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Research Article

Integrated modeling of water quantity and quality in the Araguari River basin, Brazil

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ABSTRACT. The Araguari River basin has a huge water resource potential. However, population and industrial growth have generated numerous private and collective conflicts of interest in the multiple uses of water, resulting in the need for integrated management of water quantity and quality at the basin scale. This study used the AQUATOOL Decision Support System. The water balance performed by the SIMGES module for the period of October 2006 to September 2011 provided a good representation of the reality of this basin. The parameters studied were dissolved oxygen, biochemical oxygen demand, organic nitrogen, ammonia, nitrate and total phosphorus. The coefficients of biochemical reactions, sedimentation rates and sediment dissolved oxygen release for this period were calibrated and validated in the quality modeling using the GESCAL module. A sensitivity analysis indicated that the coefficients of carbonaceous matter decomposition, nitrification, water temperature, and sediment oxygen demand interfered more significantly in the variables of state. To prevent eutrophication in the Nova Ponte reservoir and in the other cascade reservoirs, the local River Basin Committee should adopt restrictive actions against the use of agricultural fertilizers. On the other hand, in the sub basin of the Uberabinha River, new alternatives for public water supply to the city of Uberlândia and improvements in the treatment efficiency of the main wastewater treatment plant (WWTP) should be proposed, since the biochemical oxygen demand, ammonia and total phosphorus failed to meet the requirements of COPAM (2008) in the driest months.

Keywords: water, modelling, AQUATOOL, Araguari River, basin, Brazil.

Modelación integrada de cantidad y calidad del agua en la cuenca del río Araguari, Brasil

RESUMEN. La cuenca del río Araguari tiene un enorme potencial de recursos hídricos. Sin embargo, la población y crecimiento industrial han generado numerosos conflictos de interés, privados y colectivos, en los usos múltiples del agua, dando lugar a la necesidad de una gestión integrada de la cantidad y calidad del agua a nivel de la cuenca. En este estudio se utilizó el Sistema de Soporte de Decisión AQUATOOL. El balance hídrico realizado por el módulo SIMGES, para el período de octubre 2006 a septiembre 2011 proporcionó una buena representación de la realidad de esta cuenca. Los parámetros estudiados fueron el oxígeno disuelto, demanda bioquímica de oxígeno, nitrógeno orgánico, amonio, nitrato y fósforo total. Los coeficientes de las reacciones bioquímicas, tasas de sedimentación y demanda de oxígeno disuelto del sedimento para este período fueron calibrados y validados en la modelación de calidad del agua, mediante el módulo GESCAL. El análisis de sensibilidad indica que los coeficientes de degradación de la materia orgánica, nitrificación, temperatura del agua y demanda de oxígeno del sedimento interfirieron más significativamente en las variables de estado. Para evitar la eutrofización en el embalse de Ponte Nova y en el resto de los embalses en cascada, el Comité Local de la Cuenca del Río debería adoptar medidas restrictivas contra el uso de fertilizantes agrícolas. Por otra parte, en la subcuenca del Río Uberabinha, nuevas alternativas para el suministro público de agua a la ciudad de Uberlandia y mejoras en la eficiencia del tratamiento de la principal Estación Depuradora de Aguas Residuales (EDAR) deben ser considerados, ya que la demanda bioquímica de oxígeno, amonio y fósforo total no han cumplido con los requisitos de la COPAM (2008) en los meses con más sequías.

Palabras clave: agua, modelación, AQUATOOL, cuenca río Araguari, Brasil.

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INTRODUCTION

In developing countries, such as Brazil, which lack financial resources for basic sanitation and proper wastewater treatment, the problem of dissolved oxygen consumption in waterways after wastewater has been discharged into them is still significant, justifying the use of the assimilative capacity of waterways to complement the treatment process. Sustainable development and rational water use require the existence of a proper relationship between water quantity and quality. In this context, joint mathematical modeling allows for the diagnosis and prediction of impacts resulting from multiple water uses and the discharge of pollutant loads.

Numerous researchers have designed a variety of models and Decision Support Systems (DSS) that are useful for water resource planning and management at the basin scale. It is well known that the main focus of computational tools is quantitative water resource management and planning, considering the increasing demands and need to implement optimal rules for the operation of water resources. In this context, with different mathematical complexities, the main quantity models that stand out are: HEC-HMS (Klipsch & Hurst, 2007; Fan *et al*., 2009) and the MIKE SHE (McMichael *et al*., 2006) models, designed to simulate the precipitation-runoff processes of watershed systems which integrate all the important processes of the hydrologic cycle at catchment scale. HEC-ResSim and WRAP (Wurbs, 2005) models are used to model reservoir operations at one or more reservoirs and the interactions with rivers. MODFLOW (Rodriguez *et al*., 2008; Xu *et al*., 2012) and IRAS (Salewicz & Nakayama, 2004; Matrosov *et al.*, 2011) models are used to simulate flow of groundwater through aquifers interactive river-aquifer simulation. However, environmental concerns regarding water quality at the basin scale, driven by the continuous discharge of domestic and industrial wastewater, have led to the design of increasingly complete water quality models (De Paula, 2011). These models have been in use since the development of Streeter & Phelps's classical model (Streeter & Phelps, 1925), which is a benchmark in the history of sanitary and environmental engineering. Several other models have been designed with increasing complexity and number of modeled variables. Those models can be used to simulate different water quality problems. For example, while the Qual2E model (Palmieri & De Carvalho, 2006; Chapra, 2008) and its updated version Qual2K model (Von Sperling, 2007; Chapra *et al*., 2008; De Paula, 2011) are used to model water quality in river and stream, WASP model (Lai *et al*., 2012; Zhang & Rao, 2012; Yenilmez & Aksoy, 2013) has been used to examine eutrophication in lakes or streams and heavy metal pollution in rivers. AQUATOX model (Mamaqani *et al*., 2011; McKnight *et al.,* 2012) is a valuable tool in ecological risk assessment for aquatic ecosystems.

This brief review reveals the marked existence of river and reservoir water quality models that are not linked with any DSS in the quantitative management and planning of water resources. According to Paredes-Arquiola *et al.* (2010a), many scientific researches disregard the interactions between qualitative and quantitative aspects in water resource management at the basin scale. Due to this situation, many researchers around the world, *e.g.*, Dai & Labadie (2001), Paredes & Lund (2006), Argent *et al.* (2009), Zhang *et al.* (2010), Paredes-Arquiola *et al.* (2010a, 2010b), Zhang *et al.* (2011), Sulis (2013) and Welsh *et al.* (2013), are focusing on relating water quality within a DSS in water management at a basin scale.

According to the State Environmental Foundation, the state of Minas Gerais has the highest water resource potential in Brazil and accounts for the generation of 18.5% of all the electricity produced in the country. Nevertheless, there is a lack of scientific research on the integrated management of water quantity and quality at the basin scale. Many water resource management proposals have been put forward by local river basin committees. However, these proposals are not underpinned by integrated studies of water quantity and quality in lentic and lotic environments, but instead focused only on the implementation of quantitative and qualitative telemetric information systems, on user registration and updating, on the creation of criteria for granting water rights, on charging for the use of water and on payment to the surrounding municipalities, watercourse guidelines, conflict prognosis between demands and capacities, and the creation of environmental protection units.

In this context, based on the AQUATOOL Decision Support System (DSS), this article presents an integrated modeling of water quantity (using the SIMGES module) and quality (using the GESCAL module) of the three main watercourses of the Araguari River basin (Araguari, Quebra-Anzol and Uberabinha rivers). Based on water flow and water quality data monitored by the National Water Agency (ANA), the Minas Gerais Water Management Institute (IGAM) and the Minas Gerais Electric Company (CEMIG), this article presents the results of the water balance and calibration of the water quality model for the period of October 2006 to September 2009, and its validation for the period of October 2009 - September

2011. The calibration and validation of the biochemical reaction coefficients, sedimentation rates and sediment oxygen demand will serve as a basis for future studies on quantitative or qualitative interventions in this basin.

The coefficients that are part of the natural self-purification process of a watercourse, be it lentic or lotic, have distinct influences on the final water quality in the water system. Thus, using the factor model, this study performed a sensitivity analysis of the four main coefficients of biochemical reactions involved in the modeling (the re-aeration coefficient K_a, decomposition coefficient of CBOD K_d, coefficient of decomposition of organic nitrogen KN_{oa}, and coefficient of ammonia nitrification KN_{ai}), of the water temperature (*Temp*) and the sediment oxygen demand (S_{OD}).

MATERIALS AND METHODS

AQUATOOL DSS

There are few computational tools or models that simulate water quality linked to quantity at a basin scale. Andreu *et al.* (1996) developed a DSS called AQUATOOL, which is an interface for editing, simulating, reviewing and analyzing basin management simulation models, including a lentic and lotic water quality simulation module, that is widely used in Europe, Africa, Asia and Latin America (Paredes-Arquiola *et al.*, 2010a, 2010b; Nakamura, 2010; Sulis & Sechi, 2013).The GESCAL and SIMGES modules are intercon-nected, sharing georeferenced quality and quantity data through a graphical interface (Paredes-Arquiola *et al.,* 2010a). Thus, hypothetically considering a basin with multiple and transient uses, water quality can be simulated for any simulated outfall, recharge and environmental flow scenario.

SIMGES module

In this study, the quantitative water management module SIMGES was used in the water balance model in the Araguari River basin. In this water balance was considered the flow in rivers and reservoirs at the basin scale, based on the spatial and quantitative definition of outfalls (point wise outfall for irrigation, industries and human consumption). Simulations were performed by means of a network flow optimization algorithm, which controls the surface flow within the basin while aiming to minimize the deficits and maximize the liquid levels in reservoirs to meet irrigation, human consumption and hydropower demands.

GESCAL module

In order to simulate water quality linked to quantitative management in lentic and lotic environments previously defined in the SIMGES module, Paredes-Arquiola *et al.* (2009) developed the water quality module GESCAL. Although GESCAL allows modeling eutrophication, temperature, toxics and conventional contaminants, in our case, due to the lack of data and planning purpose of the study, the contaminants modeled were DO, CBOD, organic nitrogen, ammonia, nitrate and total phosphorus. In the modeling process adopted in this study, the relationship between nitrogen cycle and carbonaceous organic matter and the effect on dissolved oxygen, and total phosphorus as an arbitrary parameter was considered, according to the scheme illustrated in Fig. 1.

Study area: Araguari river basin

The Araguari River basin (Fig. 2) is located in the western region of the state of Minas Gerais, Brazil (18°20'-20°10'S, 46°00'-48°50'W). Headwaters are located in Serra da Canasta National Park, in the municipality of São Roque de Minas, covering 475 km to its mouth in the Parnaíba River (which is a tributary of the Grande River, that belongs to Transnational Paraná River basin). This basin covers an area of approximately 22,000 km^2, with altitudes ranging from 465 m to 1,350 m and rainfall exceeding 1600 mm year^{-1}. The weather condition is warm, with the dry season between May and September and a wet season between October and April (Rosa *et al.,* 2004). It has a resident population of approximately 1.2 million, distributed in 18 municipalities, 14 of which discharge their wastewater into the basin (Fig. 2). Only the municipalities of Araxá, Nova Ponte, Patrocínio and Uberlândia (which accounts for approximately 70% of the total population in the basin) have wastewater treatment plants (WWTPs), while the other 10 municipalities discharge their untreated wastewaters directly into the surface water bodies. According to the IGAM, surface and groundwater demands allocated in 2006 for human consumption, irrigation, industry, and livestock watering were 250.6 and 3.6 hm^3 year^{-1}, respectively.

This basin has six hydroelectric power stations (HP), the four largest ones located on the Araguari River with cascade reservoirs (Fig. 2). The first one, situated on the upper Araguari River, is a regulation reservoir with a storage capacity of 12,792 hm^3 (Nova Ponte HP), while the other three reservoirs, located on the lower Araguari River, are trickle reservoirs (from up to downstream, Miranda HP, Capim Branco HP 1, and Capim Branco HP 2). There are also two small hydroelectric power stations (SHP) situated on the

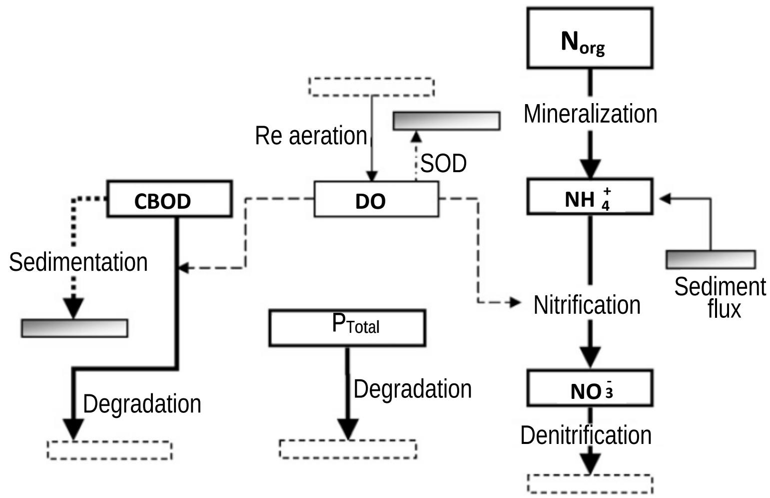


Figure 1. Relationship among the modeled quality parameters.

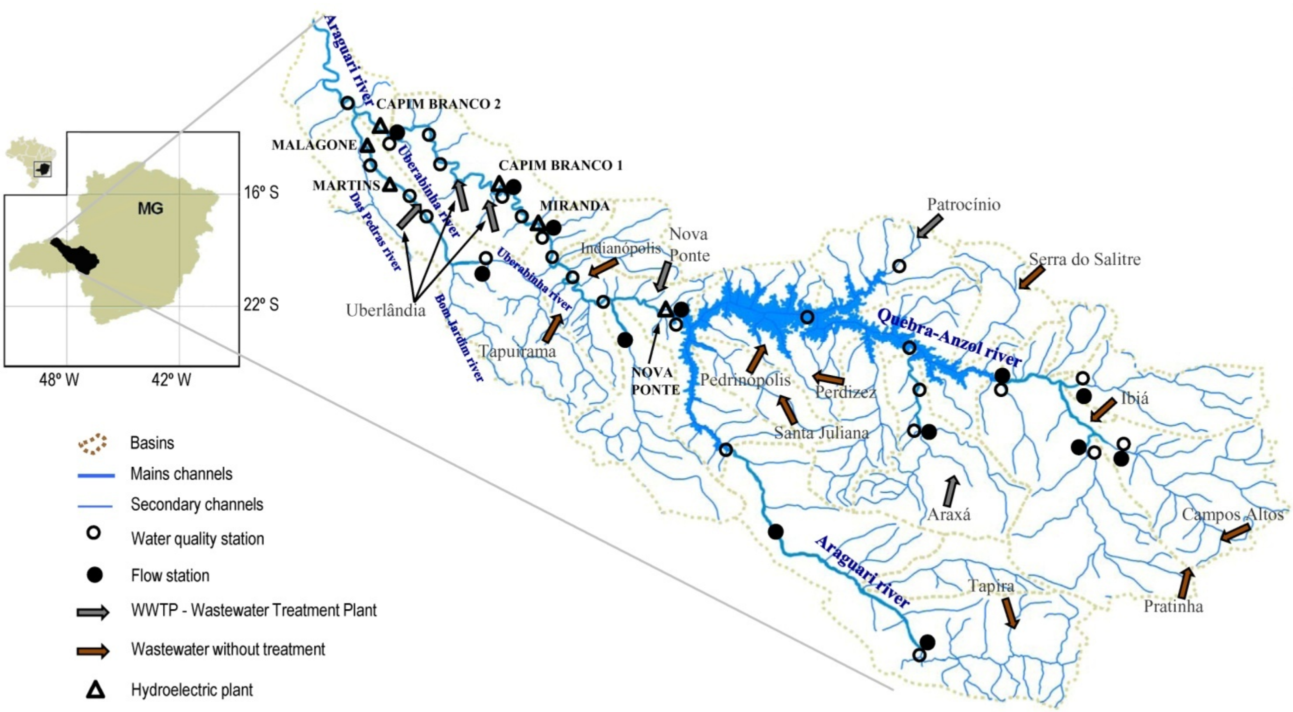


Figure 2. Location of the Araguari river basin (18°20'-20°10'S, 46°00'-48°50'W).

Uberabinha River (Martins SHP and Malagone SHP). However, in the 2006-2011 period they had not yet entered into production that, for modeling purpose, make us to consider this region as a simple river segment.

In the 1980s, the joint effect of economic valuation of soybeans and the scientific discovery of suitability of the crop to the soil of the Araguari River, transformed the region through the practice of a modern agriculture, associated with the intensive use of phosphate fertilizers and agrochemicals. Also, the presence of phosphate rocks in the region contributes to the existence of that nutrient from their natural deposits (EPE, 2006; Rosolen *et al.*, 2009; Flauzino *et al.*, 2010; Danelon *et al.,* 2012). Figure 2 shows that the basin may be divided into 18 sub basins, whose main economic activities are agriculture, aquaculture, farming, mining, power generation, manufacturing, agribusiness and tourism.

Quantity modeling

The initial procedure in the quantity modeling was to outline the topology of the model using AQUATOOL, which basically corresponds to the situational diagram of the Araguari River basin, including the unscaled elements of the model, as illustrated in Figure 3. To improve visualization, the elements that represent the smaller tributaries and the diffuse distribution along the Quebra-Anzol, Araguari and Uberabinha rivers were removed from Figure 3.

In the quantity and quality modeling processes, the three main watercourses of this basin (Araguari, Quebra-Anzol and Uberabinha rivers) were divided into 20 segments, each of which was identified by a numbered node upstream and another numbered node downstream (Fig. 3).

Data input

Based on the water flow data monitored by the National Water Agency and the Minas Gerais Electric Company (Fig. 2), a text file was arranged containing the model's quantity input data for the calibration and validation periods. According to Figure 3, all the tributaries and point wise discharges of domestic wastewater with and without the wastewater treatment plant (WWTP) are identified as inputs.

Quebra-Anzol and Araguari rivers

The quantity data of the upper Araguari River and upper Quebra-Anzol River were used directly as input data in the simulation. However, the diffuse and point wise inputs from the other tributaries were obtained from the specific outfall in $m^3 s^{-1} km^{-2}$ (Eq.1), taking into account the existing quantity data of the upper Araguari and Quebra-Anzol rivers and of the four cascading hydroelectric plants (data on turbine flow, downstream flow and volume variations in the reservoir, which enabled the flow upstream from each hydropower plant to be estimated).

$$Q_i = \left[\frac{\left(Q_{downstream} - Q_{upstream} \right)}{\sum A_n} A_i \right] \quad (1)$$

where:

Q_i = inflow i

$Q_{upstream}$ = flow at any point upstream

$Q_{downstream}$ =flow at any point downstream from the inflow Q_i;

A_n = total area between two monitoring stations,

A_i = area contribution of the inflow i, obtained by means of a GIS tool that enables the simultaneous acquisition of the area from the perimetral outline.

Uberabinha River

Existing data for the upper Uberabinha River were used directly as input data in the simulation of the model. The absence of water flow data from the mouth of this sub basin and from the two small hydroelectric plants precluded the use of the specific discharge method to estimate the diffuse and point wise flow rates. Thereby a specific rainfall-runoff model is needed for the water balance in this sub basin.

The curve number method (CN) for urban sub basins was used in our study (SCS, 1986). This is a distributed model widely accepted worldwide due to the reduced number of parameters and their relationship with the physical characteristics of the basin (Tucci, 2005; Rezende, 2012).

The HBV model developed by Bergström (1995) was used for the rural sub basins. This is a semi-distributed model that is part of a range of models which use the most important surface runoff processes by means of a simple structure and with a reduced number of parameters. The model functions on a daily or monthly time scale and uses precipitation, ground-level air temperature and average monthly evapo-transpiration as input data (Hundecha & Bárdossy, 2004; Das *et al.,* 2006). Detailed descriptions of the equations used in the HBV model are given by Bergström (1995) and Paredes-Arquiola *et al.* (2011).

The parameters of the HBV model were calibrated using the evolutionary algorithm for calibration, SCE-UA (Shuffled Complex Evolution method, University of Arizona) (Duan *et al.*, 1992). To this end, the results of the time series of surface flow obtained from the HBV model were compared with the existing time series of surface flow in the upper Uberabinha River. Self-calibration was performed adapting the original code of the SCE-UA algorithm from Duan *et al.* (1992) and reprogrammed in a Visual Basic platform. Each assessment of the objective function implies the execution of the HBV model. This algorithm has been used successfully to solve nonlinear problems in various applications of hydrological models at the basin scale (Paredes-Arquiola *et al*., 2011).

In our study, the model was applied to the sub basin corresponding to the single water flow monitoring station existing in the upper Uberabinha River (Fig. 2), whose area of contribution is 801.6 km^2. Due to the similarity of climate, geology, land use and

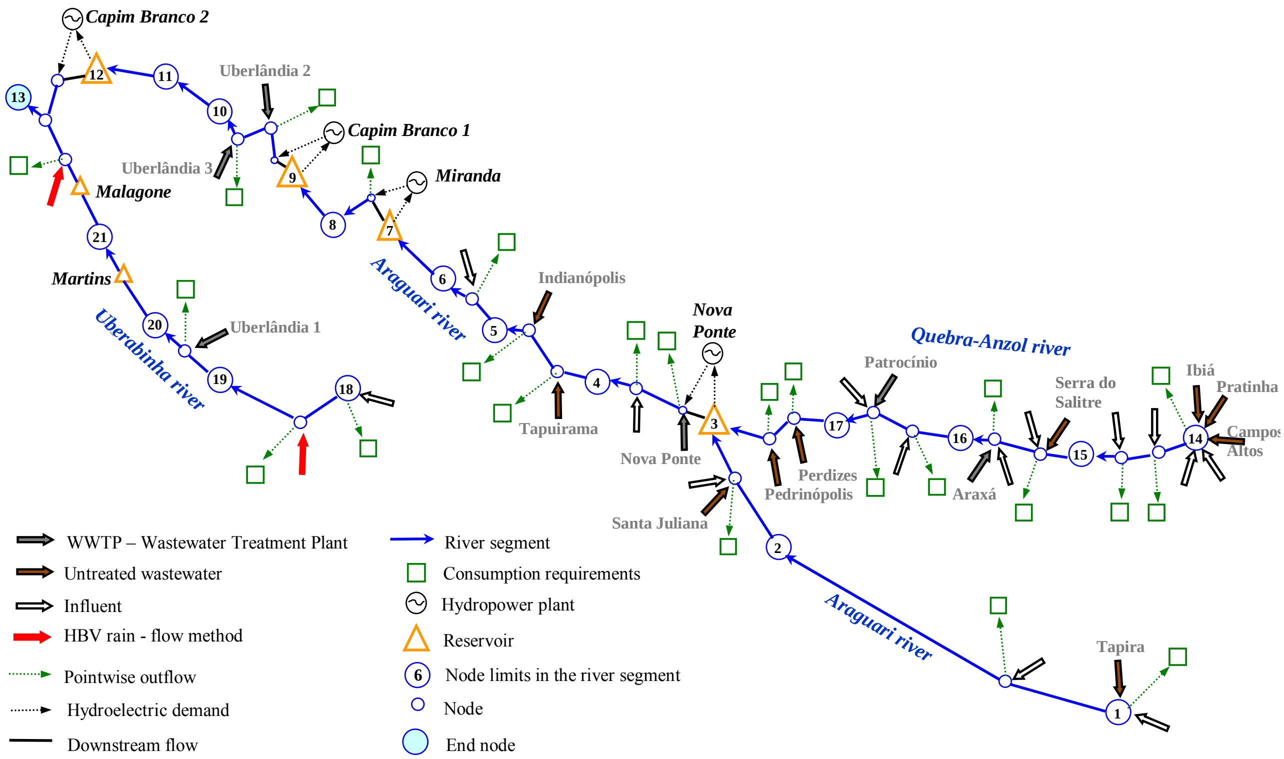


Figure 3. Model topology applied to the Araguari River basin.

occupation throughout the Uberabinha River sub basin, the initially calibrated parameters for this sub basin were used as input data to estimate the surface flow into the other rural sub basins. As it can be seen in Fig. 2, the Bom Jardim River sub basin (394.6 km^2) and the Das Pedras River sub basin (389.4 km^2) are the main rural sub basins.

WWTP

The WWTP's inflows were calculated using the drinking water flow distribution equation multiplied by the coefficient of return, which, according to the Brazilian standards ABNT: NBR 9649 (1986) and ABNT: NBR 14486 (2000), is set to 0.80 for these situations in which there are no observed data available.

Point wise demand with and without consumption

The data on granted and georeferenced surface water demands for human consumption, irrigation, industry, and livestock watering were obtained from the IGAM, based on 2006 data. Data relating to variable requirements for hydroelectric purposes were obtained from CEMIG.

Water balance

The water balance was determined using the SIMGES module after completion of the topographic map, along with inputs of quantity data required for each element of the model, which include the point wise surface consumption demands, point wise requirements for hydroelectric purposes without consumption, point wise entries of tributaries, point wise effluents with and without WWTP, and the diffuse inputs from the main rivers (Quebra-Anzol, Araguari and Uberabinha). Various input data on storage reservoirs and hydroelectric plants are also essential in modeling, such as the dead volume of each reservoir (hm^3), volume set aside in each reservoir at the beginning of the simulation (hm^3), maximum storage capacity in each reservoir (hm^3), base depth (m), minimum turbine depth (m), energy coefficient (GW hm^3 m^{-1}), maximum turbine requirement (m^3 s^{-1}), evapo-transpiration for each month, and bathymetric data of the reservoirs.

Quality modeling

In AQUATOOL, quality modeling with the GESCAL module is performed after quantity modeling. Another text file was created containing data on the water quality of tributaries and point wise discharges of WWTP treated and untreated domestic wastewater. The text file was introduced into the GESCAL module to start the simulations.

The data on water quality of the tributaries and the WWTPs were obtained from IGAM and CEMIG.

With respect to the 10 municipalities that discharge their untreated wastewaters directly into the water courses (approximately 30% of the total population of this basin), the water quality was estimated based on the characteristics of raw wastewater. The per capita gross load of BOD of 54 g day^{-1} was adopted based on the recommendation of the Brazilian standard ABNT: NBR 12209 (2011), in the absence of available measured data. Likewise, the per capita gross pollutant loads of organic nitrogen, ammonia, nitrate, and inorganic and organic phosphorus were estimated, to be 5.0, 7.0, 0.5, 1.0 and 1.5 g day^{-1}, respectively. These estimates are based on the numerous experimental results reported by several authors, such as Tchobanoglous *et al.* (2003) and Von Sperling (2007). The number of inhabitants per municipality was obtained from census of the Brazilian Institute of Geography and Statistics (IBGE, 2013).

The simulated water quality parameters are: dissolved oxygen, biochemical oxygen demand (BOD_5), organic nitrogen, ammonia, nitrate and total phosphorus. Due to the absence of eutrophication in the reservoirs for the time series under study, the modeling of water quality assumed thoroughly mixed reservoirs, for which the simulations were performed adopting only the upper region of the epilimnion. Although we thought that the behavior of the water quality in the reservoirs are enough defined with the model, overall, based on the available data, new information regarding temperature profiles and dynamics of nutrients could improve the model of the reservoir. Generally, the model is related to phosphorous and the internal sediment source of phosphorous. In this case, the developed CSTR model could be incremented to two layer model and could include the effect of the sediment, improving the knowledge of the system and the robustness of the model.

Fig. 4 shows the line diagram of the integrated modeling of water quantity and quality in the Araguari River basin. This plot shows the longitudinal distance between all the elements of the model, the longitudinal distance of the 20 river segments, and the location of the water quality monitoring stations used in the calibration model and its validation process. To calibrate the model in each segment of the river, existing water quality data was used in the node downstream from the segment (Figs. 3, 4). The GESCAL module allows the re-aeration coefficient in each segment of the river to be obtained by the Covar method (Von Sperling, 2007; Paredes-Arquiola *et al.,* 2009) or through the direct introduction of its value in the calibration process. The Covar method (empirical equations that depend on the mean flow velocity and the net depth) showed a good fit between observed and simulated dissolved oxygen data only in the headwater segments of the rivers involved. Table 1 identifies the 20 segments, the longitudinal length of each segment, and the hydraulic relationships used in the headwater segments.

Calibration, validation and sensitivity analysis

In this study, the coefficients of biochemical reactions, sedimentation rates and sediment oxygen release in the 20 segments identified in Figures 3 and 4 were calibrated through a process of trial and error. The coefficients of reactions and sedimentation rates include: re-aeration, decomposition of carbonaceous organic matter, sedimentation rate of carbonaceous organic matter, hydrolysis of organic nitrogen, sedimentation rate of organic nitrogen, ammonia nitrification and denitrification, phytoplankton growth, phytoplankton death/respiration, phytoplankton sedimentation rate, organic phosphorus decay rate and organic phosphorus sedimentation rate.

A sensitivity analysis was performed of all the segments defined in Figures 3 and 4 in view of the changes in the input values of the four main previously calibrated coefficients of reactions (re-aeration coefficient K_a, coefficient of carbonaceous organic matter decomposition K_d, decomposition coefficient of organic nitrogen KN_{oa}, and coefficient of ammonia nitrification of KN_{ai}), sediment oxygen demand S_{OD} and water temperature *Temp*.

Unlike what was done in the calibration process, in which each segment was calibrated separately, using the data observed in the node downstream from the segment as the base for calibration, the sensitivity analysis joined two or more sequential segments in some cases in which the simulated and calibrated values of the node downstream from the last sequential segment were used as the standard in the analyses. The analyses of sequential segments were organized as follows: Araguari segments (1), (2), (3-4-5-6), (7-8) and (9-10-11) correspond, respectively, to the nodes 2, 3, 7, 9 and 12; Quebra-Anzol segments (1) and (2-3-4) correspond, respectively, to the nodes 15 and 3; finally, Uberabinha segments (1), (2-3) and (4) correspond, respectively, to the nodes 19, 21 and 13.

The factor method used in the sensitivity analysis enabled the assessment of changes in the concentrations of quality parameters based on the simulta-

Table 1. Identification of the 20 segments, longitudinal length (L) of each segment, and hydraulic relationships used in the headwater segments. Q: average flow ($m^3 s^{-1}$); u: average velocity ($m s^{-1}$); h: average depth (m); b: width of the transverse section (m); α1, β1, α2, β2, α3 and β3 are coefficients of the potential relationships of u = f(Q), h = f(Q) and b = f(Q), adjusted by optimizing the Nash-Sutcliffe efficiency coefficient (Nash & Sutcliffe, 1970).

Segment	Between nodes	L (km)	$u = \alpha_1.Q^{\beta 1}$	$h = \alpha_2.Q^{\beta 2}$	$b = \alpha_3.Q^{\beta 3}$
Araguari 1	1-2	131.42	α_1=0.135; β_1=0.446 α_1=0.200; β_1=0.468	α_2=1.472; β_2=0.240 α_2=0.171; β_2=0.516	α_3=5.017; β_3=0.314 α_3=29.338; β_3=0.017
Araguari 2	2-3	47.32	---	---	---
Araguari 3	3-4	25.82	---	---	---
Araguari 4	4-5	20.57	---	---	---
Araguari 5	5-6	12.58	---	---	---
Araguari 6	6-7	18.50	---	---	---
Araguari 7	7-8	9.38	---	---	---
Araguari 8	8-9	23.40	---	---	---
Araguari 9	9-10	25.30	---	---	---
Araguari 10	10-11	21.30	---	---	---
Araguari 11	11-12	27.83	---	---	---
Araguari 12	12-13	16.75	---	---	---
Quebra-Anzol 1	14-15	90.02	α_1=0.470; β_1=0.258 α_1=0.198; β_1=0.452 α_1=0.025; β_1=0.661	α_2=0.161; β_2=0.674 α_2=0.312; β_2=0.505 α_2=0.789; β_2=0.320	α_3=13.237; β_3=0.068 α_3=16.225; β_3=0.043 α_3=51.554; β_3=0.020
Quebra-Anzol 2	15-16	33.62	---	---	---
Quebra-Anzol 3	16-17	41.16	---	---	---
Quebra-Anzol 4	17-3	42.76	---	---	---
Uberabinha 1	18-19	26.68	α_1=0.240; β_1=0.391 α_1=0.066; β_1=0.713 α_1=0.053; β_1=0.738	α_2=0.214; β_2=0.580 α_2=0.736; β_2=0.227 α_2=0.742; β_2=0.261	α_3=19.496; β_3=0.029 α_3=20.692; β_3=0.059 α_3=25.347; β_3=0.002
Uberabinha 2	19-20	3.15	---	---	---
Uberabinha 3	20-21	17.93	---	---	---
Uberabinha 4	21-13	29.74	---	---	---

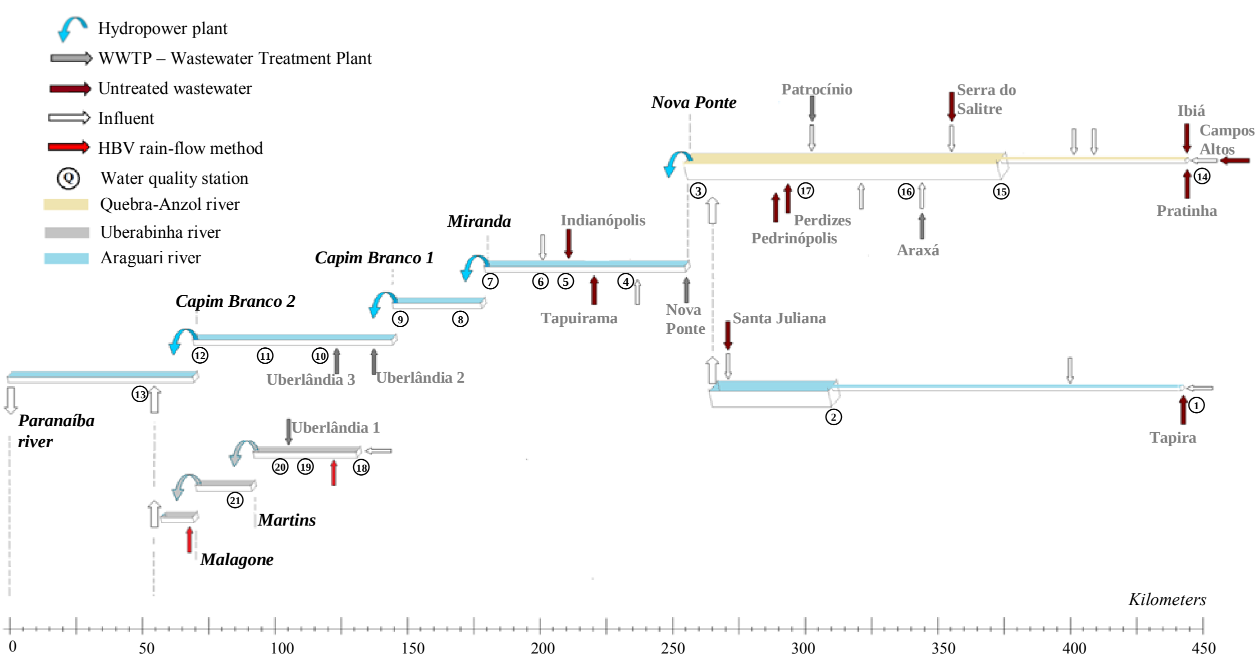


Figure 4. Single line diagram of the model.

neous variation of K_a, K_d, KN_{oa}, KN_{ai}, and S_{OD} by ± dual-level analysis. According to Loucks *et al.* (2005) and Nakamura (2010), in dual-level analysis, 2^n different simulations are performed, where *n* is the number of coefficients. However, for each river segment, *1* x *2* x 2^n simulations were made, in which the number *1* corresponds to the number of + and – pairs, the first number 2 corresponds to the two simulations +10% and -10%, and *n* corresponds to the number of coefficients (*n* is equal to 4 in the segments that have no sediment oxygen demand S_{OD}). With respect to temperature, a relative method was used to assess changes in the concentrations of quality parameters on the isolated variation by +10% and -10% from water temperature.

RESULTS

Quantity modeling

Figure 5a illustrates the variation of simulated flow during the period of calibration and validation of the main sections in the basin. The flow at the mouth of Uberabinha River varies from 54.28 to 310.81 hm^3 $month^{-1}$. In the upper Araguari River (node 2) and upper Quebra-Anzol River (node 15) vary, respectively, from 80.06 to 603.56 hm^3 $month^{-1}$ and from 83.89 to 761.98 hm^3 $month^{-1}$, while at the mouth of the Araguari River basin (node 13) the flow varied from 799.23 to 2654.52 hm^3 $month^{-1}$.

Figures 5b, 5c and 5d, respectively, illustrate the longitudinal profiles of the simulated flows of the Araguari, Quebra-Anzol and Uberabinha rivers in the driest and rainiest months, along with the maximum flow observed, minimum flow observed, average flow observed and 25-75% percentile observed. Downstream to the Nova Ponte reservoir, the box-plot graph (Fig. 5) shows that the extreme model scenarios-driest and rainiest months-are between 25-75% percentiles. In the upper Quebra-Anzol and Uberabinha Rivers, it is observed that the extreme model scenario in the driest month is between minimum observed and 25% percentile observed and the extreme model scenario in rainiest month is between maximum observed and 75% percentile observed.

Quality modeling

Figures 6 and 7 show longitudinal profile of simulated quality parameters in the driest and rainiest months, and average values, maximum and minimum flow rates observed and 25-75% percentiles observed in the period of calibration and validation in the Araguari, Quebra-Anzol and Uberabinha rivers. In the three major rivers, the longitudinal profile of simulate 10% from their calibrated value, which is called a quality parameters always remained within the minimum and maximum values observed in all the nodes studied.

Table 2 presents the calibrated values of the main coefficients of biochemical reactions (K_a, K_d, KN_{oa}, KN_{ai} and K_{phosph}), the sedimentation rates (V_{Sd}, V_{SNo} and $V_{Sphosph}$) and sediment oxygen demand (S_{OD}) in each river segment. The values in this table are within limits recommended in the literature (Chapra, 2003; Von Sperling, 2007; Paredes-Arquiola *et al.*, 2009). Also in Table 2, the values set at -1 for K_a in some segments indicate that this coefficient was estimated by the Covar method. Note that there was sediment oxygen demand in much of the basin, ranging from nodes 2 (upper course of Araguari River) and 15 (upper course of Quebra-Anzol River) to node 9 (Capim Branco HP 1).

According to Figure 8, a comparison was made for the main coefficients found in this paper with values from the literature. k_a values upstream to the Nova Ponte reservoir are similar to the found by Paredes-Arquiola *et al.* (2010a, 2010b), Nakamura (2010) and Salla *et al.* (2013), which varied between 0.5 and 6.4 day^{-1}, k_d values presented two bands, a range between 0.001 to 0.1 day^{-1} (similar to Paredes-Arquiola *et al.*, 2010a) and another range from 0.1 to 0.6 day^{-1} (similar to Paredes-Arquiola *et al.*, 2010b; Nakamura, 2010; and Salla *et al.*, 2013). With respect to S_{OD}, the same range of values found in this study was found in Paredes-Arquiola *et al.* (2010a), which varied between 0.10 and 0.23 day^{-1}. In all references consulted KN_{oa} coefficient ranged from 0.002 to 0.6 day^{-1}. The range of values found in this study to KN_{ai} (0.007 to 0.2 day^{-1}) is within the limits found by Paredes-Arquiola *et al.* (2010a, 2010b) and Salla *et al.* (2013).

The low value of the constants of biochemical reactions (Table 2) are associated with the high pollutant dilution capacity due to high surface water flows in all the river segments under study and to the low pollutant loads discharged point wise by the 13 aforementioned municipalities (Figs. 3, 4). The models that have been calibrated are intended for basin planning so that the aim is not to obtain the same adjustment to specific models or detail of water masses, as general data have been used. This approach allows to consider a reasonable fit between the time series of the simulated and observed values of water quality parameters studied here, with the best results achieved in the upper course of Araguari River, the upper course of Quebra-Anzol River and in Uberabinha River, according to the results indicated by the most representative nodes of this basin (Fig. 9).

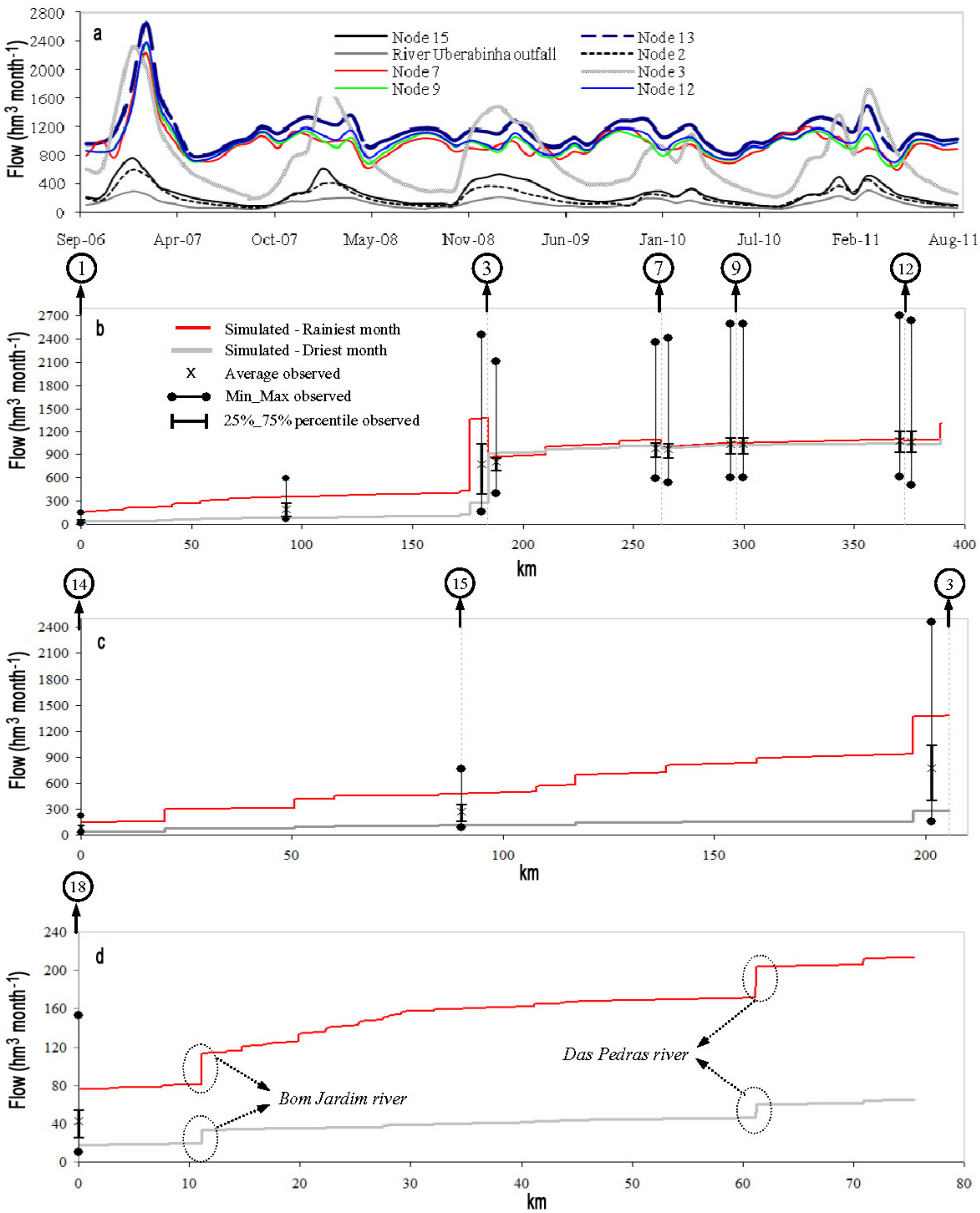


Figure 5. a) Variation of the simulated flow over the period of calibration and validation at the main points in the basin. Longitudinal profile of the simulated flows in the driest and rainiest months, with values of average, maximum and minimum flow rates observed and 25-75% percentiles observed in b) Araguari River, c) Quebra-Anzol River, and d) Uberabinha River.

In this study, a analysis was made of the sensitivity of the variables of state to changes of +10% and -10% in the values of the coefficients of re-aeration K_a, decomposition of carbonaceous organic matter K_d, decomposition of organic nitrogen KN_{oa} and ammonia nitrification KN_{ai}, water temperature *Temp* and for

Table 2. Calibrated coefficients: K_a: re-aeration, K_d: decomposition of carbonaceous matter, KN_{oa}: nitrogen mineralization, KN_{ai}: ammonia nitrification and K_{phosph}: decomposition of total phosphorus; Sedimentation rates: V_{Sd}: carbonaceous organic matter, V_{SNo}: organic nitrogen and $V_{Sphosph}$: particulate phosphorus; S_{OD}: sediment oxygen demand.

Segment	Between nodes	K_a (day^{-1})	S_{OD} (g m^{-2} day^{-1})	K_d (day^{-1})	V_{Sd} (m day^{-1})	KN_{oa} (day^{-1})	V_{SNo} (day^{-1})	KN_{ai} (day^{-1})	K_{phosph} (day^{-1})	$V_{Sphosph}$ (m day^{-1})
Araguari 1	1-2	-1	---	0.02	0.01	0.02	0.001	0.01	0.01	0.001
Araguari 2	2-3	2.0	0.10	0.5	0.05	0.05	0.05	0.007	0.01	0.001
Araguari 3	3-4	0.3; 0.4	0.10; 0.12	0.2; 0.3	0.01	0.02; 0.05	0.001; 0.05	0.01	0.3	0.1
Araguari 4	4-5	0.3	0.14	0.2	0.01	0.05	0.05	0.01	0.3	0.1
Araguari 5	5-6	0.3	0.16	0.2	0.01	0.05	0.05	0.01	0.3	0.1
Araguari 6	6-7	0.3	0.19	0.2	0.01	0.05	0.05	0.01	0.3	0.1
Araguari 7	7-8	0.10; 0.15	0.10	0.02	0.01	0.002	0.2	0.01	0.02	0.001
Araguari 8	8-9	0.10	0.12	0.02	0.01	0.002	0.2	0.01	0.01	0.001
Araguari 9	9-10	0.1	---	0.02	0.01	0.002	0.2	0.01	0.01	0.001
Araguari 10	10-11	0.1	---	0.02	0.01	0.002	0.2	0.01	0.01	0.001
Araguari 11	11-12	0.1	---	0.02	0.01	0.002	0.2	0.01	0.01	0.001
Araguari 12	12-13	0.1	---	0.05	0.1	0.002	0.2	0.01	0.2	0.1
Quebra-Anzol 1	14-15	-1	---	0.02	0.01	0.05	0.001	0.1	0.01	0.001
Quebra-Anzol 2	15-16	-1	0.21	0.6	0.1	0.01	0.05	0.1	0.2	0.1
Quebra-Anzol 3	16-17	2.0	0.22	0.4	0.05	0.01	0.05	0.1	0.2	0.1
Quebra-Anzol 4	17-30	4.0	0.23	0.5	0.1	0.05	0.05	0.007	0.2	0.1
Uberabinha 1	18-19	-1	---	0.02	0.01	0.2	0.001	0.1; 0.2	0.01	0.001
Uberabinha 2	19-20	0.04; 0.08	---	0.04; 0.06	0.01	0.2;0.4	0.001; 0.01	0.1	0.01	0.001
Uberabinha 3	20-21	0.04	---	0.06	0.01	0.4	0.01	0.01	0.01	0.001
Uberabinha 4	21-13	0.04; 0.1	---	0.05; 0.06	0.01; 0.1	0.002;0.4	0.01; 0.2	0.01	0.01;0.02;0.03	0.01;0.1

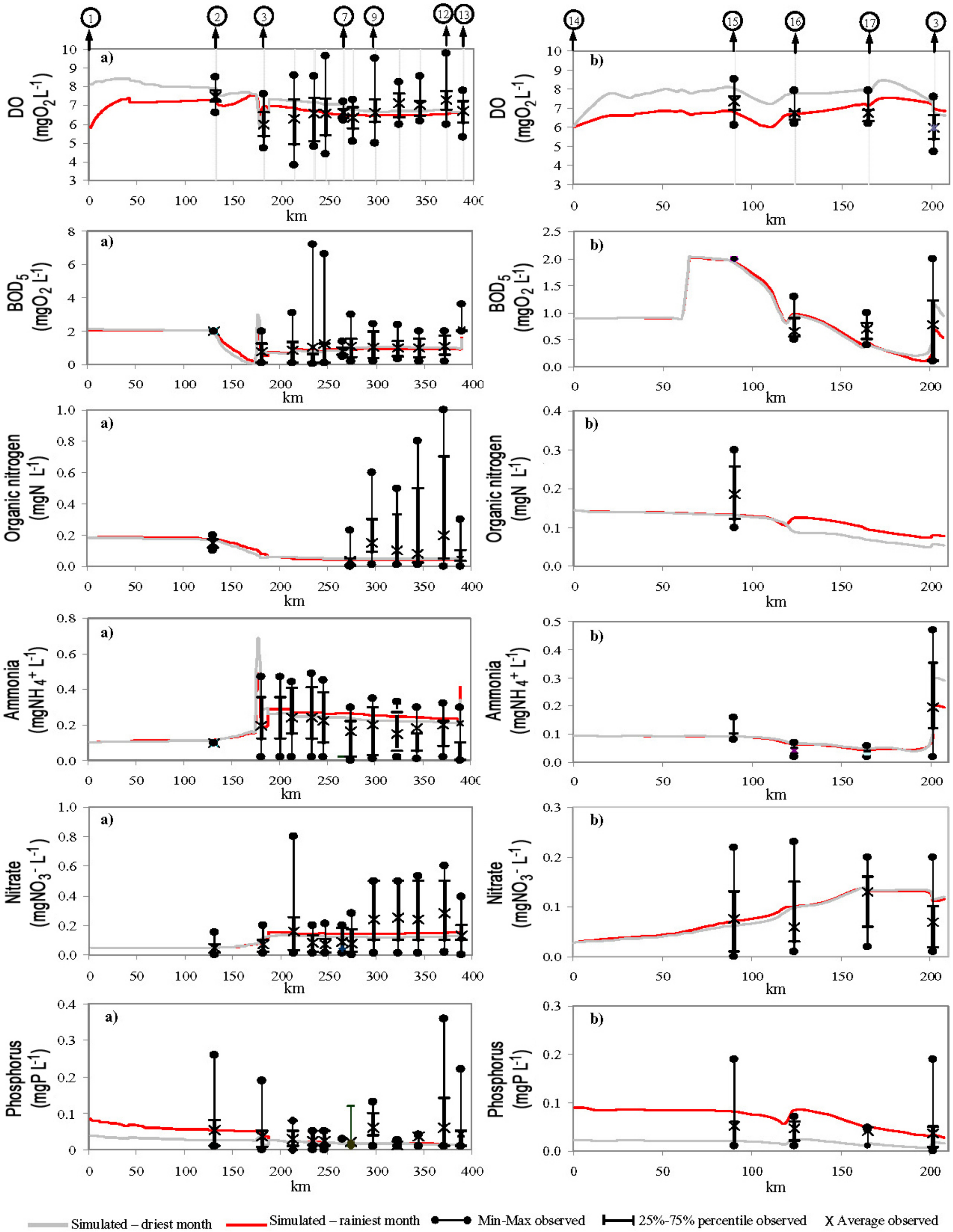


Figure 6. Longitudinal profile of simulated quality parameters in the driest and rainiest months, and values of average, maximum and minimum flow rates observed and 25-75% percentile observed in the period of calibration and validation: a) Araguari River, b) Quebra-Anzol River.

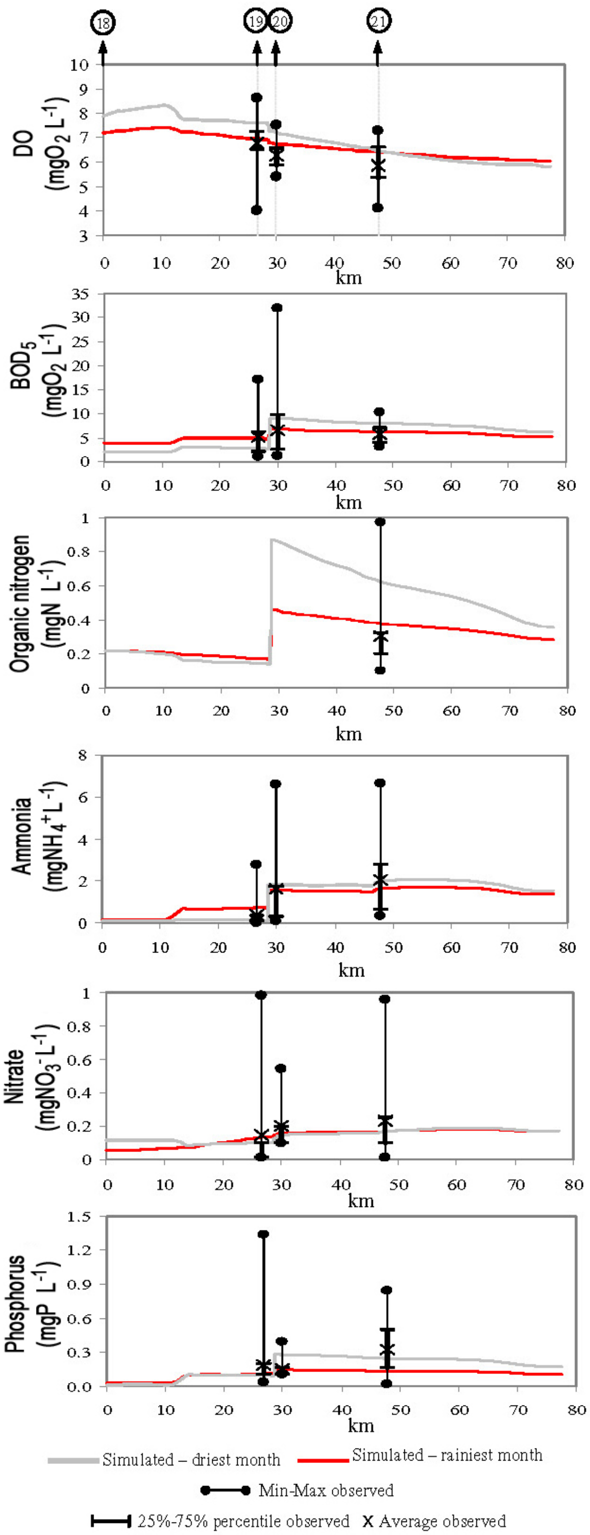


Figure 7. Longitudinal profile of the simulated quality parameters for the rainiest and driest months, and values of average, maximum and minimum flow rates observed and 25-75% percentiles observed in the period of calibration and validation in Uberabinha River.

some segments, also the sediment oxygen demand S_{OD}.

Figure 10 illustrates the percentage of variation of the parameters DO, BOD_5, organic nitrogen, ammonia and nitrate as a function of the segments. In general, it was found that variations in the coefficients and in sediment oxygen demand display a low sensitivity with respect the previously calibrated results, while water temperature generated the largest one. With regard to the parameter DO, the highest sensitivities occurred as a result of changes in S_{OD} and *Temp* in the segments of the Nova Ponte reservoir. With respect to S_{OD}, the parameter DO ranged from -2.1 to +10% S_{OD} and +1.9 to -10% S_{OD} in Araguari segment 2 and from -3.8 to +10% S_{OD} and +3.3 to -10% S_{OD} in Quebra-Anzol segments 2, 3 and 4. With respect to *Temp*, the parameter DO has reached -6.4 to -10% *Temp* in Araguari segment 2 and +6.7 to +10% *Temp* in Quebra-Anzol segments 2, 3 and 4. The variation of K_a generated little sensitivity in the calibrated results of DO (≤ 1.2% in all the segments).

The parameter BOD_5 showed sensitivity only in Araguari segment 2 and Quebra-Anzol segments 2 a 4 (Nova Ponte reservoir) and Araguari segments 3 a 6 (between Nova Ponte HP and Miranda HP) due to variations in the coefficient K_d and *Temp*. With respect to K_d, the parameter BOD_5 ranged from -5.2 to +10% K_d and +5.6 to -10% K_d in Araguari segment 2; -4.8 to +10% K_d and +5.0 to -10% K_d in Araguari segments 3-6; and -2.8 to +10% K_d and +3.6 to -10% K_d in Quebra-Anzol segments 2-4 (Fig. 10). With respect to *Temp*, the parameter BOD_5 has reached -15.0 to -10% *Temp* in Araguari segment 2 and -4.8 to -10% *Temp* in Quebra-Anzol segments 2-4 (Fig. 10).

The highest variations in the organic nitrogen occurred due to variations in the coefficient KN_{oa} and water temperature *Temp*. The higher sensitivities observed where of ± 1.7% in Quebra-Anzol segments 2 to 4 and of ± 2.1% in Uberabinha segments 2 and 3 due to variations in the coefficient KN_{oa}. With respect to *Temp*, organic nitrogen has reached -5.4 to -10% *Temp* in Araguari segment 2 and -4.4 to -10% *Temp* in Uberabinha river segments 2 and 3 (Fig. 10).

Ammonia showed low sensitivity (≤1.1%) due to variations in the coefficients KN_{oa} and KN_{ai}. With respect to water temperature *Temp*, the ammonia has reached -2.1 to +10% *Temp* and -3.2 to -10% *Temp* in Quebra-Anzol segment 1.

And nitrate showed the highest sensitivity due to variations in the coefficient KN_{ai} and water temperature *Temp, s*howed the highest sensitivity of ± 6.4% in Quebra-Anzol segments 2 to 4 and of ±3.4%

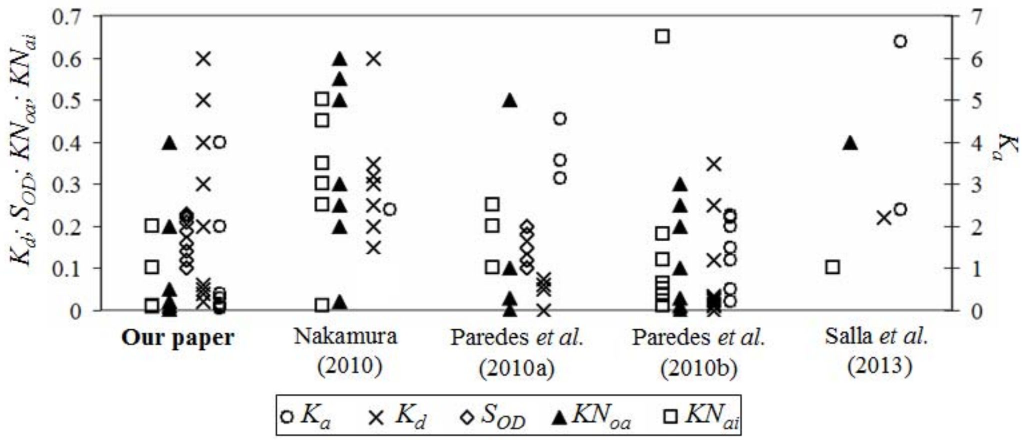


Figure 8. Comparison of the main coefficients found in this paper with literature values.

in Uberabinha segments 2 and 3 due to variations in the coefficient KN_{ai}. With respect to *Temp*, the nitrate has reached +19.3 to +10% *Temp* and +27.5 to -10% *Temp* in Quebra-Anzol segment 1.

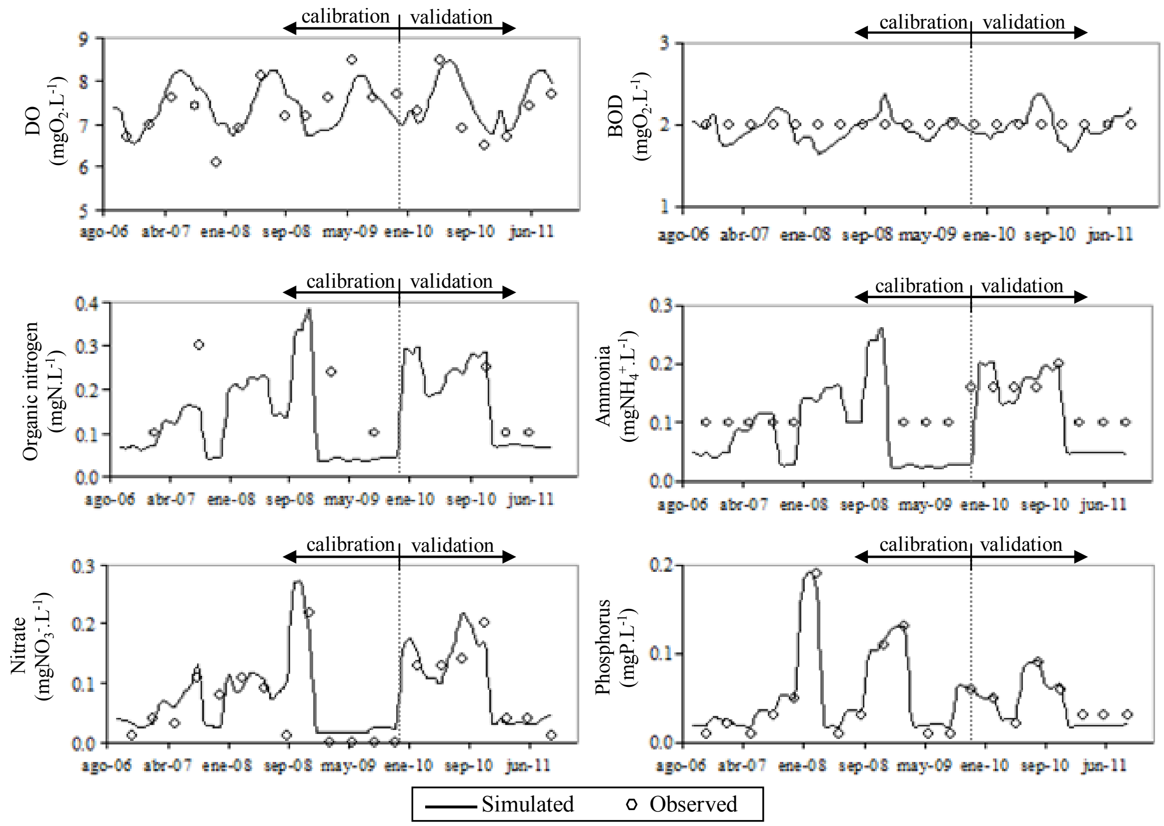
DISCUSSION

In the quantity simulations performed in the SIMGES module, from October 2006 to September 2011, the adjustments were satisfactory for scale work used in this paper, in which we tried to represent the mean behavior of the system. In Figure 5a, the greater amplitude of oscillation of the flow in the Nova Ponte HP (node 3) compared to the Miranda HP (node 7), Capim Branco HP 1 (node 9) and Capim Branco HP 2 (node 12) indicates the regulatory behavior of the Ponte Nova reservoir vis-à-vis the other three cascade reservoirs. The regulatory behavior of the Nova Ponte reservoir (node 3) is also shown in Figure 5b. An analysis of node 3 reveals that there is storage of liquid volume in the rainy season and release during the dry months, which causes a considerable decrease in the difference in flow between the rainy and dry seasons (note the segments upstream and downstream from node 3).

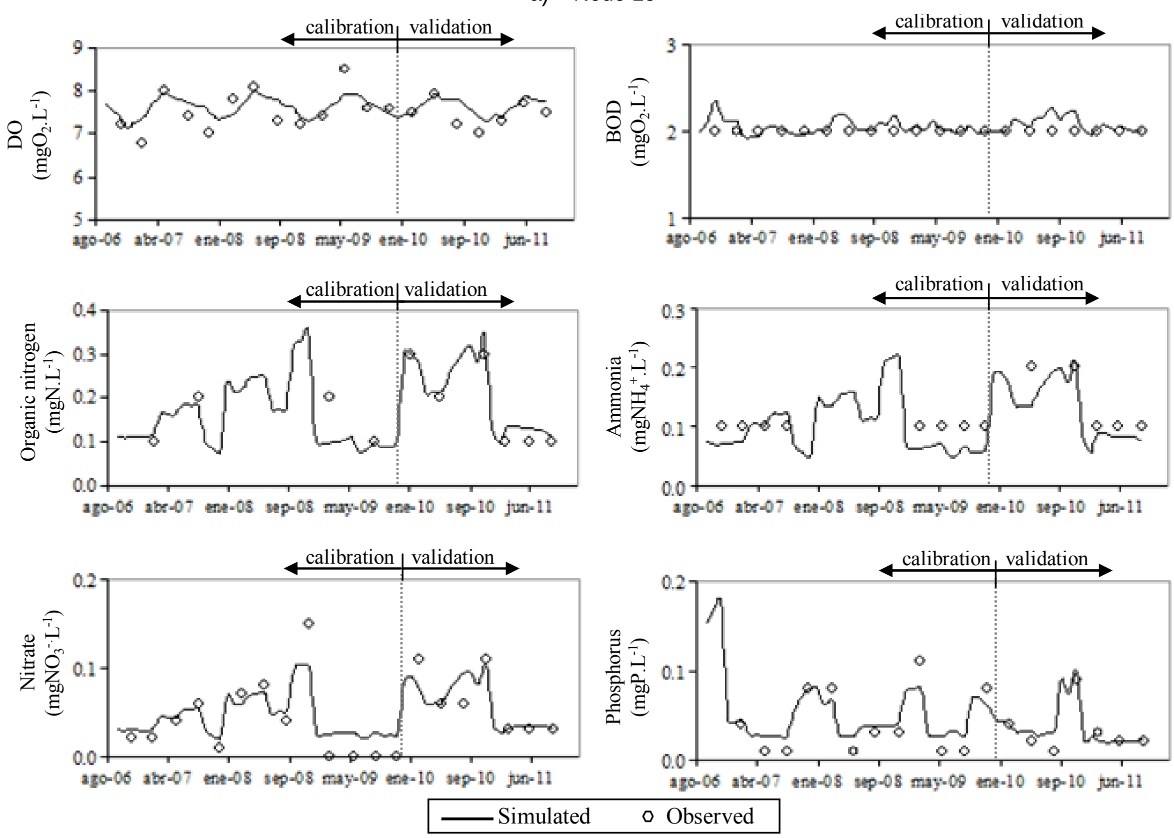
In Brazil, water bodies are classified by CONAMA (2005). In addition to this resolution, the state of Minas Gerais has its own Joint Regulatory Resolution (COPAM, 2008), which is similar to CONAMA (2005) with respect to the parameters studied here. According to the COPAM (2008), the Araguari, Quebra-Anzol and Uberabinha rivers are Class 2 rivers, for which the following limits with respect to the quality parameters studied here must be observed: dissolved oxygen ≥5.0 mg O_2 L^{-1}; BOD_5 ≤5.0 mg O_2 L^{-1}; ammonia ≤3.7 mg NH_4^+ L^{-1}; nitrate ≤10.0 mg NO_3^- L^{-1}; phosphorus (lentic environment) ≤0.03 mg P L^{-1}; phosphorus (intermediate environment) ≤0.05 mg P L^{-1}; and phosphorus (lotic environment) ≤0.10 mg P L^{-1}.

However, a general analysis of the longitudinal profiles of the quality parameters simulated for the rainiest and driest months (Figs. 6, 7) reveals discrepancies with regard to the parameters BOD_5 in the Uberabinha River (Fig. 7) and total phosphorus in the Uberabinha, Araguari and Quebra-Anzol rivers (Figs. 6, 7). In Uberabinha River, downstream from the site where the municipality of Uberlândia discharges its treated wastewater, to the mouth of Uberlandia River (called Uberabinha segments 3 and 4), the BOD_5 and total phosphorus show Class 3 behavior. The BOD_5 ranged from 5.1 to 6.8 mg O_2 L^{-1} in the rainiest month and from 6.2 to 9.1 mg O_2 L^{-1} in the driest month. The total phosphorus parameter for lotic environments ranged from 0.10 to 0.14 mg P L^{-1} in the rainiest month and from 0.17 to 0.28 mg P L^{-1} in the driest month. The higher concentrations of BOD_5 and total phosphorus in the driest month are associated with the lower capacity for natural self-purification and dilution of pollutants due to reduced flows. This problem will increase due to the increasing population of this municipality.

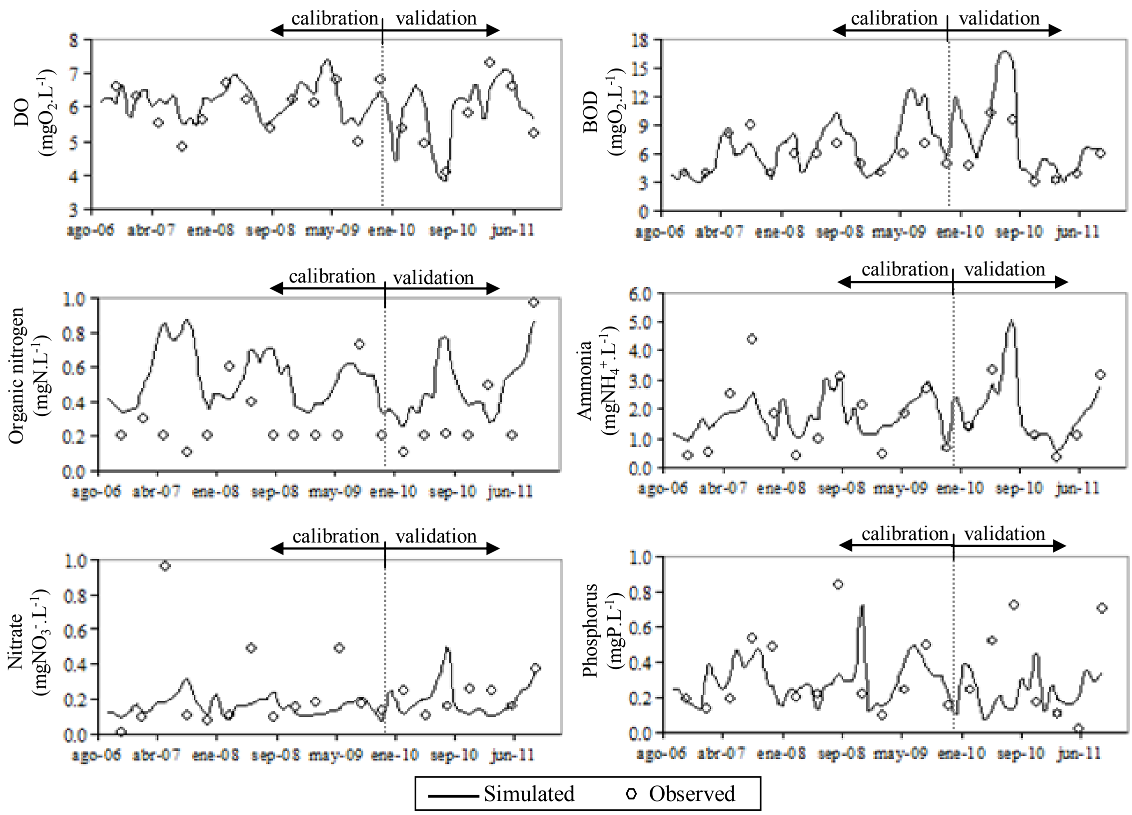
In the Araguari and Quebra-Anzol rivers, the simulated profiles of the parameter total phosphorus show non-compliance with the COPAM (2008) in the Araguari 2, Quebra-Anzol 3 and Quebra-Anzol 4 segments. These segments, which correspond to the flooded areas of the Nova Ponte reservoir, behave like lentic environments, in which phosphorus ranged from 0.04 to 0.06 mg P L^{-1} in the rainiest month and from



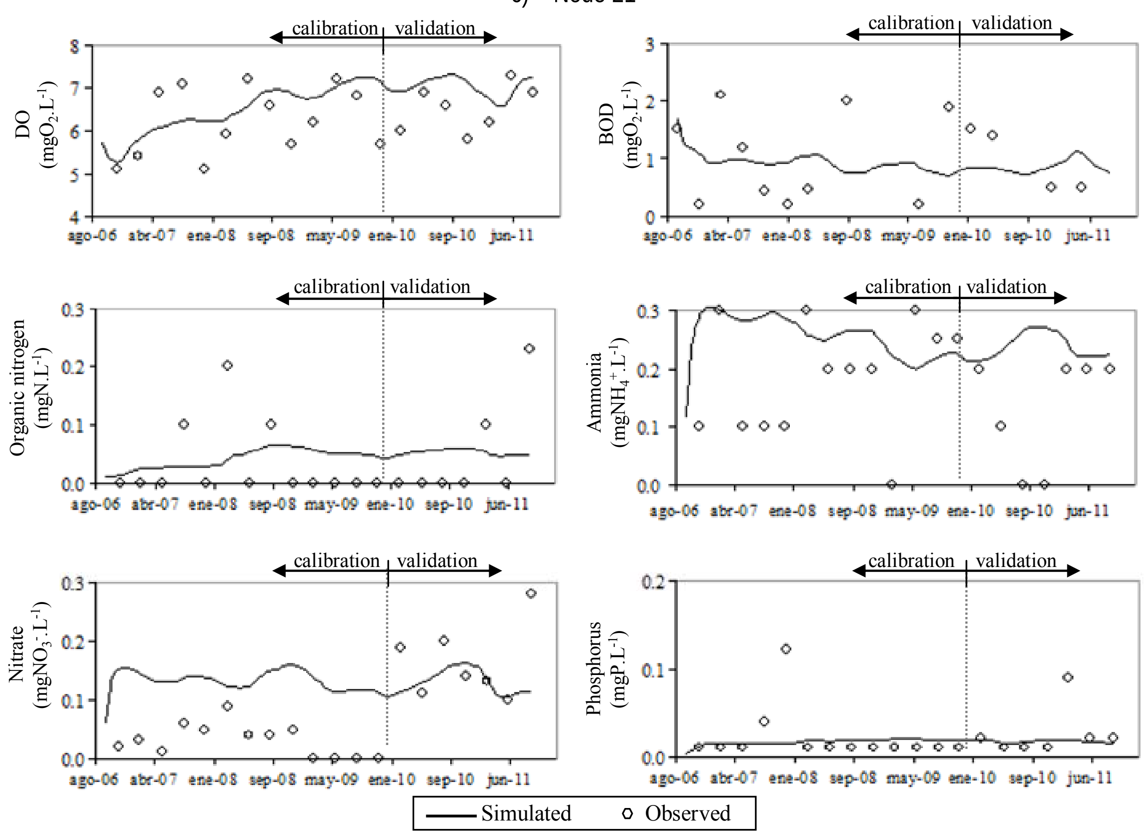
a) – Node 15



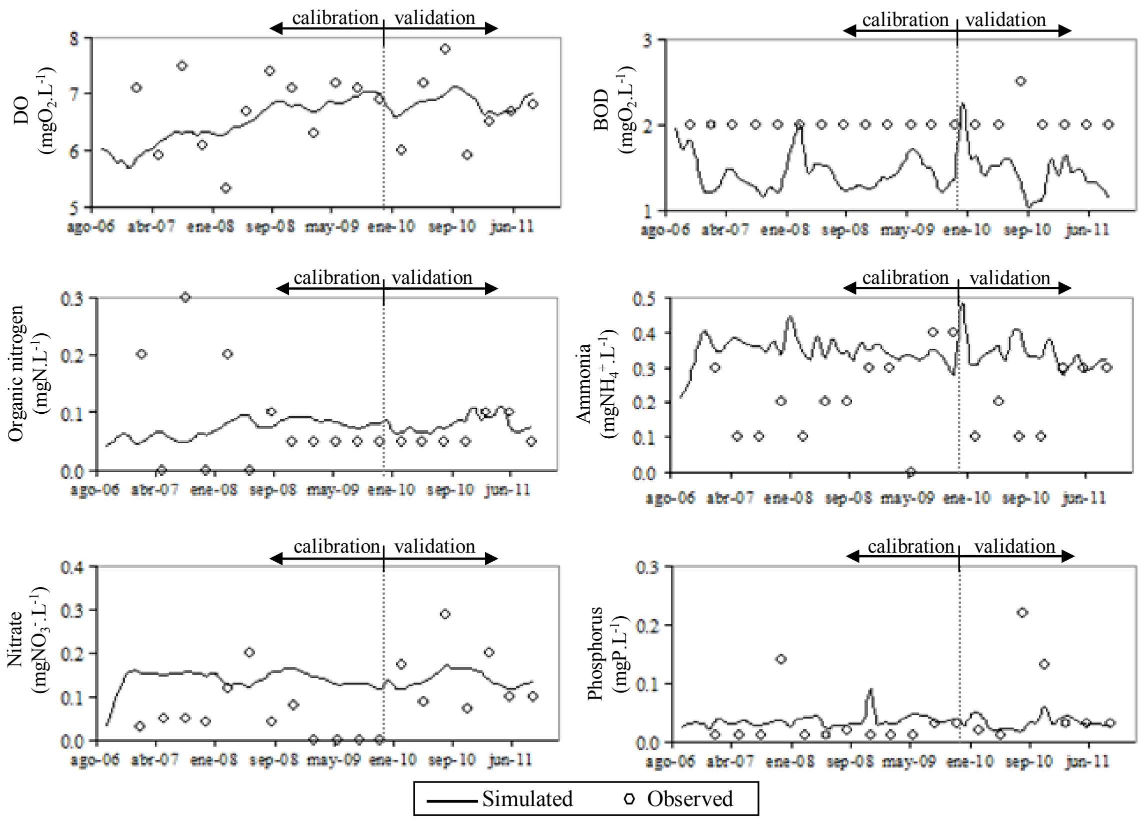
b) – Node 2



c) – Node 21



d) – Node 8



e) – Node 13

Figure 9. Time series of simulated and observed values in: a) Node 15, b) Node 2, c) Node 21, d) Node 8, and e) Node 13.

0.02 to 0.04 mg P L^{-1} in the driest month in the Araguari segment 2, and from 0.03 to 0.09 mg P L^{-1} in the rainiest month in the Quebra-Anzol segments 1, 2 and 3. In this region of the Araguari River basin, the higher concentrations of total phosphorus in the rainiest month are associated with land use in terms of the excessive application of this nutrient in annual and perennial crops. In the period of this study, land use for pasture, and annual and perennial crops represented approximately 53% of the area of contribution to the sub basin of the Quebra-Anzol River, according to the Committee of Araguari river basin.

An overall analysis of the time series of observed values of quality parameters (Figs. 6, 7) reveals a behavior that does not comply with the recommendations of the COPAM (2008) on certain dates within the period studied. In Uberabinha River, the parameter DO showed values of less than 5.0 mg O_2 L^{-1} on only four occasions in the dry months, downstream from Uberlandia's municipal wastewater treatment plant (nodes 20 and 21). Point wise DO values of less than 5.0 mg O_2 L^{-1} were found in Araguari River segments 3, 4 and 5, indicating the influence of the bottom discharge of Nova Ponte reservoir (lower concentrations of dissolved oxygen). BOD_5 values far exceeding the maximum of 5.0 mg O_2 L^{-1} were found only in Uberabinha River downstream from the municipality's WWTP, which reached up to 32.0 mg O_2 L^{-1} to observed data in node 20, However, the box-plot graph (Fig. 7) shows that the extreme model scenarios –driest and rainiest month– are between 25 and 75% percentile observed in node 20. Ammonia values exceeded the maximum of 3.7 mg NH_4^+ L^{-1} only in Uberabinha River, also downstream from the municipality's WWTP, which reached up to 11.0 mg NH_4^+ L^{-1} in a single month without rain. The nitrate parameter was in compliance with the COPAM (2008) in the analyzed time series. However, in most of the nodes, the total phosphorus parameter presented values not in compliance with the maximum of 0.03 mg P L^{-1}, except for nodes 4, 5, 6, 10, 14, and 18.

The calibrations in the upper courses of Araguari and Quebra-Anzol rivers (Figs. 9a, 9b) showed satisfactory fits to the DO, nitrate and total phosphorus parameters. As for organic nitrogen, the reduced number of observed data precluded a good assessment of the fit. The time series of observed data of the

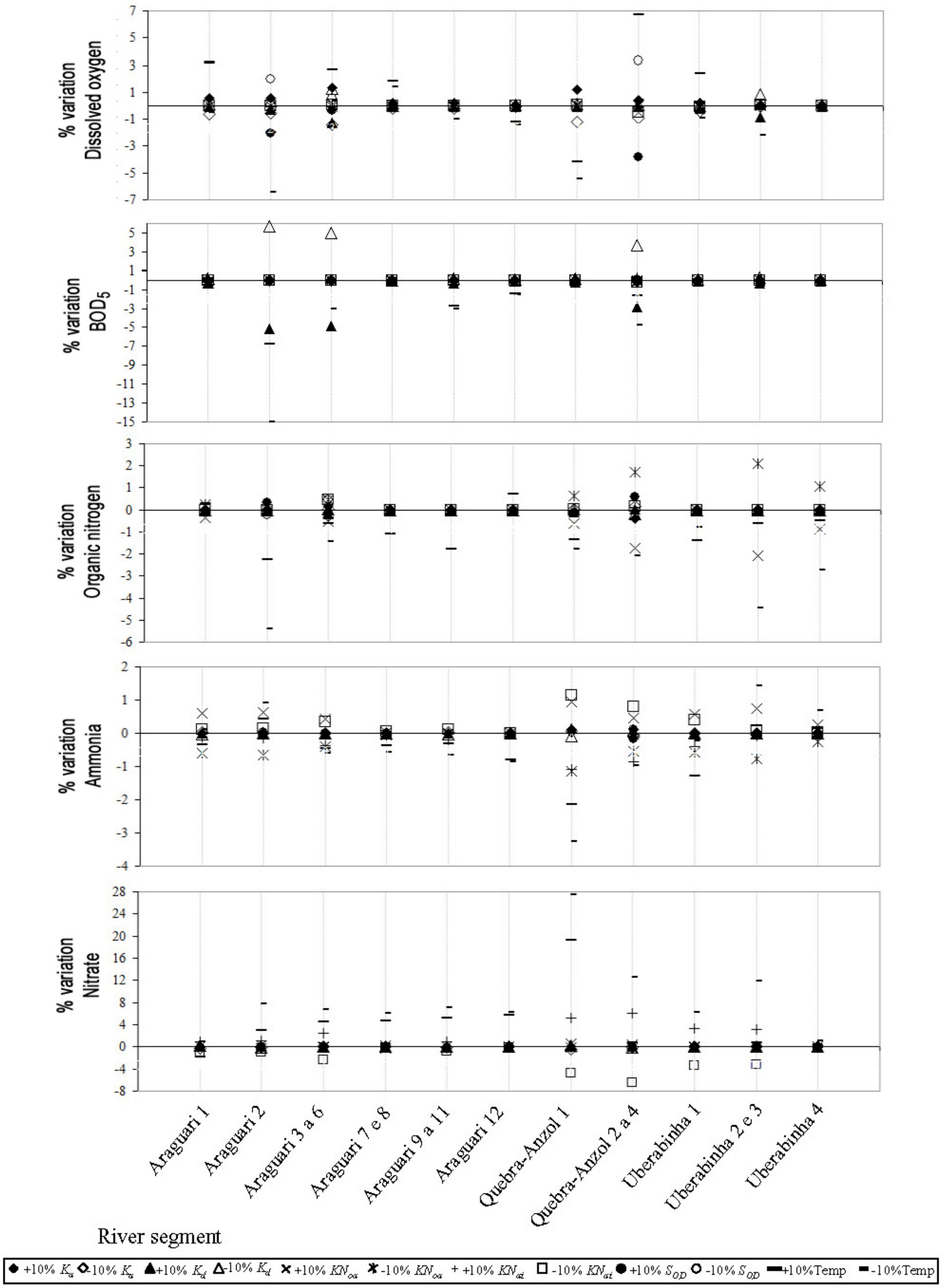


Figure 10. Sensitivity Analysis – Percentages of variation of the DO, BOD_5, organic nitrogen, ammonia and nitrate parameters as a function of the segments of river.

BOD_5 and ammonia parameters showed practically constant values, which also made it difficult to assess the fit between observed and simulated data, indicating the possibility that the laboratory measurements of these parameters have methodological limitations.

Figure 9c shows the time series of simulations and observed data at node 21, located downstream from Uberlandia's municipal WWTP at the lower course of Uberabinha River. The calibrations achieved satisfactory results for the DO, BOD_5, ammonia, nitrate and total phosphorus parameters, despite a few observed data scattered of the ammonia, nitrate and phosphorus parameters. The quality of the observed data for the nitrogen parameter hindered their fit to the simulations, as indicated by a comparison of the oscillatory behavior of the data observed for ammonia and its fixed behavior and with the value of 0.2 mg N L^{-1} for 60% of the data observed for nitrogen. Calibrations in the middle and lower course of Araguari River (Figs. 9d, 9e) showed different behaviors in relation to the nodes located in the upper course of Araguari River and in Uberabinha River. In general, the time series of observed data are highly scattered in these regions of the basin, which hindered the satisfactory fit of the simulations, except for the of dissolved oxygen and phosphorus parameters.

The model was validated from October 2009 to September 2011, as indicated in Figure 9. The fits between simulated and measured data were satisfactory for the upper courses of Quebra-Anzol and Araguari rivers for most of the parameters (Figs. 9a, 9b), except for ammonia in node 15 for the year 2011 (Fig. 9a). As for node 21 (Fig. 9c), the validation was not satisfactory for organic nitrogen and phosphorus due to the marked dispersion observed in the time series. With regard to the validation of the model for the middle and lower course of Araguari River (Figs. 9d, 9e), the same findings as those recorded during the period of calibration persisted.

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