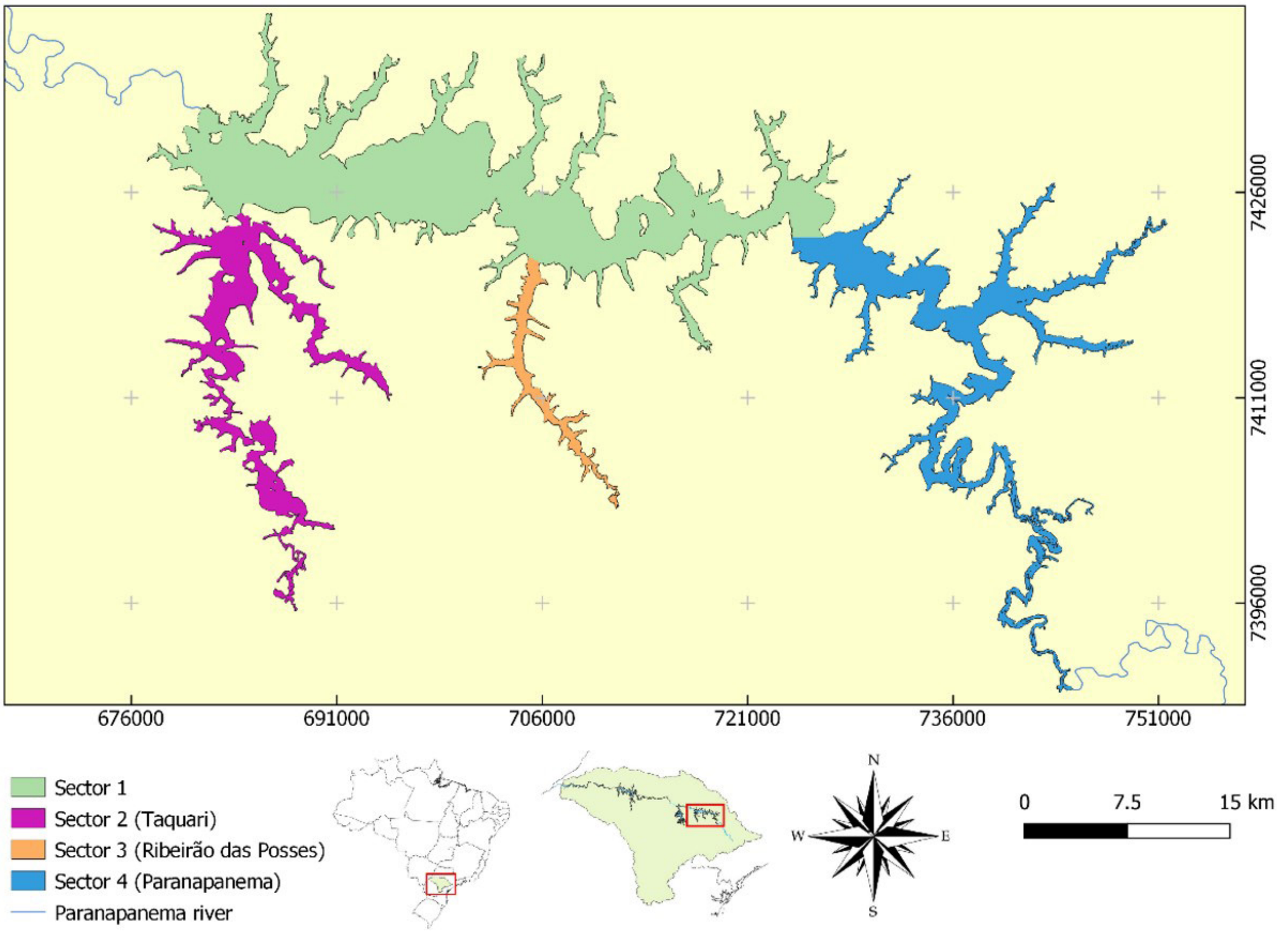

Figure 4. Sectors applied in the "model B".

B. The creation of four different regions decreases the model limitation of uniformity along the whole reservoir. Sector 1 is the deepest part of the reservoir, close to the dam. Sector 2 is the Taquari river entry, while sector 3 is the entrance of Ribeirão das Posses. Sector 4 includes the entrance of the Paranapanema river.

The sectors were defined in the context of the reservoir zoning proposed by Agência Nacional de Águas e Saneamento Básico (2020), which aimed to divide different reservoir areas as a function of their characteristics. The number of sectors were defined as the total number of the largest sub-basins covering 80% of total reservoir's drainage area. The definition of sector was the result of spectral clustering of equidistant points inside the reservoir area. Thus, the result is a clustering based on the morphological aspects of the reservoir and the basin.

The outlet flows and concentrations of the sectors 2, 3 and 4 were considered as input values for the sector 1, as showed by Equation 7.

$$\overbrace{c_{out\ i+1}}^{\text{Sector 1}} = \frac{c_{out\ i} + \frac{\Delta t}{v_{i+1}}\left(\overbrace{Q_{in\ i+1} c_{in\ i+1}}^{\text{Sector 1}} + \overbrace{Q_{out\ i+1} c_{out\ i+1}}^{\text{Sector 2}} + \overbrace{Q_{out\ i+1} c_{out\ i+1}}^{\text{Sector 3}} + \overbrace{Q_{out\ i+1} c_{out\ i+1}}^{\text{Sector 4}}\right)}{1 + \frac{\Delta t}{v_{i+1}}\left[Q_{out\ i+1} + kV_{i+1} + vA_{s\ i+1} + \frac{\Delta V}{\Delta t}\right]} \quad (7)$$

Due to the lack of observed data for comparison of the results of each sector, the choice of the parameters *k* and *v* followed the same values applied for model A for the Jurumirim reservoir. The parameters were the same for all sectors.

The flow series of the sectors was estimated based on the flow series of the inflow and outflow of the reservoir. However, to divide the flow of the reservoir between the sectors, it was considered that each sector received a percentage of the flow. This proportions were defined as functions of the drainage area of the tributaries of each sector. Table 2 shows the proportions of the areas, which were applied to the calculations of the flow series of the sectors.

The estimation of the load series followed the same process. The synthetic load series was given by the concentration of the synthetic series multiplied by the area proportions and to the flow. Then, the concentrations were obtained from the loads by the inverse process (dividing by the flow). The volumes and areas were obtained by an algorithm that considers the bathymetry and the water level of the reservoir.

Three-dimensional model: Delft3D

The three-dimensional modeling considered in the comparison with the zero-dimensional model was conducted by Agência Nacional de Águas e Saneamento Básico (2020) on

Delft3D mathematical model. In the horizontal direction, 98.646 cells were defined (401 in x direction in the Cartesian plan, 246 in y direction in the Cartesian plan). In the vertical direction, 10 layers were considered. The time step of the simulation was 30 seconds, in order to assure the Courant criteria and the stability of the numerical solution. In this case, the initial level was -2 m and the initial temperature was 20ºC. The phosphorus concentration series considered in the comparison were the vertical depth averaged results simulated in the exit of each sector. Figure 5 illustrates the morphologic grid, the bathymetry and the output monitoring points in which the daily series were evaluated. The values selected for the analysis were the average concentrations of the water column.

Evaluation of phosphorus results

In order to evaluate the magnitude of the phosphorus values, they were compared to the phosphorus limits for lentic environment (lakes and reservoirs) of the Brazilian regulation CONAMA 357/2005 (Brasil, 2005). The classes are defined in the Water Quality Classification Framework procedure considering the water uses defined for the waterbody. Classes 1 and 2, for example, designate the uses of "direct contact recreation", "aquiculture" and "aquatic community protection", while a waterbody classified as class 3 does not imply this water uses, considered as more noble. The phosphorus limits for each class are shown in Table 3. More details about the activities indicated by each class can be consulted in Agência Nacional de Águas e Saneamento Básico (2022).

RESULTS AND DISCUSSIONS

Model A

The calibration of the model consisted in the process of comparing the boxplots of several simulated series with the boxplot of the measured data. The simulated series were calculated considering the first order decay coefficient (k) of 0 s^{-1}, 0.001 s^{-1}, 0.005 s^{-1} and 0.010 s^{-1}. The apparent settling velocity (v) values were 0 $m.s^{-1}$, 0.001 $m.s^{-1}$ and 0.010 $m.s^{-1}$.

Figure 6 shows the calibration boxplots. In the right, the last boxplot shows the observed data in the water quality stations of Jurumirim reservoir. Table 4 shows the simulated medians and the difference from observed data. The median of the series simulated considering $k = 0.005$ s^{-1} and $v = 0.010$ $m.s^{-1}$ (blue box highlight) has smaller difference (0.0016 $mg.L^{-1}$) from the median of observed data (0.025 $mg.L^{-1}$), which corresponds to 6.4% of the observed value. Therefore, those parameters values were selected for the model simulations of Jurumirim reservoir.

Table 2. Proportions of the drainage areas of each sector.

Sector	Proportion of the drainage area
Sector 1 (Dam)	8.4%
Sector 2 (Taquari)	25.3%
Sector 3 (Ribeirão das Posses)	2.3%
Sector 4 (Paranapanema)	64.0%
Total	100.0%

Table 3. Phosphorus limits for lentic environment (Brasil, 2005).

Class	Water uses	Phosphorus limits for lentic environment ($mg.L^{-1}$)
Class 1	Noble uses	0.020
Class 2	-	0.030
Class 3	-	0.050
Class 4	Less noble uses	No limit

Figure 5. Morphologic grid, bathymetry and output monitoring points from Delft3D model used for comparison between models.

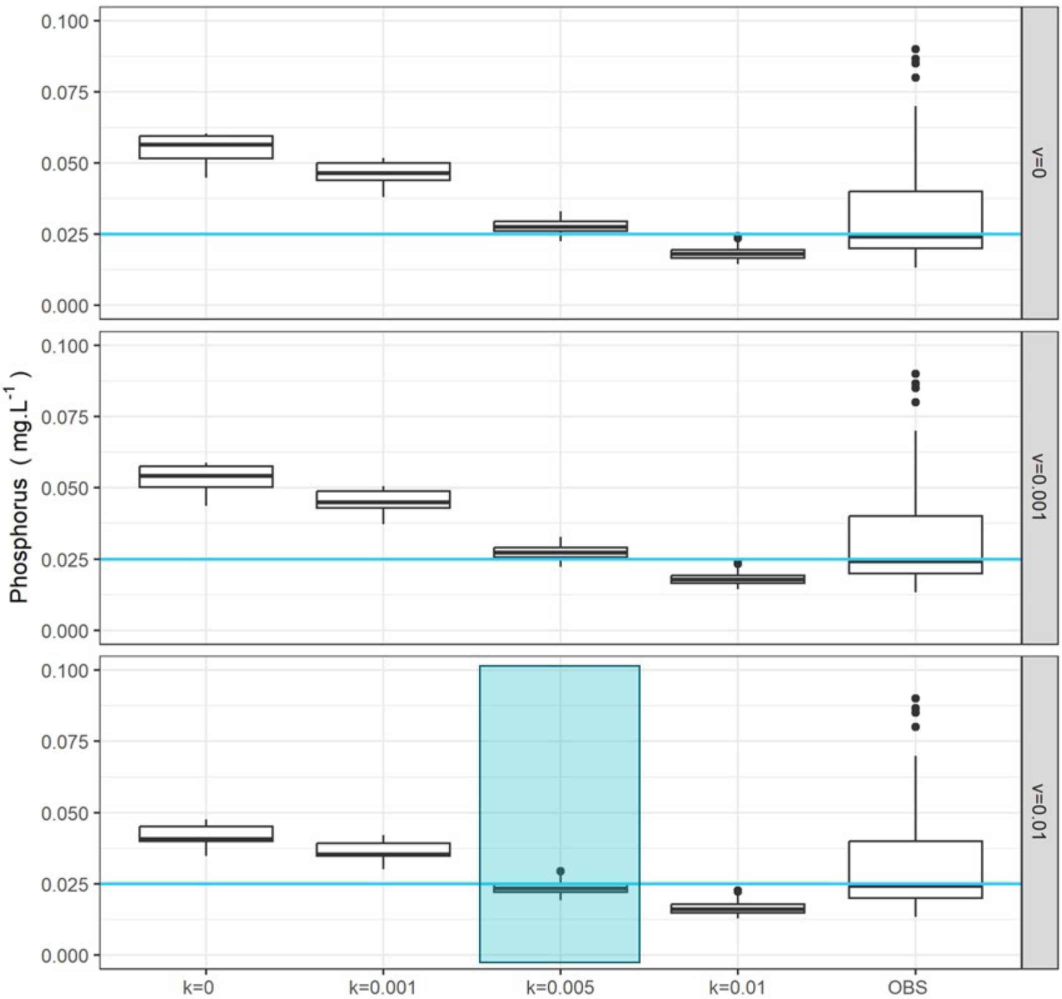

Figure 6. Boxplots of the sensibility analysis of the model parameters (k: s^{-1} and v: m.s^{-1}) – Jurumirim reservoir (the blue line represents the median of observed data and the blue box highlight represents the selected series).

Table 4. Simulated medians and difference from observed data. Values in bold represent the parameters selected for the model simulations.

k (s^{-1})	***v*** (s^{-1})	**Simulated (mg.L^{-1})**	**Difference (mg.L^{-1})**
0	0	0.0565	0.0315
0	0.001	0.0542	0.0292
0	0.010	0.0407	0.0157
0.001	0	0.0466	0.0216
0.001	0.001	0.0449	0.0199
0.001	0.010	0.0353	0.0103
0.005	0	0.0276	0.0026
0.005	0.001	0.0272	0.0022
0.005	**0.010**	**0.0234**	**0.0016**
0.010	0	0.0181	0.0069
0.010	0.001	0.0178	0.0072
0.010	0.010	0.0160	0.0090

The time series result for each calibration strategy is presented in Figure 7. The figure includes the results of two year simulation (2011 and 2012). The background color divides the years in the time axis. The first year (2011) was omitted of further graphics and not considered in the final results, due to the warm up time discard. As it can be seen in Figure 7, the first months of 2011 had increasing phosphorus values until the stability was reached. It took some months to reach stable results, depending on the parameters used in each simulation. The simulated series selected in the calibration phase was the one with $k = 0.005$ s^{-1} and $v = 0.010$ m.s^{-1}. In this series, the stability was reached in may/2011.

Figure 7 also works as a sensibility test for the *k* and *v* parameters. The smaller the parameters are, the bigger the phosphorus concentration is, since the terms of reaction and sedimentation are reduced.

The input synthetic series and output modeled concentrations of the year 2012 are shown in Figure 8. The synthetic series (input) has more variation in their values, since the numbers are generated in a partially deterministic autoregressive process, in which the following value is proportional to the previous one, but there is the statistical noise. The output concentrations, on the contrary, are continuous series, since the generated number is always a function of the previous value. The increasing values of the output series variation can be justified by the variation on

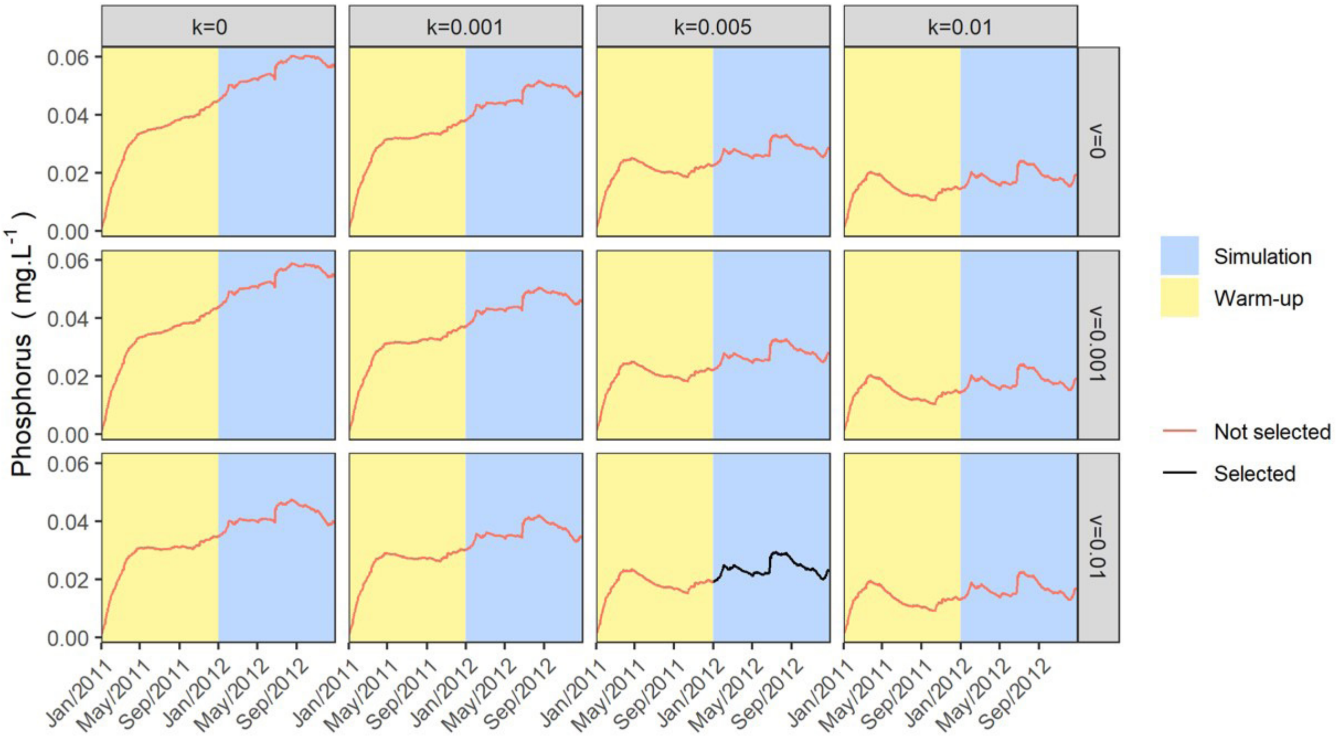

Figure 7. Time series of the sensibility analysis of the model parameters (k: s^{-1} and v: m/s).

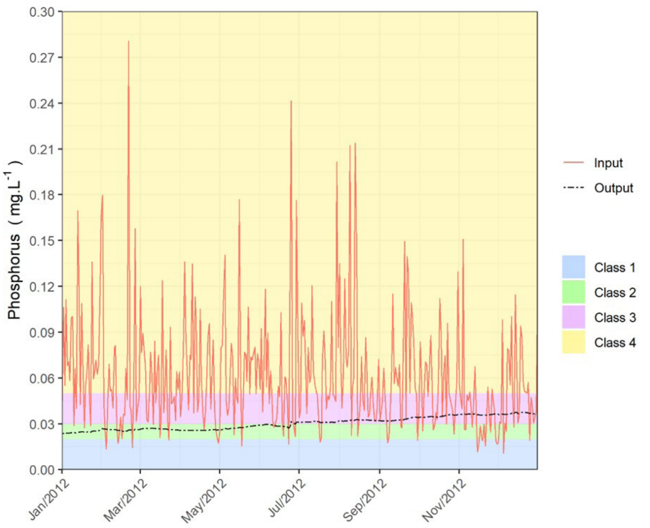

Figure 8. Input and output phosphorus concentrations: base scenario.

the input load. The class limits from CONAMA 357 legislation are represented in background colors.

For the reference scenario (B12) (Figure 8), the values of the output concentration were below the CONAMA regulation limit for Class 2 of 0.03 mg.L^{-1} in the first semester. However in second semester the values surpassed the limit. The increase in the phosphorus concentrations that happened in June reflected the flow values occurred in that period and the decay in reservoir volume. The inflow and outflow series are exhibited in Figure 9.

Those values can help in the interpretation of some aspects of the output concentration series. The phosphorus increase in June, for example, can be explained by the largest inflow and nutrient load in that month, as well as the maintenance of higher values can be explained by the volume reduction in the second semester, which can be justified by the outflow surpassing the inflow from August to December (Figure 9). The decay in volume increased the nutrient concentration and contributed to the output concentration.

Figure 10 shows the box plots of input and output concentrations for all scenarios described in Table 1. The input synthetic series concentrations grow as the sceneries become more critic. The concentrations stand below the Class 2 limit during half of the evaluated time in B12 scenery. In T25, A25, T35 and A35, all the values were higher than the Class 2 limit. In the more extreme scenario (A35), the phosphorus concentration reached 0.09 mg.L^{-1}.

Model B

In this item, the zero-dimensional model is applied to the four sectors of the Jurumirim reservoir. The flow series of the sectors (Figure 11) were obtained proportionally considering the drainage areas (Table 2).

The resulting volume and area time series were presented in Figure 12. It is worth to take into account the fact that this estimation presented some imprecisions.

The input synthetic series and the output of the model are exhibited in Figure 13. Considering the B12 scenery, sector 1 values varied from 0.05 mg.L^{-1} to 0.09 mg.L^{-1}. The concentrations

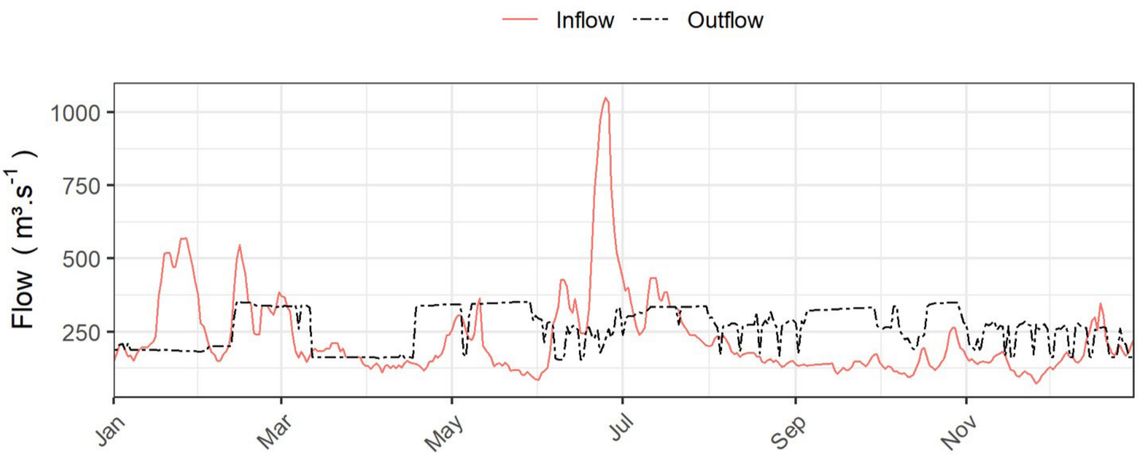

Figure 9. Inflow and outflow of the model for Jurumirim reservoir.

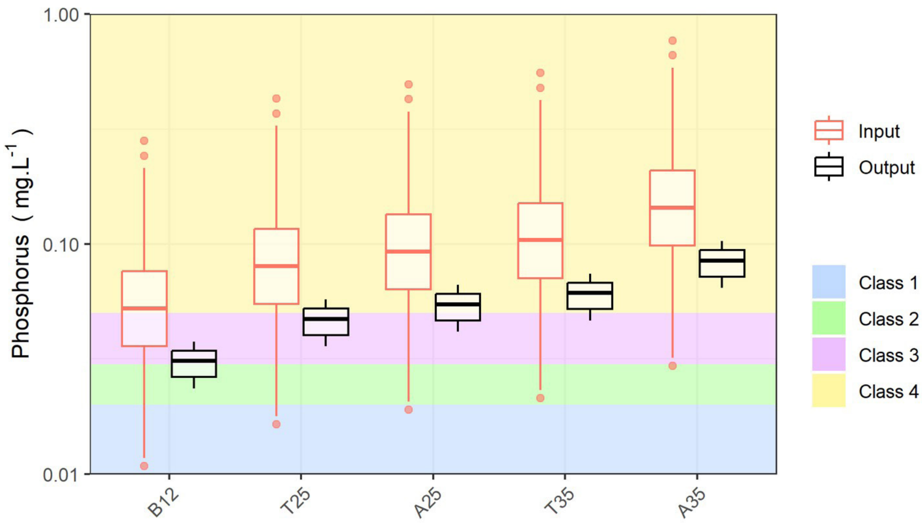

Figure 10. Input and output phosphorus concentrations: base, tendential and accelerated scenarios.

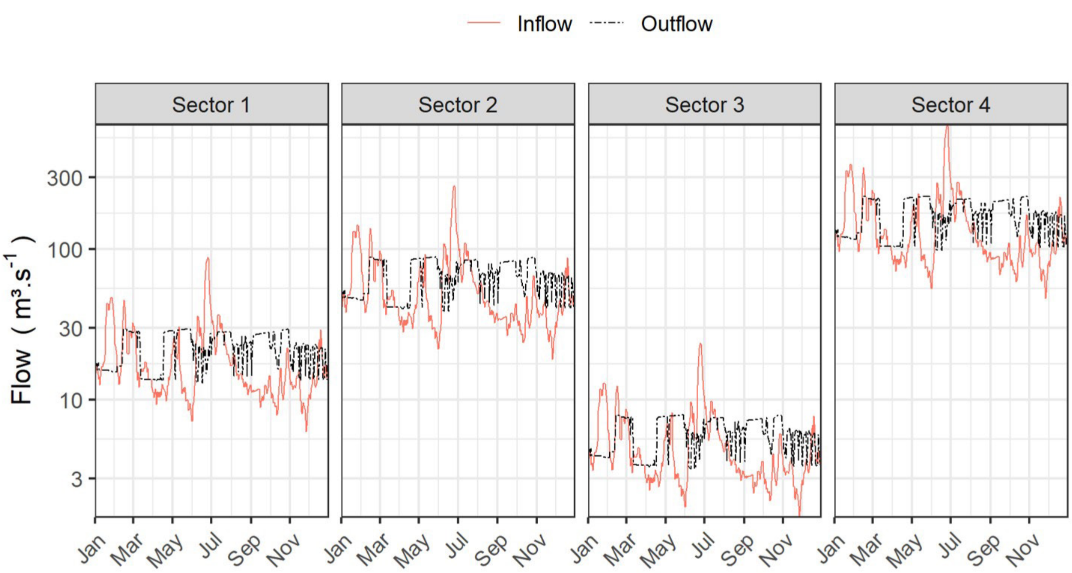

Figure 11. Inflow and outflow of the four sectors of Jurumirim reservoir.

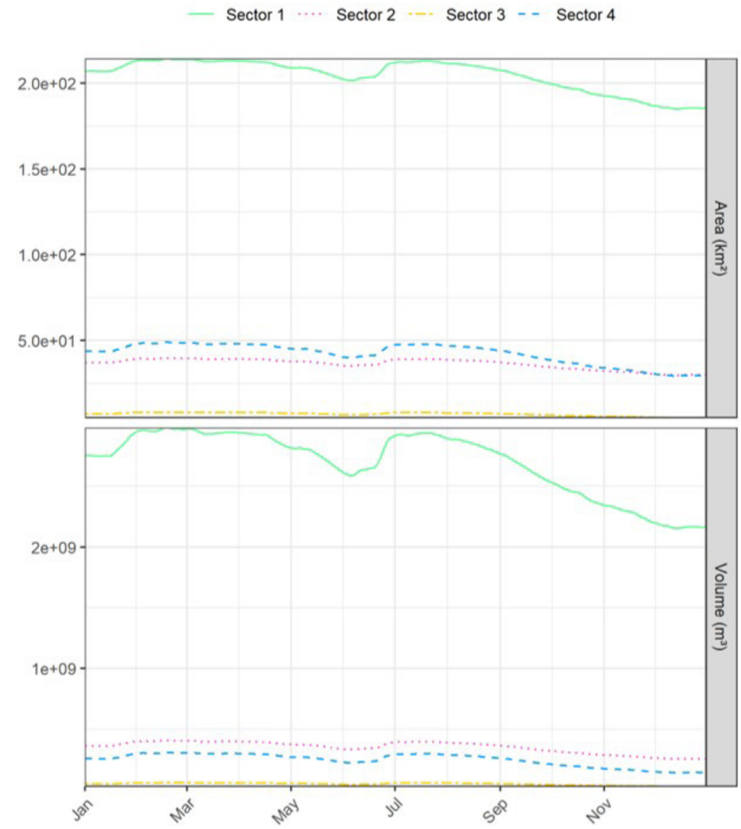

Figure 12. Volumes and areas for each sector of Jurumirim reservoir.

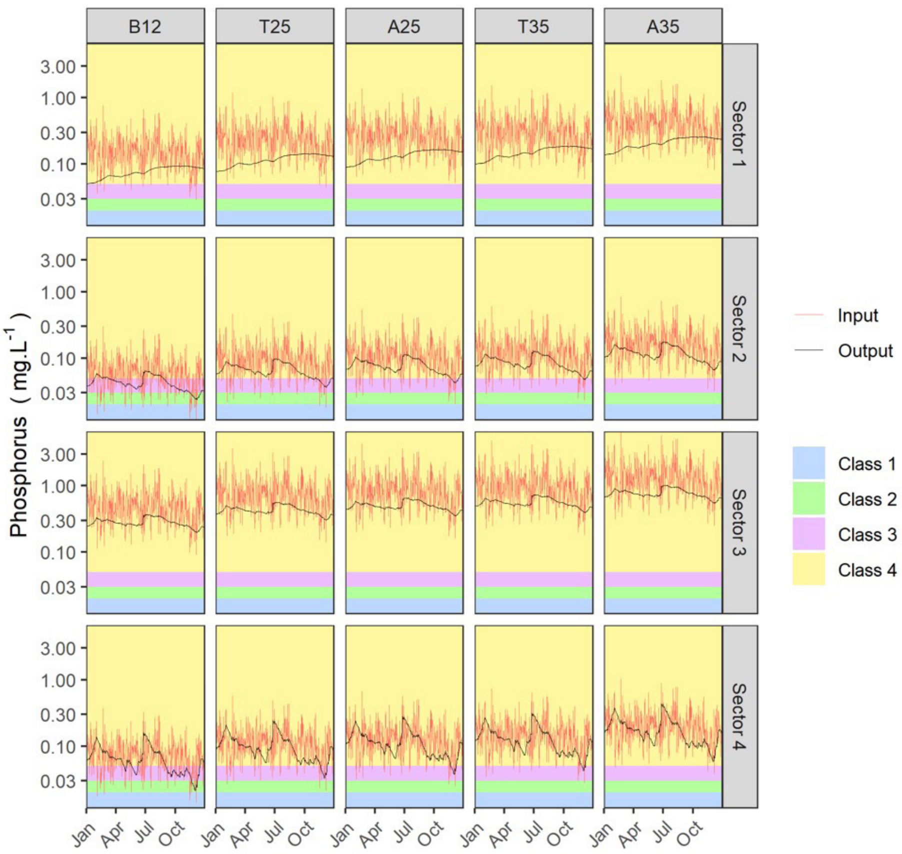

Figure 13. Input and output phosphorus concentrations of the four sectors of Jurumirim reservoir.

on sector 2 varied from 0.02 mg.L^{-1} to 0.06 mg.L^{-1}. On sector 3, phosphorus values varied from 0.2 mg.L^{-1} to 0.37 mg.L^{-1}. Finally, on sector 4 the minimum concentration was 0.02 mg.L^{-1} and the maximum concentration was 0.16 mg.L^{-1}. The high nutrient values on sector 3 can be justified by the phosphorus emissions in this region, which main use is industrial, as opposed to sector 2, which is mostly used by agriculture, pasture and fish-farming (Agência Nacional de Águas e Saneamento Básico, 2022).

Figure 14 provides a comparison of the output time series of the sectors for the year 2012 (B12 scenario). Sector 3 (Ribeirão das Posses) has the most expressive phosphorus concentrations, which exceeded 0.3 mg.L^{-1} during 31% of the time. In sector 2 (Taquari) the maximum concentration was 0.06 mg.L^{-1} and in sector 4 (Paranapanema), the values were below 0.10 mg.L^{-1} during 88% of the evaluated period. The sector closer to the dam (sector 1) considers the other sector's concentration as input values. Thus, the variation in the time series is smaller. The concentrations on Sector 1 variated from 0.05 mg.L^{-1} to 0.09 mg.L^{-1}.

Regarding the load time series (Figure 15), sector 3 no longer present the highest values. Although the high concentrations are in that location, its contribution to the reservoir is minor due to smaller flows. The highest loads are in the sector 1 (closer to the dam), because this sector, in addition to the output load of other sectors, receives load of the north side of the reservoir. The contributions

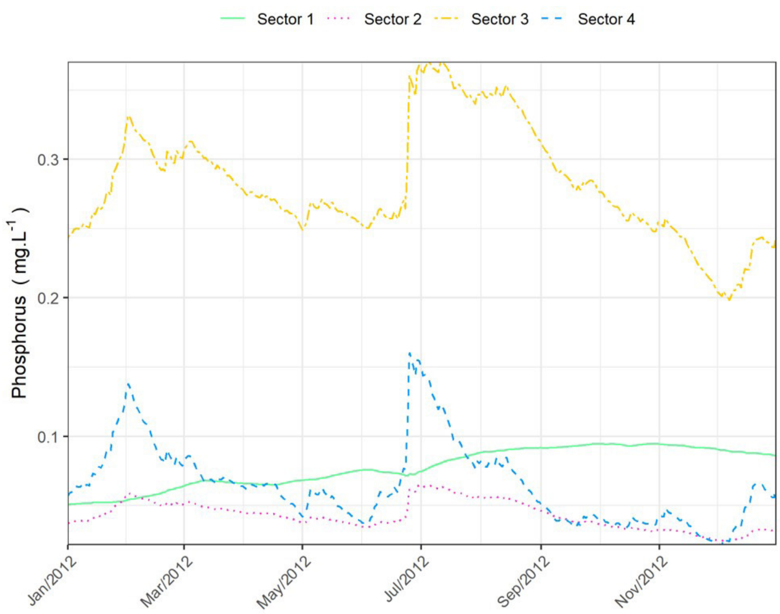

Figure 14. Phosphorus concentrations in the four sectors of Jurumirim reservoir (B12).

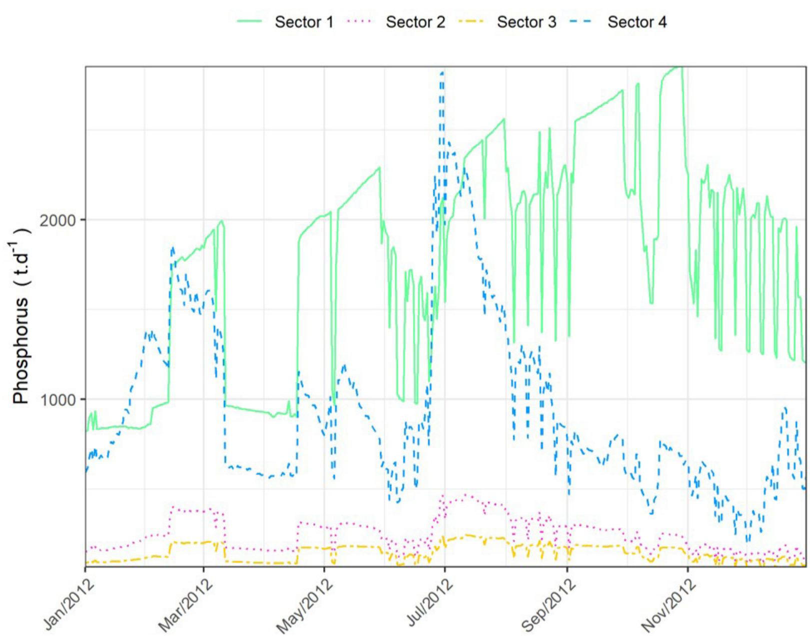

Figure 15. Phosphorus loads in the four sectors of Jurumirim reservoir.

of sector 2 (Taquari) and sector 3 (Ribeirão das Posses) are not as significant as the load of the sector 4 (Paranapanema river).

Comparison of the zero-dimensional models with a three-dimensional model

The output concentrations of the zero-dimensional models and Delft3D model were presented in Figure 16. The final results of model B correspond to the sector 1 results, since its output location is close to the dam and its calculation consider the output results of the other three sectors as described in Equation 7.

Model A concentrations for the scenery B12 varied from 0.02 to 0.03 mg.L^{-1}, while model B concentrations varied from 0.050 mg.L^{-1} to 0.095 mg.L^{-1}. The concentrations from model Delft3D varied from 0.055 mg.L^{-1} to 0.070 mg.L^{-1}. Figure 16 compares the time series of the three models in the scenery B12.

Regarding the phosphorus limits, the results of all models exceeded Class 1 limit (0.02 mg.L^{-1}). Model B and Delft3D results exceeded the Class 3 limit (0.05 mg.L^{-1}) in the whole simulated time. In Figure 16, the background color represents the legislation limits.

The mean concentrations of all scenarios and the average deviations are exhibited in Table 5. This values show that model B and Delft3D had closer results compared to model A, since its average deviations were smaller than the other models compared. It points out how the reservoir division in model B was favorable to the model precision.

The time series of the result of each sector for the scenery B12, comparing the model B with Delft 3D are illustrated in Figure 17. The magnitude of the concentrations simulated for Jurumirim reservoir sectors was similar for both models. The behavior throughout the time, however, is distinct. One possible cause for this phenomena is that the hydrodynamic effects on sector 3 are more significant than sectors 1, 2 and 4, as well as the approximations and simplifications of the zero-dimensional model.

The boxplots in Figure 18 reinforce that the order of magnitude was similar for the sceneries B12 and A35, which presented the smallest and the biggest phosphorus concentrations, respectively.

Although the simulated series are numerically different (Figure 16), in the point of view of planning and management of reservoirs, the magnitude of the values can be considered compatible, considering the similar order of magnitude (between 0.2 mg.L^{-1} and 0.4 mg.L^{-1} for sector 3, scenery B12, for example). The proposed 0D model with sectors (model B) is able to show the differences of the four regions, even though the lower values such as the series of sector 1 and 2 are different from the 3D model.

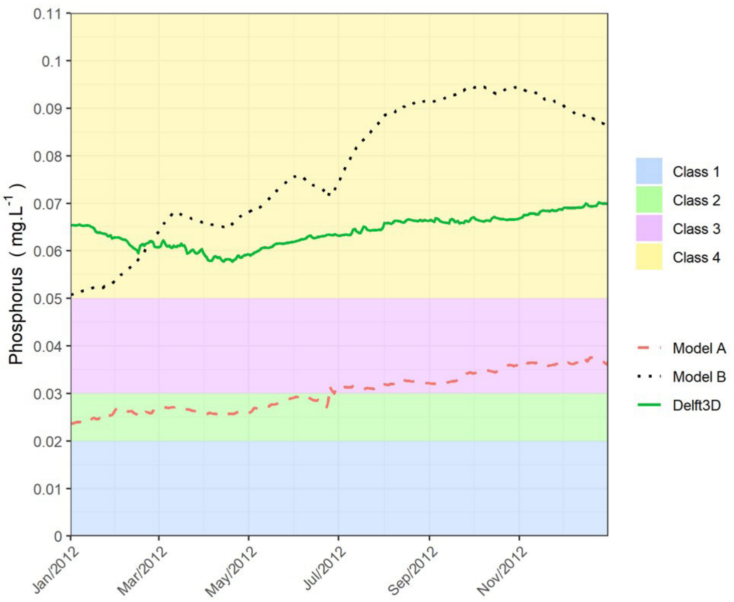

Figure 16. Comparison of the concentrations of zero-dimensional models and DELFT3D.

Table 5. Comparison of model A, model B and the three-dimensional model.

Scenery	Average concentration (mg.L^{-1})			Average deviation (%)		
	Model A	Model B	Delft3D	Delft3D and Model A	Delft3D and Model B	Model A and Model B
B12	0.030	0.077	0.064	59%	13%	60%
T25	0.046	0.118	0.102	50%	22%	60%
A25	0.054	0.137	0.129	53%	19%	60%
T35	0.060	0.153	0.104	55%	18%	60%
A35	0.083	0.212	0.164	43%	30%	60%

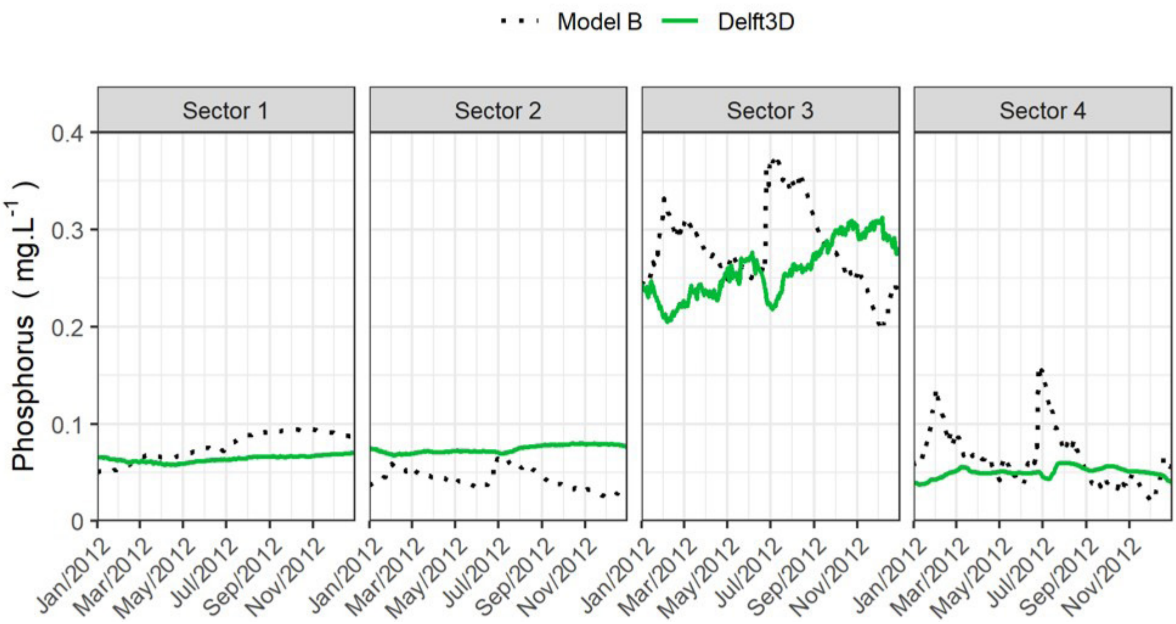

Figure 17. Comparison of Model B and DELFT3D – Sectors – Time series.

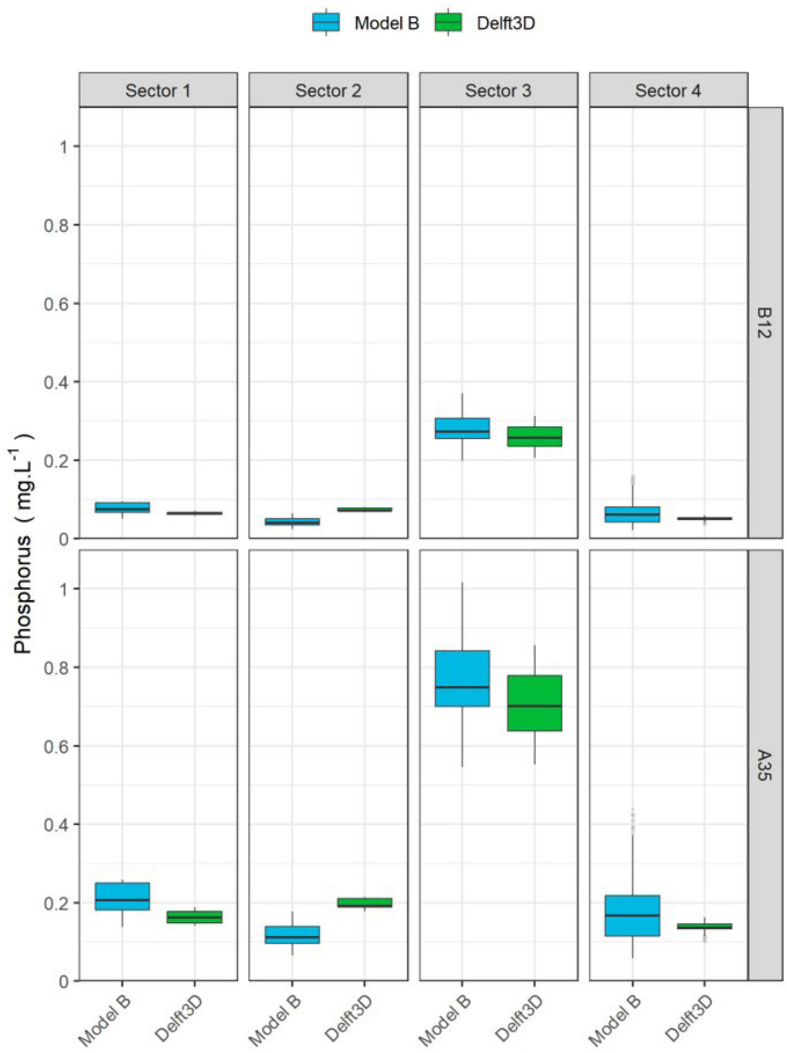

Figure 18. Comparison of Model B and DELFT3D – Sectors – Boxplot.

IMPLICATIONS AND LIMITATIONS

The similar results of the zero-dimensional (0D) and three-dimensional (3D) models show that simplified numerical schemes are important potential tools to be considered for initial analysis of water quality dynamics in reservoirs and for management purposes. It is recommended that more studies are made in this context in order to consolidate the quality and the equivalency of the simulated results.

One possible reason that justify the difference of models A and B results can be the simplification of the flows and concentrations distribution based on the drainage area. The verification of the mass balance of each sector may contribute to the future applications of the 0D model in reservoir sectors. In addition, the calculation method of areas and volumes of each sector presented some imprecisions. These imprecisions possibly led to overestimation of the concentration results of model B (reservoir modelled with sectors).

Another simplification adopted in this study was the same first order decay coefficients (*k*) and apparent settling velocities (*v*) for all sectors. In future applications, it can be improved based on another possible ways to estimate k, as studied by Araujo et al. (2022). Besides, the parameters estimation can consider the morphological characteristics of each sector. In Sector 1, for example, these parameter values can be modified in order to represent the strongest lentic characteristics of this region. Besides, due to the uncertainties in the definitions of those parameters, it may be helpful to future studies to use a global decay coefficient, which includes both processes. Another possible alternative to represent processes is to include the sediment loading that comes from the bottom of the reservoir, according to what was done by Lima Neto et al. (2022).

Some other model details can be varied in future studies, in order to check its influence on final results, such as the heat up time, which was selected the period of a year, and the calculation of surface area of the sediments, that was estimated as being two times the water surface area. The seasonal components can also be explored in future studies.

FINAL CONSIDERATIONS

The present research contributes to the challenge of simplifying the modelling processes. The results obtained for model B (reservoir modelled with sectors) were in the same magnitude of the results of a 3D simulation and fulfilled the goal of applying a 0D model in the case study of Jurumirim reservoir. The 0D simulation with sectors was capable of identifying the reservoir region that outstands in the context of planning and management (Sector 3 – Ribeirão das Posses).

The choice of which model one should use depends on the purpose of the modelling. If the goal is to address specific locals, a 3D model should be used due to the spatial precision. It is worth remembering that this precision is conditioned to the quality of field measurements used as input and calibration data. Zero-dimensional models, however, are useful for pointing out the general concentration dynamics of each sector. For planning and management purposes, such as the Water Quality Classification Framework of waterbodies, as well for a fast evaluation of the effects of the reservoir, the simplified approach is a valuable tool to spare time and resources.

This model created for water resources planning and management is capable of representing the reservoir dynamics for this purpose with reasonable precision. Its use is recommended for the wide number of Brazilian reservoirs that still were not submitted to the Water Quality Framework Process and do not have a large database of water quality monitoring results.

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