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Deterministic and probabilistic modeling of microbiological quality using the QUAL-UFMG: a water resource management tool applied on the slope waters of the Grande River, Brazil

Clécio Eustáquio Gomides [a,*], Mateus Pimentel de Matos[b], Ronaldo Fia[b] and Alysson Rodrigo Fonseca[c]

[a] Department of Water Resources, Federal University of Lavras – UFLA, University Campus, P.O. Box 3037, Lavras, MG CEP 37200-900, Brazil
[b] Department of Environmental Engineering, Federal University of Lavras – UFLA, University Campus, P.O. Box 3037, Lavras, MG CEP 37200-900, Brazil
[c] Department of Agronomic Engineering, State University of Minas Gerais – UEMG, University Campus, 3001 Paraná Avenue, Divinópolis, MG CEP 35501-170, Brazil
*Corresponding author. E-mail: cleciogomides@yahoo.com.br, clecio.gomides1@estudante.ufla.br

CEG, 0000-0002-8566-2913

ABSTRACT

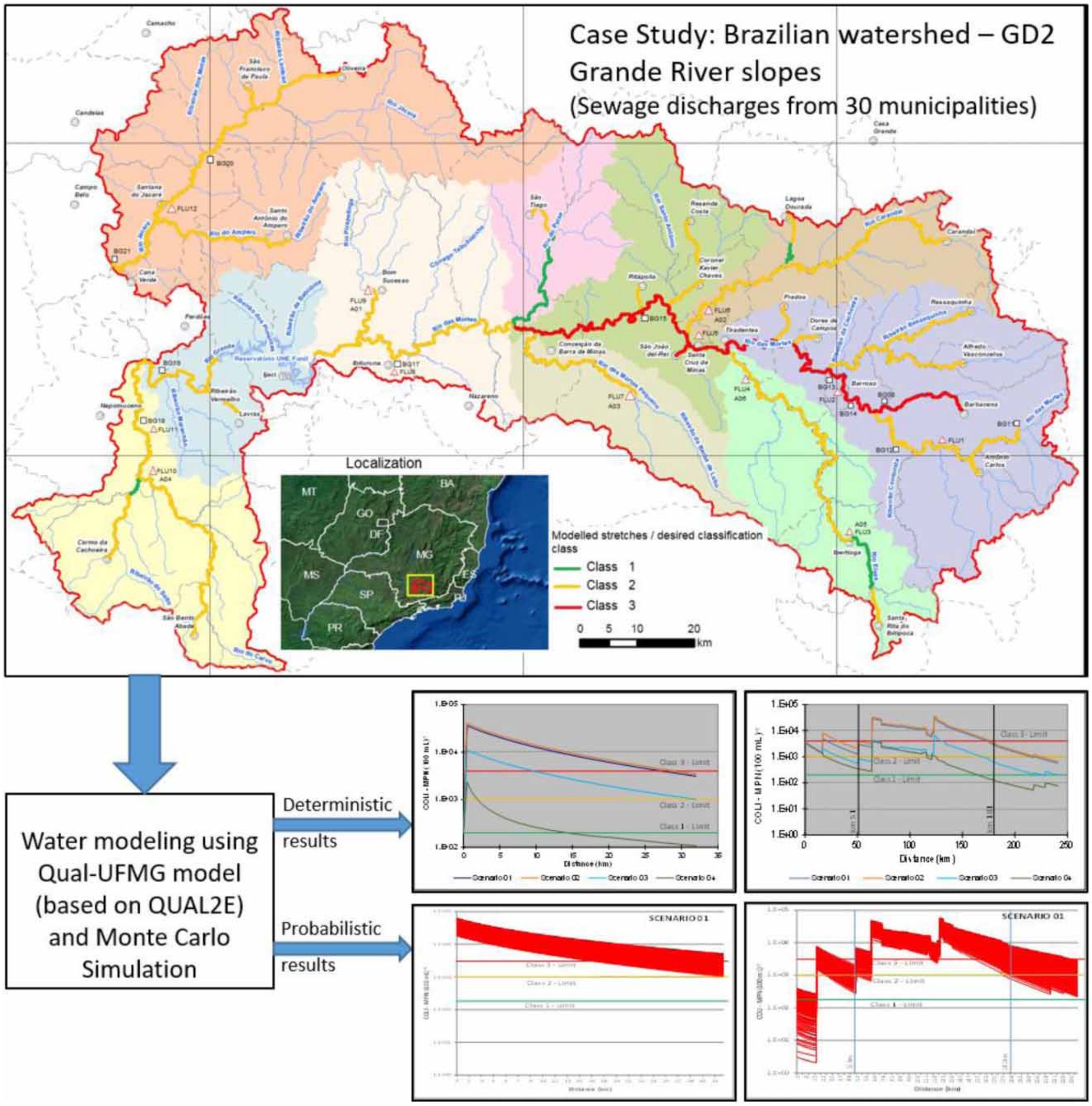
The present work presents a methodology for modeling the quality of surface water, aiming at the management of hydrographic basins and the best allocation of resources in the treatment of sanitary sewage, considering the predominant uses of water and microbiological quality. The QUAL-UFMG model was used, composed of Excel spreadsheets, where visual basic for applications (VBA) routines were implemented, enabling deterministic and probabilistic modeling through Monte Carlo simulations. The proposed methodology was applied to a Brazilian hydrographic basin, called the GD2 Planning Unit (Grande River Slopes), considering the discharges of sanitary sewage from 30 municipal seats and approximately 740,000 inhabitants. Four scenarios were studied: the current situation (C-01), the trend for the year 2033 (C-02), compliance with environmental legislation (C-03) and compliance with the main uses of the basin (C-04). The results showed that for C-01 and C-02, the water quality, in terms of thermotolerant coliforms, in most stretches does not meet the defined uses. Even complying with the provisions of environmental legislation (C-03), which do not provide for disinfection, only the largest watercourses would have adequate quality for use. Complete service would only be achieved in C-04, which provides for universal sewage treatment with disinfection for the vast majority of municipalities.

Key words: mathematical modeling, self-purification, sewage treatment, thermotolerant coliforms, water pollution

HIGHLIGHTS

- The joint analysis of deterministic and probabilistic modeling proved to be an interesting tool in watershed management.
- The secondary level of sewage treatment is not sufficient to reach the necessary quality of watercourses.
- Normally, the obligations related to the treatment of sewage, as foreseen in the legislation, are not sufficient to guarantee the necessary quality for the foreseen uses of the water.

GRAPHICAL ABSTRACT



1. INTRODUCTION

Brazil has a population of approximately 213.3 million inhabitants (IBGE 2022) and is a country with dimensions similar to those of a continent, which results in very different regional conditions in some aspects. The greatest water availability is found in the North region, which has the lowest population density. On the other hand, the Southeast concentrates the largest portion of the population and does not have the same water availability, which leads to greater demand, a greater amount of discharges and less dilution capacity of water bodies (Ana 2009). It is known that the disposal of untreated or insufficiently treated effluents in water sources can cause a series of damages to the aquatic environment (Ashouri & Rafei 2018; Bui *et al.* 2019; Liu *et al.* 2022), such as, for instance, contamination by pathogenic organisms, which is a problem, especially in developing countries (Pujol-Vila *et al.* 2016; Andersson *et al.* 2018; Madani *et al.* 2021).

The presence of etiological agents of waterborne diseases affects some of the main uses intended for it, such as drinking water supply, irrigation and bathing (Von Sperling 2014a; Alegbeleye *et al.* 2016; Madani *et al.* 2021), which may lead to an increase in the number of ill people and/or imply the technical and financial impossibility of water resource use. As it is costly and economically unfeasible to quantify the presence of all possible causes of diseases, monitoring is done using groups of organisms that are indicators of fecal contamination, the group of thermotolerant coliforms, along with detection methodologies for quantification of the bacteria *Escherichia coli* (*E. coli*), are the most used in the assessment of health hazards (Batista & Harari 2016; Silva *et al.* 2021).

1.1. Coverage of sanitary sewage services in Brazil

According to the thematic diagnosis of water and sewage services (SNIS 2021), only 63.2% of the sewage generated in Brazil is collected and the percentage of treatment is even lower, at 50.8%, with unequal service among large urban centers (with higher rates) and smaller towns (with low population coverage). Even in locations that have wastewater treatment plants (WWTPs), it is considered that there is low removal of pathogenic organisms, since the occurrence of tertiary treatment with disinfection is very infrequent (Ferreira *et al.* 2021; SNIS 2021).

Aiming to guarantee surface waters quality compatible with their uses, according to their framework class, Federal Law No. 14.026 (Brasil 2020) established the new Legal Framework for Sanitation in Brazil, determining, among other things, that public basic sanitation services must guarantee 90% of the population with sewage collection and treatment by 31 December 2033. It should be noted, however, that this legal provision does not establish criteria regarding the minimum efficiency of removal of the various contaminants existing in the sewage, especially the fecal contamination indicator organisms.

1.2. The importance of surface water quality modeling

It is of crucial importance to know the behavior of disease-transmitting agents in a water body, from the moment it is discharged to the places where it is used, in order to infer forms of control or to estimate points where the water collection can be installed for different uses. It is known that most of these agents have in the human intestinal tract the optimal conditions for their growth and reproduction. Once subjected to the adverse conditions prevailing in the water body, they tend to decrease in number, characterizing the so-called decay (Von Sperling 2014b; Madani *et al.* 2021). Thus, depending on the degree of contamination of a watercourse, the reduction in the count of these pathogenic organisms may be greater or dependent on a long stretch of recovery.

Water quality models are important tools for the effective management of water resources, assisting in decision-making by providing water quality simulations for a variety of management actions (Koo *et al.* 2020; Bello & Haniffah 2021; Kaufman *et al.* 2021; White *et al.* 2021). Furthermore, these models reduce the need for water collection and analysis, reducing costs in terms of resources and time (Von Sperling 2014b; Quijano *et al.* 2017; Bui *et al.* 2019). It is noteworthy that the monitoring of water quality in Brazil is quite limited, with a small number of sampling points, monitored variables and short historical series (ANA 2009). As a guide for assessing water quality using these models, it is necessary to have pertinent legislation and established parameters, such as the framework classes of water bodies.

1.3. Framing of surface watercourses and the legal framework for sanitation

The framework aims to ensure that the water quality is compatible with the most demanding uses for which it is intended and to reduce the costs of combating pollution, through permanent preventive actions (Machado *et al.* 2019; Costa 2021). With specific regard to fresh water, there are five classes, fundamentally established in accordance with the predominant uses of water resources (Brasil 2005; minas Gerais 2008): the special class, which cannot receive sewage discharges and serves to preserve the natural balance of aquatic communities; and Classes 1–4, the first of which has more restrictive parameters of quality and destination for more noble uses, with an increase in the permissiveness of variable values in the following classes.

The minimum efficiencies and maximum concentrations defined in the legislation must be observed when discharging wastewater into receiving bodies, as well as respecting the non-alteration of the watercourse class in which the stretch was classified, according to the intended uses (Classes 1–4). However, due to the inefficiency of sanitation services in many locations, the river is often in a condition inferior to what it should be, making it difficult to meet the legal requirements for the disposal of treated wastewater. This is the case in many hydrographic basins, such as the Rio Grande Basin and its planning units, such as GD2 (water slopes of the Rio Grande), with a high degree of contamination (in certain stretches), as observed in studies such as Amâncio *et al.* (2018). Thus, actions must be taken to improve the quality of the watercourse, with an increase in sewage treatment rates, in addition to reviewing the frameworks in place.

1.4. Objectives of the work

The general objective of this work was to implement a mathematical model of surface water quality for thermotolerant coliforms, of simple and free use for the watershed in question, with deterministic and probabilistic results, aiming at:

(a) Checking the current basin water quality panorama, based on the few monitoring points, against the quality required for its main uses;
(b) Inferring the future situation of the basin, in case new investments in sewage collection and treatment are not adopted;
(c) Checking how the basin water quality will be if the obligations foreseen in the sanitation legal framework are met, indicating whether the quality will be compatible with the preponderant uses foreseen. Otherwise, propose the necessary interventions;
(d) Identifying stretches where the proposed framework is not being met and assessing the necessary conditions for compliance;
(e) Assessing the adequacy of the model used for the management of Brazilian watersheds.

2. METHOD

2.1. Modeled watershed

Brazil has eight large hydrographic basins and the São Francisco River Basin, together with the Paraná River Basin, covers a large part of the most populated region of the country (ANA 2009). One of the main subbasins of the Paraná River is the Grande River Basin, which is subdivided into 24 Water Resources Planning and Management Units – UPGRH (IGAM 2013). For the present work, one of these planning units was selected, named GD2 (waters slopes of Rio Grande), which comprises the areas drained by Mortes, Jacaré and Cervo Rivers.

GD2 is located in the southern region of Minas Gerais, between parallels 20° 30′ –22°, south latitude and 43° 30′–45°30′ west longitude, having as its highest point the headwaters of the Mortes River, on the border between the municipalities of Barbacena and Senhora dos Remédios, on the slopes of Mantiqueira, at approximately 1,200 m altitude. The lowest point is the mouth of Jacaré River (JAR), at Furnas Reservoir, on the border between the municipalities of Campo Belo and Cana Verde, at an altitude of approximately 780 m. As the climate is tropical altitude, with a rainy and a dry season, there are dry periods with little or no rainfall. The basin's drained area is 10,533 km^2, divided into 10 subbasins (Figure 1). In its interior, there are lands of 42 municipalities and of these, 30 discharge their sanitary effluents in the watercourses (IGAM 2013).

Table 1 shows a summary of the sewage systems in the basin, in which it is observed that only 13 municipalities have some form of sewage treatment. Of the total urban population of the basin (541,576 inhabitants), 95% are served with sewage collection, however, only 21.7% of the collected sewage is treated (without disinfection) before being discharged into the receiving bodies, a situation that is worrying. Of the total discharges generated, 67.7% correspond to the four largest municipalities in the basin (Barbacena, São João Del-Rei, Lavras and Oliveira).

In the evaluation, the watercourses that receive discharges from urban areas or have water quality monitoring points were modeled and are presented in Figure 1, as well as the allocation of municipal seats with their respective points of liquid discharge.

The pollutant loads considered in the discharges are those related to sanitary sewage discharges from the urban areas of 30 municipalities located within the basin. The considered flows are shown in Table 1, and the discharges are indicated in Figure 1. As there is no systematic qualitative monitoring of sanitary sewage in the municipalities, for the deterministic modeling, the value of 10^6 MPN $(100\ \mathrm{mL})^{-1}$ was considered, which is consistent with reports in the literature (Arceivala 1981; Metcalf & Eddy 1991; Von Sperling & Von Sperling 2013; Von Sperling 2014a) and with the calibration process.

2.2. Adopted model

The model chosen was the QUAL-UFMG, which is widely used in Brazil, due to its versatility and ease of use, allowing greater applicability and good reliability (Fan *et al.* 2012; Srikrishnan & Keller 2021). It consists of an Excel platform developed by von Sperling (2014b), based on simplifications of the QUAL2E model (Brown & Barnwell 1987) and adaptation of its equations to electronic spreadsheets (De Oliveira Filho & Lima Neto 2018; Lima *et al.* 2018). For technical simplification, the algae component of its modeling and the longitudinal dispersion are excluded from the model, since advection is the main transport phenomenon in rivers. According to von Sperling (2014b), for rivers (small and large), the inclusion of the

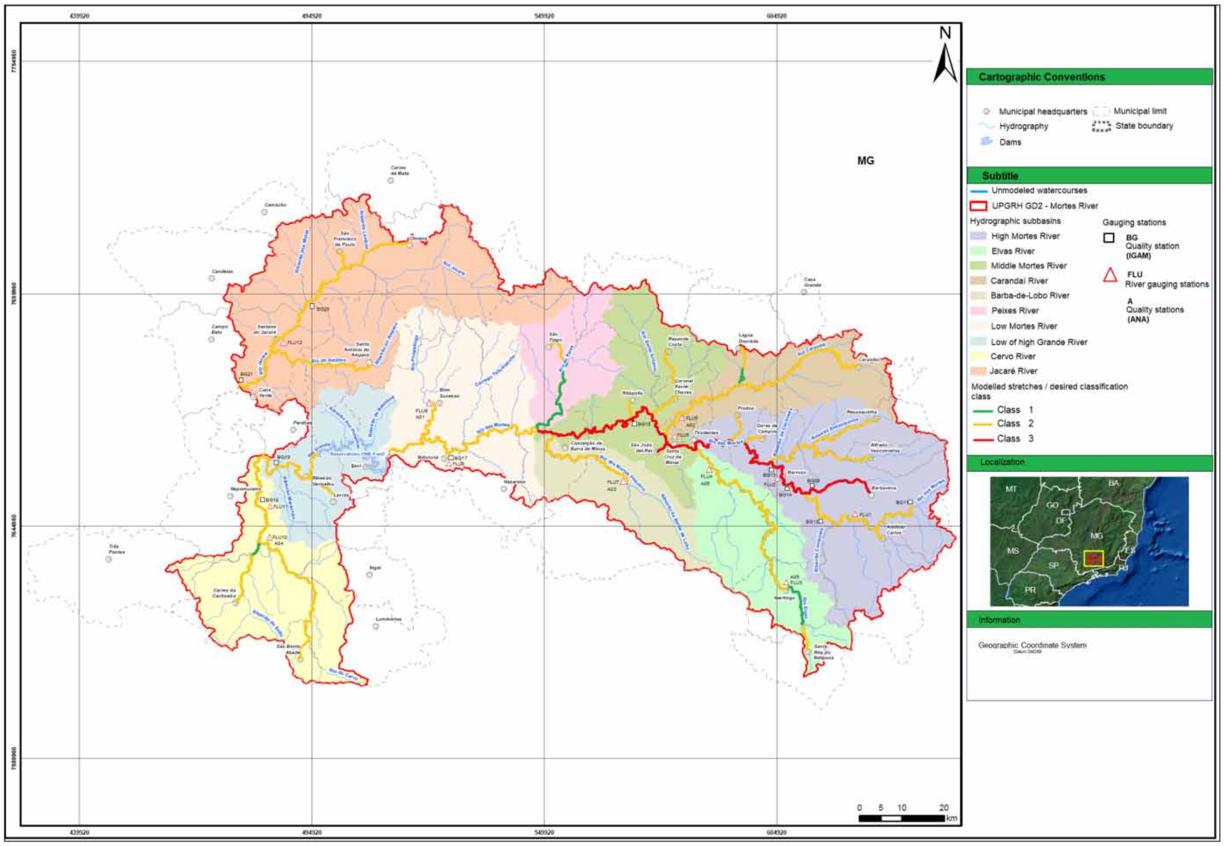


Figure 1 | Hydrographic basin, modeled sections, framework, municipal headquarters, flow and quality river stations. *Source*: Adapted from IGAM (2013).

phenomenon of dispersion is not important, at least on a large time scale (stationary conditions), as in the case of the present study. However, for verification purposes, in item 2.5, its influence is verified.

The calculations are made considering numerical integration by the Euler method (Teodoro *et al.* 2013). In QUAL-UFMG, it is possible to evaluate the dynamics of some variables; however, the study will be restricted only to thermotolerant coliforms.

In Brazilian legislation (BRASIL 2005; Minas Gerais 2008), there is no discharge standard for organisms that indicate fecal contamination. However, the respective discharge, even if treated, cannot give the receiving body the adverse characteristics of the class in which it was framed.

2.2.1. Bacterial decay kinetics

When exposed to environmental conditions that differ from those prevailing within the intestinal tract of warm-blooded animals, ideal for their development and reproduction, coliforms and other enteric organisms present natural mortality. Among the various factors that contribute to decay, we can mention mainly: sunlight, temperature, sedimentation, pH, lack of nutrients and predation (Almeida 1979; Arceivala 1981; Thomann & Mueller 1987).

The bacterial mortality rate is generally estimated using Chick's law, according to which the removal rate is directly proportional to the concentration of bacteria (Von Sperling 2014b):

$$\frac{dN}{dt} = -K_b N \qquad (1)$$

where N is the number of coliforms (ORG $(100\ mL)^{-1}$ or MPN $(100\ mL)^{-1}$); K_b is the bacterial decay rate (day^{-1}); and t is the time (day).

Table 1 | Current status of sewage systems in the basin

Municipality/subbasin	Urban population 2020	Sewage collection service (%)	Q_{med} – sewage (L s^{-1})		Treatment coverage (%)[a]
			Generated	Collected	
Upper Mortes River Basin					
Alfredo Vasconcelos	4,632	100.0	6.29	6.29	0.0
Antônio Carlos	8,069	95.0	9.68	9.20	0.0
Barbacena	126,477	91.1	122.37	111.48	31.3
Barroso	20,236	91.8	39.77	36.51	6.4
Dores de Campos	9,297	100.0	17.36	17.36	0.0
Ressaquinha	3,091	99.6	3.18	3.17	0.0
Tiradentes	6,234	62.8	12.85	8.07	0.0
Prados	6,423	97.4	6.01	5.86	100.0
Barba-de-lobo River Basin					
Conceição da B. de Minas	2,787	61	2.96	1.80	71.8
Middle Mortes River Basin					
Coronel Xavier Chaves	1,876	100.0	3.52	3.52	0.0
Resende Costa	9,280	39.4	11.80	4.65	100.0
Ritápolis	3,156	20.0	3.64	0.73	0.0
Santa Cruz de Minas	8,664	100.0	28.67	28.67	0.0
São João Del-Rei	85,556	99.5	427.98	425.84	3.2
Elvas River Basin					
Ibertioga	3,439	100.0	6.25	6.25	100
Santa Rita do Ibitipoca	2,120	90.0	2.48	2.23	0
Low of High Grande River Basin					
Ijaci	6,323	100.0	11.10	11.10	85.7
Lavras	99,846	90.6	132.32	119.88	100.0
Ribeirão Vermelho	3,748	100.0	3.59	3.59	0.0
JAR Basin					
Oliveira	37,301	100.0	50.77	50.77	10.0
Santana do Jacaré	4,623	100.0	12.72	12.72	0.0
Santo Antônio do Amparo	16,297	100.0	18.18	18.18	33.0
São Francisco de Paula	4,678	100.0	26.96	26.96	0.0
Peixe River Basin					
São Tiago	8,791	63	11.00	6.96	62.5
Low Mortes River Basin					
Bom Sucesso	14,494	99.8	21.14	21.09	100.0
Ibituruna	2,598	100.0	3.01	3.01	0.0
Carandaí River Basin					
Carandaí	20,016	100.0	41.21	41.21	0.0
Lagoa Dourada	7,343	90.0	27.75	24.97	0.0
Cervo River Basin					
Carmo da Cachoeira	9,228	84.5	11.23	9.49	0.0
São Bento do Abade	4,953	100.0	6.98	6.98	0.0

Q_{med}, average sewage flow. Source: SNIS (2021).
[a]Regarding the volume of sewage collected.

The integration of Equation (1) leads to the formula for calculating the concentration of coliforms in rivers after a time t:

$$N = N_0.e^{-Kb.t} \tag{2}$$

where N_0 is the coliform count at the starting point of the mix ($t = 0$) (MPN (100 mL)$^{-1}$); N is the coliform count after time t (MPN (100 mL)$^{-1}$); K_b is the bacterial decay rate (day^{-1}); and t is the time (day).

The mortality of microorganisms in different water bodies is generally associated with different K_b values, depending on the nature of the organism and the conditions in the aquatic environment (Arceivala 1981). Due to the dependence of several factors, the K_b values obtained in different studies in freshwater vary over a wide range. Typical values, however, are in the range of $K_b = 0.5$ a 1.5 day^{-1} (base e, 20 °C), with 1.0 day^{-1} being commonly adopted (Arceivala 1981; Thomann & Mueller 1987).

The effect of temperature on the bacterial decay coefficient can be formulated as in the following equation:

$$K_{bT} = K_{b20}.\theta^{(T-20)} \tag{3}$$

where θ is the temperature coefficient, with the value 1.07 being commonly adopted (Thomann & Mueller 1987).

2.3. River data

The flow rate considered for the dilution of wastewater into receiving bodies was the minimum, average of seven consecutive days, for a recurrence time of 10 years ($Q_{7,10}$), according to the legislation of the State of Minas Gerais (Minas Gerais 2008).

To obtain the $Q_{7,10}$, at each point of the basin watercourses, Equation (4) was used, which relates the referred flow to the upstream drainage area. This equation was obtained by the Hidrotec tool (UFV 2009), made available by the Federal University of Viçosa – UFV, which carried out hydrological studies for the 12 fluviometric stations within the basin (Figure 1).

$$Q_{7,10} = 0{,}00686 \ . A^{0{,}9495} \tag{4}$$

where $Q_{7,10}$ is the minimum flow rate, an average of seven consecutive days, for a recurrence time of 10 years (m^3 s^{-1}); A is the drainage area upstream of the point (km^2).

In this way, the flow rate of the receiving bodies was updated for each segment considered, according to its drainage area. Table 2 shows the total $Q_{7,10}$ for each of the 10 subbasins.

In order to define the velocities to be adopted in the work, regression analysis was carried out for the historical series of the 12 existing fluviometric stations within the basin. Data from the last 10 years of monitoring were considered for the dry period (April–September). Thus, equations were defined that relate the runoff flow with the watercourse velocity, for all the

Table 2 | Drainage area and $Q_{7,10}$ by subbasin

Subbasin	Area (km^2)	$Q_{7,10}$ (m^3 s^{-1})
Cervo River	1,105.0	5.32
Elvas River	866.6	4.22
Barba-de-lobo River	562.9	2.80
High Mortes River	1,816.6	8.53
Low of High Grande River	712.2	3.51
Carandaí River	676.2	3.34
Low Mortes River	1,210.8	5.80
Peixe River	511.6	2.56
Middle Mortes River	960.2	4.66
JAR	2,111.4	9.84

Source: UFV (2009).

subbasins studied. Figure 2 presents, as an example, the regression analysis for the fluviometric station FLU1, located at the upper Mortes River, close to its headwaters.

Regarding quality data, data from 11 surface water quality monitoring stations (Figure 1) operated by the *Instituto Mineiro de Gestão das Águas* (Minas Gerais Water Management Institute) – IGAM were used, with quarterly analysis and historical series since 1997 for the variables thermotolerant coliforms and temperature (IGAM 2022), and six stations operated by the National Water Agency – ANA, with data only on temperature (ANA 2022), with average values for the last 5 years during the dry season (April–October), shown in Table 3.

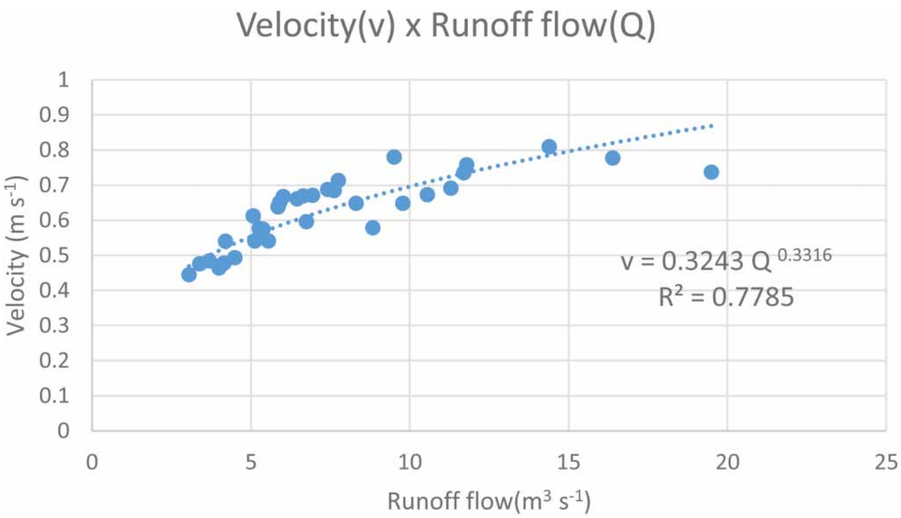


Figure 2 | Regression analysis, FLU1 river gauging station, High Mortes River.

Table 3 | Average values for model-related variables at monitoring stations (data of the last 5 years in the dry season)

	Variables	
Quality station	**Thermotolerant coliforms (MPN (100 mL)$^{-1}$)**	**Temperature (°C)**
BG – 08	1.68×10^4	17.1
BG – 11	3.65×10^3	16.4
BG – 12	5.92×10^2	17.1
BG – 13	2.76×10^4	18.3
BG – 14	9.86×10^2	17.8
BG – 15	1.15×10^4	18.9
BG – 17	4.74×10^2	17.7
BG – 18	5.58×10^2	17.4
BG – 19	2.17×10^3	20.7
BG – 20	2.44×10^3	20.5
BG – 21	3.03×10^3	20.0
A – 01	–	21.2
A – 02	–	18.9
A – 03	–	18.4
A – 04	–	17.9
A – 05	–	16.3
A – 06	–	18.1

MNP, most probable number; BG, IGAM stations; A, ANA stations.

The data presented in Table 3 were used in the calibration of the model, for $Q_{7.10}$.

None of the quality stations with data on thermotolerant coliforms are located in upstream stretches of watercourses, in places with little or no human intervention. Thus, in defining the head values for the modeled watercourses, it was decided to assume the upper limit of Class 1 (Minas Gerais 2008), that is, 200 MPN $(100\ \mathrm{mL})^{-1}$. Therefore, this was the value considered for the river, immediately before the first discharge of sanitary sewage, in all modeled watercourses.

2.4. Model calibration

Model calibration is one of the most important parts of the process. It is at this moment that the coefficients are adjusted, aiming to bring the quality data obtained closer to the data found in the monitoring stations (Gomes *et al.* 2018; Lima *et al.* 2018). In the present work, the Coefficient of Determination – CD was used, which consists of the ratio between the sum of the squared residuals and the total variance of the observed data, according to Equation (5):

$$\mathrm{CD} = 1 - \frac{\sum (Y_{\mathrm{obs}} - Y_{\mathrm{est}})^2}{\sum (Y_{\mathrm{obs}} - Y_{\mathrm{obsméd}})^2} \quad (5)$$

where Y_{obs} is the observed value; Y_{est} is the estimated value; and $Y_{\mathrm{obsméd}}$ is the mean of observed values.

The performance of a model is considered adequate and good if the CD value exceeds 0.75 and it is considered acceptable if the CD value is between 0.36 and 0.75 (Collischonn 2001). According to Thomann & Mueller (1987), the adequacy of the model will be as good as the CD value approaches 1. Calibration was performed using the Excel Solver tool, seeking to maximize CD, varying the model coefficients within the ranges reported in the literature.

The values adopted for K_{b}, for the various modeled watercourses after calibration, are presented in Table 4.

CD = 0.989 (with a relative error of 1.75%) was obtained, which shows an adequate performance.

In Figure 3, it is possible to verify the comparison between the observed and estimated values, for the monitoring stations located in the Mortes River subbasin, which includes 7 of the 10 studied subbasins. We can verify the good adequacy of the model for thermotolerant coliforms.

2.5. Verification of the longitudinal dispersion effects

To define whether the effect of longitudinal dispersion can be neglected in the simulation of the concentration of a constituent that decays according to first-order kinetics, with a decay rate K (as is the case of the present model), EPA (1985) presents the relationship expressed in Equation (6).

$$D_{\mathrm{L}} < \frac{0.04\ .\ v^{2}}{K} \quad (6)$$

where D_{L} is the coefficient of longitudinal dispersion ($\mathrm{m^2 \cdot day^{-1}}$); v is the average horizontal velocity ($\mathrm{m \cdot s^{-1}}$); K is the decay rate ($\mathrm{day^{-1}}$).

If the expression is true, it means that the concentration profile will not be affected by more than 10% if dispersion is ignored.

Values were calculated for the right portion of Equation (6) for all subbasins under study. The lowest value found (worst situation) was $1.5 \times 10^{6}\ \mathrm{m^2 \cdot h^{-1}}$, in the Peixe River subbasin ($v = 0.31\ \mathrm{m \cdot s^{-1}}$ and $K_{\mathrm{b}} = 1.0\ \mathrm{day^{-1}}$).

Table 4 | Bacterial decay rate – kb adopted in the model after calibration

	Subbasin[a]									
Coefficient	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
K_{b} ($\mathrm{day^{-1}}$)	1.0	1.0	1.0	1.5	1.0	1.0	1.5	1.0	1.3	1.1

[a]1 – High Mortes River; 2 – Elvas River; 3 – Carandaí River; 4 – Middle Mortes River; 5 – Peixe River; 6 – Barba-de-Lobo River; 7 – Low Mortes River; 8 – Low of the High Grande River; 9 – Cervo River; 10 – JAR.

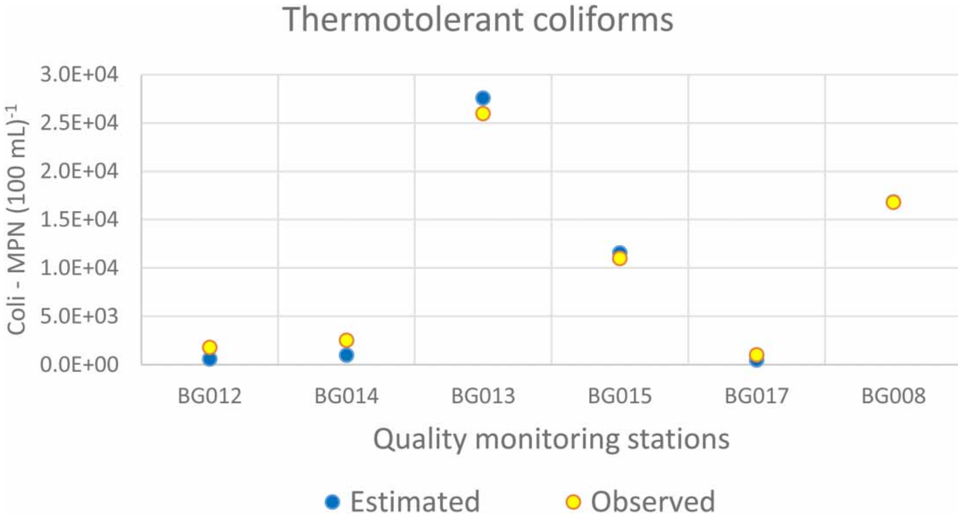


Figure 3 | Comparison between observed and estimated values, Mortes River Subbasin.

According to Arceivala (1981), typical L_D values for larger water courses and rivers are between 10^3 and 10^5 $m^2{\cdot}h^{-1}$. Therefore, as the value found (in the worst situation) is above the D_L value, it is assumed that the expression is true and that the longitudinal dispersion can be neglected.

2.6. Probabilistic model, uncertainty and sensitivity analysis

In mathematical models of water quality, there are uncertainties in the determination of input data that can significantly alter the expected results, which can lead to wrong decisions (Costa & Teixeira 2011; White *et al.* 2021). Thus, it is necessary to identify the input variables that directly affect the uncertainty of the output results of the simulation model (De Menezes *et al.* 2016; Koo *et al.* 2020; Soares & Calijuri 2021). There are many sources of inaccuracy in the modeling process, for example, those related to the estimation of coefficients, input data and system structure (Lindenschmidt & Fleischbein 2007; Khorashadi Zadeh *et al.* 2022). According to von Sperling (2014b), the uncertainty analysis allows, in addition to expressing the results in probabilistic terms, the sensitivity analysis of the model's response to the input data, allowing inferences about the importance of a given parameter or variable.

2.6.1. Uncertainty analysis and probabilistic model

In the present work, the Monte Carlo simulation technique was used (Beck 1987), which has been widely applied in the uncertainty analysis of mathematical models in general (Brum *et al.* 2022). It is based on running a large number of simulations (which can reach thousands). In each simulation of the model, a different set of values of the input data about which there is uncertainty is selected. Each value is randomly generated, according to its distribution and within a pre-specified range. The results obtained are later statistically analyzed, generating results in terms of probability (Kroese *et al.* 2014).

In obtaining random input data, the 'random' Excel function was used for each input parameter of the model that was considered to have significant variation (Equation (6)). Due to its conceptual simplicity, the uniform distribution was used:

$$\text{Value} = \text{Minimum value} + \text{RANDOM}()*(\text{Maximum value} - \text{Minimum value}) \quad (7)$$

The minimum and maximum values were obtained, respectively, through Equations (7) and (8).

$$\text{Minimum value} = \text{Average}*(1 - \text{Percentage of variation}/100) \quad (8)$$

$$\text{Minimum value} = \text{Average}*(1 + \text{Percentage of variation}/100) \quad (9)$$

For each set of random data generated, the model was run and output data were produced, which were stored in new spreadsheets. A thousand simulations were carried out, with the help of an extension, implemented at QUAL-UFMG, in (visual basic for applications (VBA)), as proposed by Brum *et al.* (2022), generating results that can be analyzed probabilistically.

Table 5 presents the input data that suffered variation, with the respective percentages considered and justifications/references.

2.6.2. Sensitivity analysis

Along with uncertainty analysis, sensitivity analysis is of crucial importance in the use of water quality models, especially when applied to water resource management. This consists of evaluating the influence of each input variable on the model's output data (Soares & Calijuri 2021). In this way, it is possible to verify which variables are more important and deserve greater investment in obtaining more accurate data (Saltelli *et al.* 2021; Khorashadi Zadeh *et al.* 2022).

The results generated in the 1,000 Monte Carlo simulations were used, applying the regionalized sensitivity analysis, as initially proposed by Spear (1980). Initially, the raw input data were separated into two samples. The first aggregated the values of the coefficients (and other input data) whose rounds generated the 50% highest values of maximum thermotolerant coliforms and the other gathered the other simulations. Then, the samples were compared to verify if they would be significantly different, using the '*t*' test for dependent samples, with a significance level of $\alpha = 0.05$. The test was performed for all model input data that showed variation. Those data that obtained a value of $p \leq 0.05$ (hypothesis test) were considered important for the process, that is, the model is sensitive to them.

The calculation process was also automated with the help of the extension in VBA proposed by Brum *et al.* (2022).

2.7. Modeled scenarios

After its calibration, the model was used to make deterministic and probabilistic simulations for the four scenarios proposed below, always considering the $Q_{7,10}$ of the receiving body. In the first scenario (C-01), the current populations, current flows and levels of sewage collection and treatment were considered, as shown in Table 1 (SNIS 2021). In the future scenario (C-02), the urban populations of the municipalities were projected for 2033 (Table 6) and the current rates of sewage collection and treatment were maintained (Table 1). In the population projection calculations, data from the last two Brazilian demographic censuses, 2000 and 2020, were considered (IBGE 2022) and a geometric progression was applied to obtain the population in 2033.

The third scenario (C-03) consisted of considering the urban populations projected for the year 2033 and a value of 90% for sewage collection and treatment, as determined by the Sanitation Legal Framework (Brasil 2020).

The standard for effluent discharge in Brazil does not include organisms that indicate fecal contamination (Brasil 2005; Minas Gerais 2008), only establishing that the discharge of effluents cannot give the receiving body adverse characteristics

Table 5 | Input data of the probabilistic model with uncertainty

Variable	Symbol	Average value	Variation (%)	Justifications/references
Sanitary sewage released				
Flow rate	Q e	VAR*	10	SNIS (2021)
Thermotolerant coliforms	Coli e	10^6 MPN (100 m L)$^{-1}$	50	50% around the value obtained in calibration
Receiving body upstream of the sewage release				
River discharge	Q r	VAR	10	UFV (2009)
Thermotolerant coliforms	Coli r	2×10^2 MPN (100 m L)$^{-1}$	100	100% around the limit value of class 1
Along the receiving body				
Velocity	V r	VAR	20 a 50	According to the R2 found in the regression
Temperature	T r	VAR	10	Historical variation of monitoring data from the nearest quality station (IGAM 2022)
Model coefficient				
Bacterial decay rate	K_b	1,00 day^{-1}	50	Arceivala (1981), Thomann & Mueller (1987), Von Sperling & Von Sperling (2013)

VAR, variable.

Table 6 | Urban population by municipality 2020/2033

Municipality	Year 2020	Year 2033	Municipality	Year 2020	Year 2033
Alfredo Vasconcelos	4,632	7,118	Oliveira	37,301	43,103
Antônio Carlos	8,069	14,808	Prados	6,423	8,857
Barbacena	126,477	148,379	Resende Costa	9,280	12,112
Barroso	20,236	22,193	Ressaquinha	3,091	4,666
Bom Sucesso	14,494	15,505	Ribeirão Vermelho	3,748	4,137
Carandaí	20,016	25,288	Ritápolis	3,156	3,198
Carmo da Cachoeira	9,228	13,407	Santa Cruz de Minas	8,664	10,145
Conceição da Barra de Minas	2,787	3,087	Santa Rita do Ibitipoca	2,120	2,439
Coronel Xavier Chaves	1,876	2,360	Santana do Jacaré	4,623	5,103
Dores de Campos	9,297	12,363	Santo Antônio do Amparo	16,297	18,158
Ibertioga	3,439	4,204	São Bento do Abade	4,953	6,793
Ibituruna	2,598	4,157	São Francisco de Paula	4,678	6,038
Ijaci	6,323	11,642	São João Del-Rei	85,556	95,787
Lagoa Dourada	7,343	9,273	São Tiago	8,791	11,337
Lavras	99,846	129,189	Tiradentes	6,234	9,659

according to its framework class. As there is no disinfection in the treatment systems already implemented and the environmental legislation does not explicitly require its implementation, it was decided to consider, in the first three scenarios, the removal of only 90%, compatible with natural sewage treatment systems (Von Sperling 2014a; Mailler *et al.* 2021). Finally, the fourth scenario (C-04) refers to the deterministic model to find the necessary efficiencies for removing thermotolerant coliforms, so that the proposed framework for the basin (CBH-GD2 2018), illustrated in Figure 1, would be reached, considering the population of 2033. The limit values for the watercourse to be in each class are presented in Table 7.

2.8. Analysis of the impact of the framework within environmental licensing

In Brazil, especially in the state of Minas Gerais, licensing environmental bodies have as a rule not to allow new discharges of effluents (even treated ones) in watercourses where the current condition is out of the framework class. Thus, the present work aims to identify the stretches of rivers where this occurs for the four scenarios studied, where the implementation of enterprises generating liquid effluents, which should be discharged there, would not be authorized.

3. RESULTS

3.1. Results of the deterministic model

In this approach, the input data of the model were fixed, being the average values for the characteristics of sanitary sewages and rivers and the values found in the calibration process for the model coefficients, as described in items 2.1–2.8.

Figure 4 presents the expected conditions for the basin, for each of the four studied scenarios, for the variable thermotolerant coliforms, according to the four framework classes.

Table 7 | Limits for thermotolerant coliforms in each framing class

Variable	Framing class 1	2	3	4
Thermotolerant coliforms (MPN 100 mL^{-1})[a]	≤200	≤1,000	≤4,000	–

[a]In 80% or more of at least six samples collected during the period of 1 year, on a bimonthly basis.
Source: Brasil (2005) and Minas Gerais (2008).

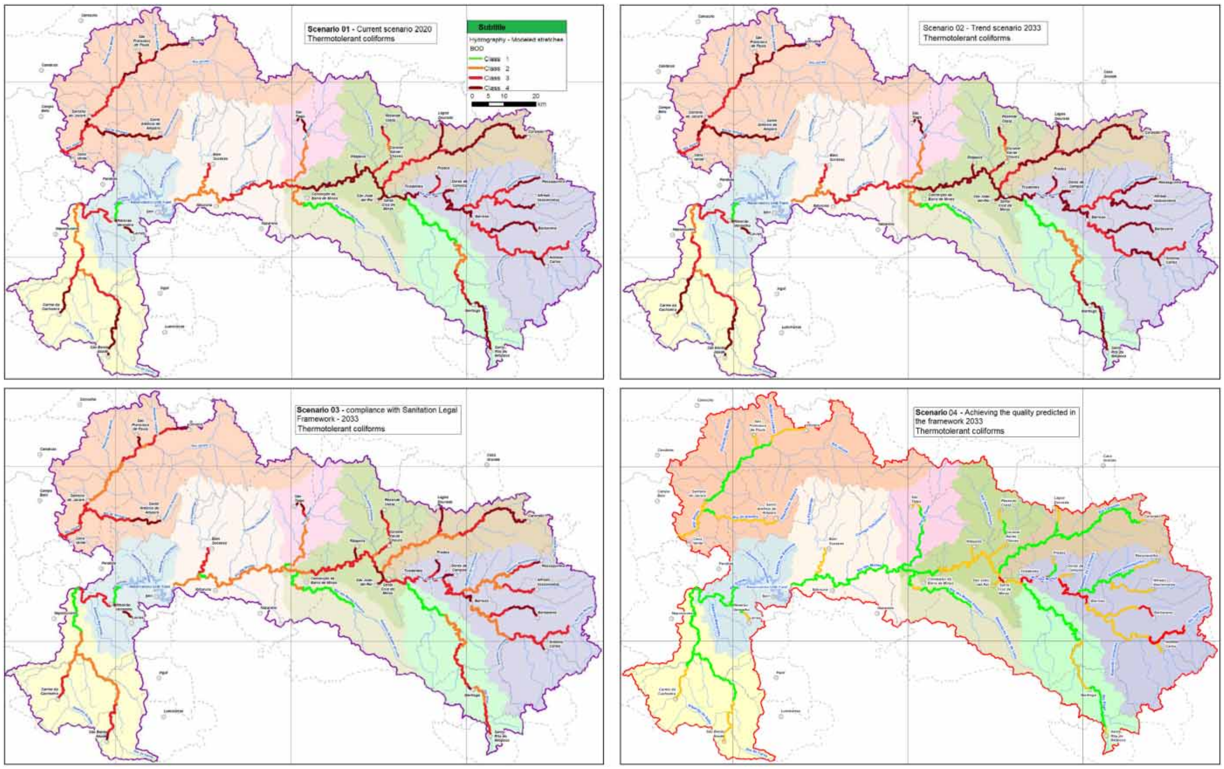


Figure 4 | Conditions for the basin, for each of the four scenarios studied, for the thermotolerant coliforms variable and according to the four framing classes. Fonte: adaptado de IGAM (2013).

For Scenarios 1 and 2, we can verify a predominance of the condition of the watercourses in Classes 3 and 4, with Class 4 being observed almost exclusively downstream of the sanitary sewage discharge points. This fact brings a special health concern since it makes the use of water for nobler uses, such as primary contact recreation and irrigation of vegetables that are consumed raw, not recommended (Brasil 2005; Minas Gerais 2008). This is a direct consequence of the release of municipal sanitary discharges without treatment or with insufficient treatment, making the water unfit for most uses, from a sanitary point of view, for long stretches.

A different situation only occurs in the lower reaches of some watercourses, such as the Elvas, Pirapetinga, Peixe and Cervo Rivers, where the large drainage area and the distance from the discharge point favor improvement of water quality. This fact shows the importance of the dilution ratio, which comes with the increase in the flow of the watercourse and the phenomenon of bacterial decay in water quality, which should always be important factors to be considered in the management of water resources.

A significant improvement can be observed in Scenario 3, with compliance with the sanitation legal framework (Brasil 2020), especially for the main bed of the Mortes River. However, this improvement is not enough to meet the proposed framework for the basin and consequently, the current and future uses of water (CBH-GD2 2018). This fact proves that even the universalization of sewage collection and treatment, if tertiary treatment with disinfection is not foreseen, is not enough, in the vast majority of cases, to safeguard the quality of the receiving bodies, from the point of view of indicator organisms of fecal contamination. Secondary treatment may only be sufficient in very specific situations, where we have a low discharge flow and a high receiving body flow, providing high dilution ratios. This can be proven, for example, by the launch of the urban headquarters of Ibituruna in the main bed of the Mortes River.

As can be seen in Table 8 and Figure 5, the main bed of the Mortes River is found, for the first two scenarios, for the most part, within Classes 3 and 4. Class 2 appears only downstream from Ibiturana, on the lower Mortes River, close to its mouth next to Funil Lake. These data confirm what has also been verified by Amâncio *et al.* (2018), the poor microbiological quality of the subbasin, affected by diffuse and, above all, punctual pollution (domestic discharges).

Table 8 | Percentage of extension of the main bed of the Mortes River within the framework classes for the thermotolerant coliforms variable

	Scenario			
Class	C- 01	C-02	C-03	C-04
1	–	–	1.2	31.7
2	10.4	6.8	41.8	37.1
3	42.2	40.6	51.8	31.3
4	47.4	52.6	5.2	–

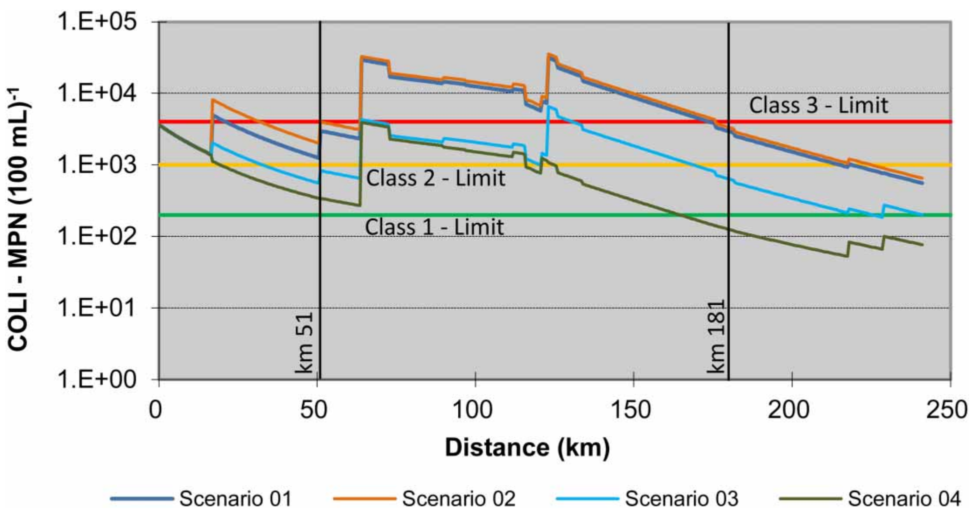


Figure 5 | Longitudinal profiles (thermotolerant coliforms) for the four scenarios studied – Mortes River.

The main bed of the Mortes River is framed (CBH-GD2 2018) between km 51 (confluence with the Caieiros stream) and km 181 (confluence with the Peixe River), in Class 3, with the remainder being Class 2.

For Scenario 3, which aims to meet the Sanitation Legal Framework (Brasil 2020), we can see significant improvement for the main bed of the Mortes River. Non-compliance with the classification only occurs only in two short stretches: just downstream of Bandeirinha Stream (with discharges from Antônio Carlos – km 17) and then downstream of Água Limpa Stream (with discharges from São João Del-Rei – km 123). Unfortunately, this situation is not repeated in the other watercourses modeled in the basin, where the actions proposed in Scenario 3 will not be sufficient to meet the framework.

Table 9 presents the sections with a situation that does not comply with the proposed framework, according to the studied scenarios.

As an example, Figure 6 shows the longitudinal profiles for the Amparo River, which receives sewage from the municipality of Santo Antônio do Amparo. A similar situation occurs in all watercourses that receive sanitary discharges near their headwaters, where the dilution flow of the discharges is low.

We can see that, in Amparo River, compliance with the framework (Class 2) will only occur in Scenario 4. In Scenarios 1 and 2, almost the entire length of the watercourse would be in Class 4. In Scenario 3, we would have Class 4 until close to km 10 and Class 3 up to its mouth on JAR.

As stated above, the efficiency of 90% in the removal of thermotolerant coliforms is not enough to comply with the framework in the vast majority of municipalities. According to the results of the deterministic modeling, for C-04 (compliance with compliance), the efficiencies shown in Table 10 would be necessary.

Only the municipalities of Barroso, Conceição da Barra de Minas, Ibituruna, Ijaci, Ribeirão Vermelho, Santana do Jacaré and Tiradentes would not require disinfection to comply with the framework and the efficiency of the removal of thermotolerant coliforms, of the order of 90%, in a secondary treatment would be enough. Some municipalities, such as Ibertioga and

Table 9 | The stretches with a situation at odds with the proposed framework

				Quality condition by scenario			
Municipality	**Watercourse**	**Subbasin**	**Framework**	**C-01**	**C-02**	**C-03**	**C-04**
Antônio Carlos	Bandeirinha	ARM	2	4	4	4,3[a]	2
Barbacena	Caieiros	ARM	3	4	4	4,3	3,2
Ressaquinha	Ressaquinha	ARM	2	4,3	4,3	4,3,2	2,1
Dores de Campos	Patusca	ARM	2	4	4	4	2
Prados	Pinhão	ARM	2	4,3	4,3	4,3	2,1
Carandaí	Carandaí	CAR	2	4,3	4,3	4,3,2	2,1
Lagoa Dourada	Tanque Grande	CAR	2	4	4	4,3	2,1
São João Del-Rei	Água Limpa	MRM	3	4	4	4	2
Resende Costa	Quilombo	MRM	2	4,3,2	4,3,2	4,3,2	2,1
Ritápolis	Paiol	MRM	2	4	4	4	2
Lavras	Ribeirão Vermelho	ABRG	2	4	4	4	2,1
São Bento Abade	Algodão/Cervo	CER	2	4,3,2	4,3,2	4,3,2,1	2,1
Carmo Cachoeira	Carmo/Salto	CER	2	4,3	4,3	3,2	2,1
Oliveira	Maracanã/Lambari	JAR	2	4,3	4,3	4,3,2	2,1
S. F. de Paula	Machadinha	JAR	2	4	4	4	2
S. A. do Amparo	Amparo	JAR	2	4,3	4,3	4,3	2,1

[a]The same watercourse can be in different classes along its length.
ARM, High Mortes River; CAR, Carandaí River; MRM, Middle Mortes River; CER, Cervo River; ABRG, Low of the High Grande River; JAR, Jacaré River.

Ressaquinha need efficiencies of around 99.99%. The urban center of Lavras, on the other hand, would need an efficiency of 99.999% to meet the Class 2 framework of the Vermelho Stream. This is mainly due to the placement of sewage discharges within the basin, in regions with a greater or lesser drainage area and, consequently, a greater or lesser dilution ratio.

The framework is made according to the predominant uses found or foreseen in the basin, reflecting the necessary and, mainly, desired water quality. However, it must be done judiciously, taking into account technical and mainly economic

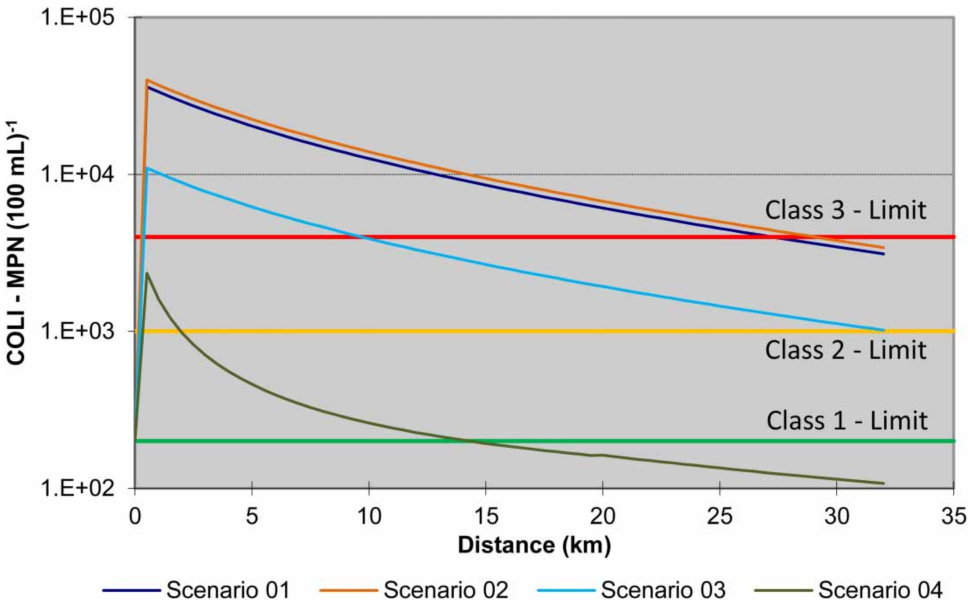


Figure 6 | Longitudinal profiles (thermotolerant coliforms) for the four scenarios studied – Amparo River.

Table 10 | Minimum efficiency to thermotolerant coliforms removal to meet the framework

Municipality	Minimum removal efficiency %	log UN	Municipality	Minimum removal efficiency %	log UN
Alfredo Vasconcelos	99.99	4	Oliveira	99	2
Antônio Carlos	99.99	4	Prados	99.9	3
Barbacena	99.9	3	Resende Costa	99.9	3
Barroso	90	1	Ressaquinha	99.99	4
Bom Sucesso	99.99	4	Ribeirão Vermelho	90	1
Carandaí	99.9	3	Ritápolis	99.9	3
Carmo da Cachoeira	99	2	Santa Cruz de Minas	90	1
Conceição da Barra de Minas	90	1	Santa Rita do Ibitipoca	99.9	3
Coronel Xavier Chaves	99	2	Santana do Jacaré	90	1
Dores de Campos	99.9	3	Santo Antônio do Amparo	99	2
Ibertioga	99.99	4	São Bento do Abade	99	2
Ibituruna	90	1	São Francisco de Paula	99.9	3
Ijaci	90	1	São João Del-Rei	99.9	3
Lagoa Dourada	99.9	3	São Tiago	99.9	3
Lavras	99.999	5	Tiradentes	90	1

criteria related to the treatment of sanitary sewage, under penalty of imposing heavy burdens on municipalities (mainly smaller ones) and sanitation companies. An example is the small municipality of Ressaquinha, which would need 99.99% efficiency in coliform removal, in addition to universal sewage collection and treatment, to comply with the framework. It should be evaluated on a case-by-case basis, bearing in mind the real and necessary uses of each stretch, as well as the existing releases of evictions and the economic capacities of each municipality. If necessary, the uses can be reviewed or even intermediate goals created. This is of fundamental importance in Brazil and other developing countries, where investments in sanitation are very limited.

3.2. Results of the probabilistic model/uncertainty analysis

In this item, the results of the probabilistic modeling will be presented. Longitudinal profiles were generated for all simulations performed, creating uncertainty band graphs (Brum *et al.* 2022). Due to Excel's technical limitations, for these graphs, the profiles were presented only for the first 250 simulations (out of 1000 Monte Carlo simulations).

In calculating the probability (P) of compliance with the classification, Equation (10) was used.

$$P = (\text{number of simulations that met the standard}/1{,}000) * 100 \quad (10)$$

The Brazilian environmental legislation (Brasil 2005; Minas Gerais 2008), in general, does not deal with the discharge standard and compliance with the framework in a probabilistic way. Analyses are usually made in absolute terms, such as attendance and non-attendance. Also, no bibliographical references were found to guide acceptable values for the probability of meeting the framework. In this way, it is up to the water resources manager, based on their reality and the risks they are willing to assume, to define the probability of meeting the framework in which they will work. Here is an interesting knowledge gap to be filled in future studies.

In the specific case of the thermotolerant coliforms variable, the legislation (Minas Gerais 2008) determines that the class limit should not be exceeded by at least 80% of at least six annual samples, with a bimonthly frequency. Thus, in the absence of other references, it can be assumed that the probability of meeting the framework, for this parameter in question, will be accepted if it is at least 80%.

In Figures 7 and 8, respectively, uncertainty band graphs are presented, for the longitudinal profiles of thermotolerant coliforms, along the main beds of the Mortes and Amparo Rivers.

We can verify that up to km 17, where it receives Bandeirinha Stream with discharges from Antônio Carlos, the probability (P) of Class 2 compliance is 100%, for the four studied scenarios. After this first significant discharge of sanitary sewage, meeting the framework is compromised, for the first three scenarios, but mainly for the first two, where the probability of meeting the framework, right after the confluence, is nil. For the third scenario, this probability is around 50%.

The probability of complying with the framework varies downstream, as phenomena related to bacterial decay occur and new discharges of sanitary sewage happen. A little downstream, just after the confluence with Caieiros Stream, bringing sewage from Barbacena, the compliance probabilities are approximately 60% for C-01 and C-02 and 100% for C-03.

In general, the probabilities of compliance with the framework for Scenarios 1 and 2 are practically nil, with some short stretches where there is some probability of compliance.

Regarding C-03, we can verify that it will not be enough for the entire length of the Mortes River. Right at the confluence with the Bandeirinha Stream (km 17), the probability of compliance is only 32.8%. At km 64, where it receives sewage from Barroso, the probability of compliance is only 44.5%. At the confluence with the Água Limpa Stream, carrying sewage from São João Del-Rei, the probability of compliance is only 6.7%. Thus, treatment efficiencies for the Municipalities of Antônio Carlos, Barroso and São João Del-Rei should be greater. Right after the confluence with the Peixe River, the probability is 76.1%.

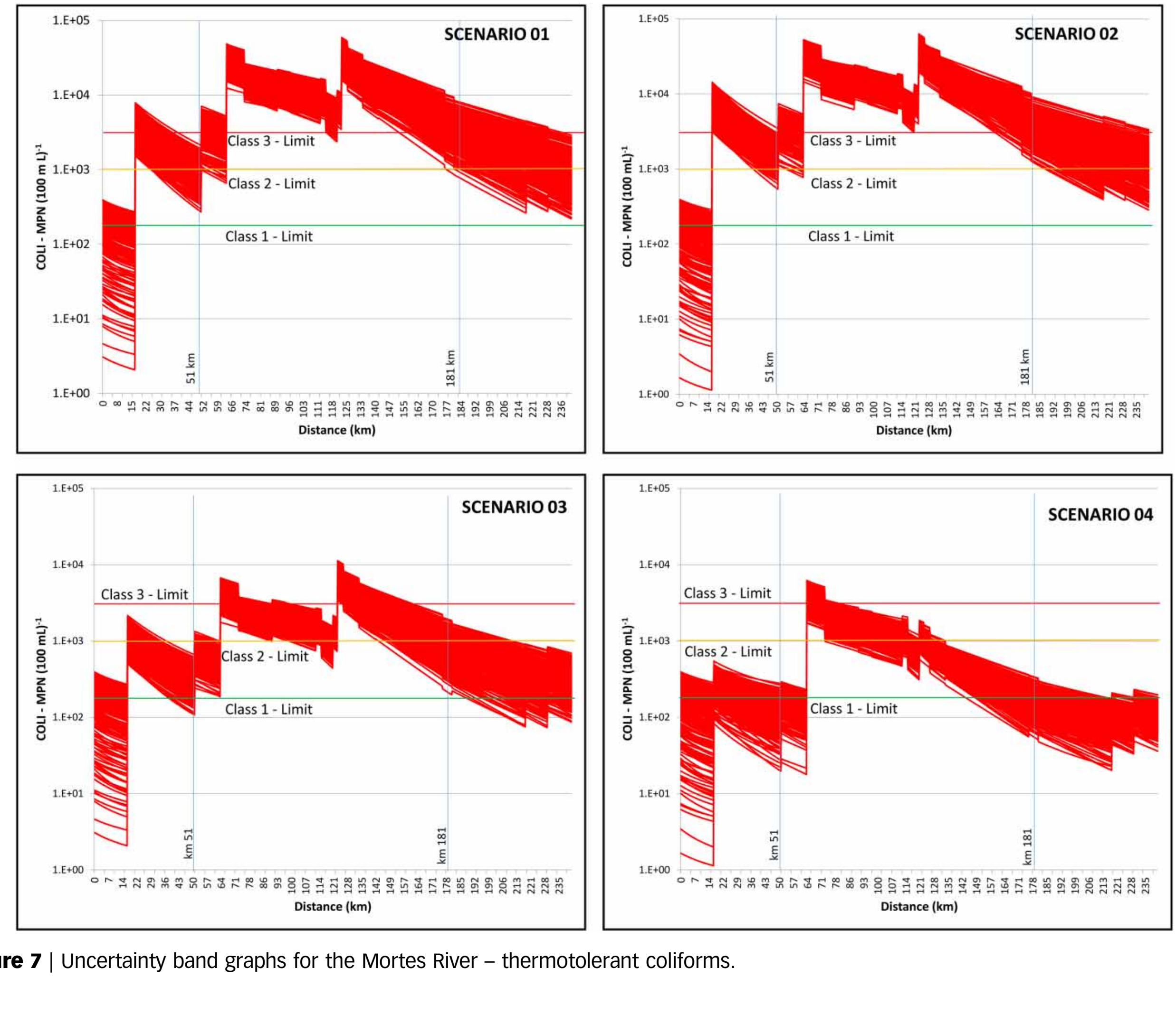


Figure 7 | Uncertainty band graphs for the Mortes River – thermotolerant coliforms.

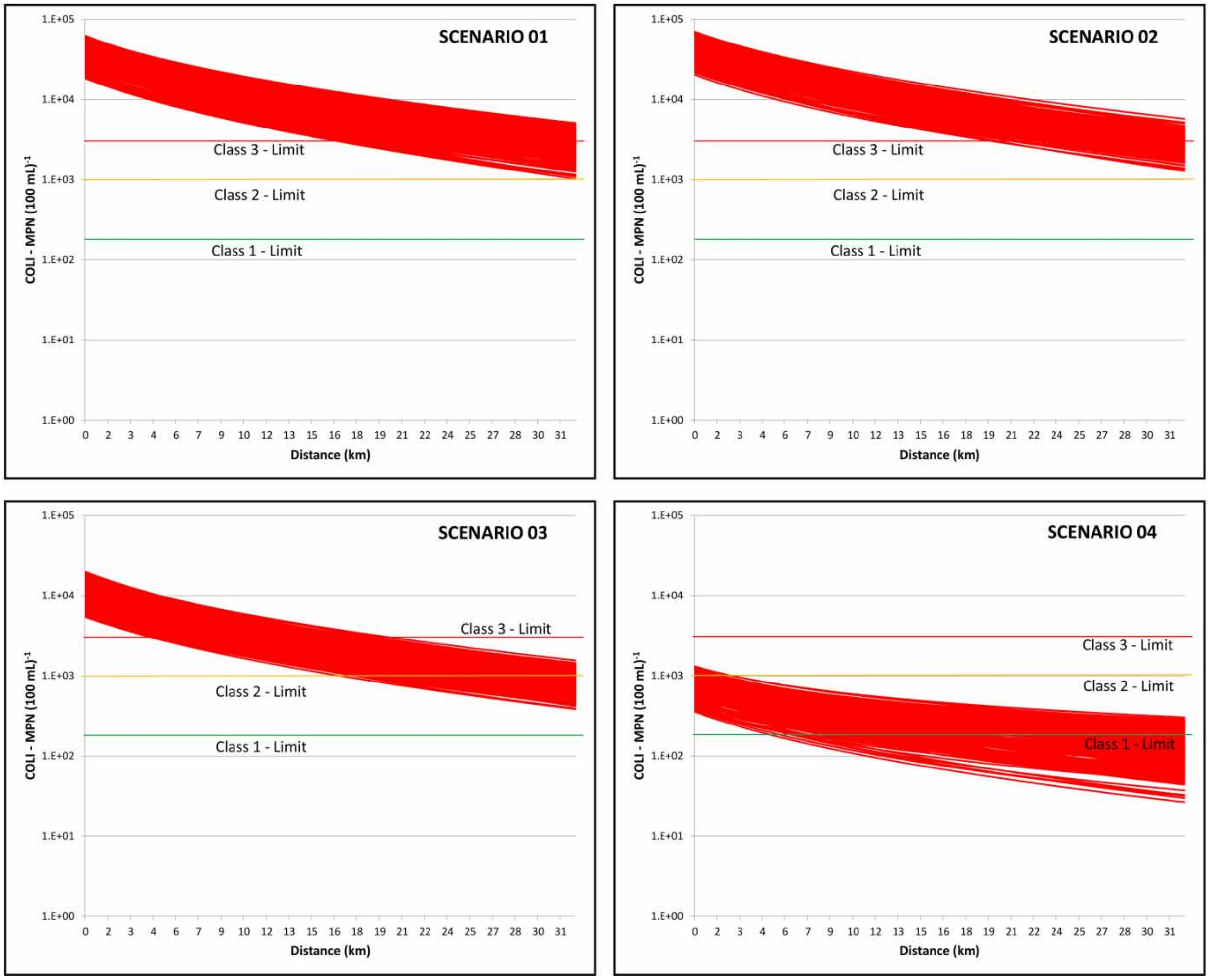


Figure 8 | Uncertainty band graphs for the Amparo River – thermotolerant coliforms.

In Scenario 4, we have a 100% probability of compliance for almost the entire length of Rio Mortes. The only exception is just downstream from the urban center of Barroso, where the probability of compliance is 57.1%, but which returns to 100% just 9 km downstream.

For the Amparo River, which receives the discharges from the urban center of Santo Antônio do Amparo, the probability of meeting the framework (Class 2) is nil, in the first two scenarios, in all its extension. In Scenario 3, there is some probability of compliance starting at km 15.6, reaching 50% at km 28.9 and a maximum of 70.2% at its mouth, at km 32.

As for Scenario 4, we have 89.1% just downstream of the discharge point, reaching 100% 2.65 km downstream.

Table 11 presents a summary of the results of the probabilistic model, for all modeled watercourses, according to each scenario.

We can see that the probability of complying with the framework, for C-01 and C-02, except for the Barba- de-Lobo River, is zero for all watercourses, which shows the poor quality of the water from a sanitary point of view. As phenomena related to bacterial decay occur, the situation improves downstream. Pinhão, Quilombo, Elvas, Sujo, Pirapetinga and Algodão watercourses have a 50% probability of compliance a few kilometers downstream. Only Quilombo, Elvas and Sujo watercourses, due to their large extensions, manage to reach a 100% probability of compliance. Barba-de-Lobo River has excellent sanitary quality, even receiving discharges from Conceição da Barra de Minas, which treats only 71.8% of its sewage, without disinfection, due to its great dilution capacity, which does not occur in the rest of the watercourses. The

Table 11 | Summary of probabilistic model results

	Scenario 01			**Scenario 02**			**Scenario 03**			**Scenario 04**		
Watercourse	***P***	**km 50%**	**km 100%**	***P***	**km 50%**	**km 100%**	***P***	**km 50%**	**km 100%**	***P***	**km 50%**	**km 100%**
High Mortes River Basin												
Bandeirinha	0.0	–	–	0.0	–	–	0.0	–	–	80.0	–	–
Caieiros	0.0	–	–	0.0	–	–	0.0	13.0	–	83.3	–	1.4
Loures	0.0	–	–	0.0	–	–	0.0	17.2	–	52.7	–	12.9
Ressaquinha	0.0	–	–	0.0	–	–	0.0	13.2	–	87.0	–	1.4
Patusca	0.0	–	–	0.0	–	–	0.0	–	–	100.0	–	–
Pinhão	0.0	7.7	–	0.0	8.2	–	0.0	8.2	–	100.0	–	–
Barba-de-lobo River Basin												
Barba-de-Lobo	100.0	–	–	100.0	–	–	100.0	–	–	100.0	–	–
Middle Mortes River Basin												
Água Limpa	0.0	–	–	0.0	–	–	0.0	–	–	100.0	–	–
Quilombo	0.0	7.7	14.9	0.0	9.2	–	0.0	14.8	–	100.0	–	–
Paiol	0.0	–	–	0.0	–	–	0.0	–	–	100.0	–	–
Elvas River Basin												
Elvas	0.0	27.6	51.5	0.0	29.4	55.5	0.0	7.3	48.7	100.0	–	–
Low of the High Grande River												
Ribeirão Vermelho	0.0	–	–	0.0	–	–	0.0	–	–	100.0	–	–
Rio Grande	0.0	–	–	0.0	–	–	0.0	–	–	100.0	–	–
JAR Basin												
Maracanã/Jacaré	0.0	–	–	0.0	–	–	0.0	14.5	49.4	10.6	1.5	2.6
Machadinha	0.0	–	–	0.0	–	–	0.0	–	–	100.0	–	–
Amparo	0.0	–	–	0.0	–	–	0.0	28.9	–	89.1	–	2.7
Peixe River Basin												
Sujo/Peixe	0.0	9.0	34.6	0.0	10.7	–	0.0	9.0	13.4	100.0	–	–
Low Mortes River												
Pirapetinga	19.6	8.1	–	15.2	9.9	–	15.2	9.9	–	82.7	–	5.6
Carandaí River Basin												
Carandaí	0.0	–	–	0.0	–	–	0.0	43.3	–	100.0	–	–
Tanque Grande	0.0	–	–	0.0	–	–	0.0	–	–	97.9	–	0.8
Cervo River Basin												
Algodão/Cervo	0.0	27.9	–	0.0	32.3	–	0.0	12.1	23.0	37.2	0.7	2.0
Salto	0.0	–	–	0.0	–	–	0.0	9.0	–	100.0	–	–

P, Probability of complying with the framework just downstream of the mixing point (50 m).
km 50%, Distance required, on the river, for a 50% probability of service to occur.
km 100%, Distance required, on the river, for a 100% probability of service to occur.
(–) The watercourse distance is not enough.

$Q_{7,10}$ at the point of discharge is 2,360 L s^{-1}, for a current sewage discharge of 1.8 L s^{-1}, which gives a dilution ratio of 1,311 times. In Scenario 2, we can see a worsening of the situation, with the increase in distances needed for the purification of watercourses to occur.

In Scenario 3, where 90% of the sewage is collected and treated, however, without disinfection, we see that right downstream from the discharge points, the situation of non-compliance with the framework does not change, with zero probability of compliance equal to the first two scenarios. The improvement in water quality can only be seen downstream, reducing the necessary distance to 50 and 100% probability of complying with the framework. However, even in this scenario, some watercourses do not have sufficient distance.

In Scenario 4, where disinfection was considered, with the efficiencies shown in Table 10, we have a 100% probability of meeting the framework, just downstream of the discharge point, in the vast majority of modeled watercourses. Some watercourses have a probability of compliance greater than 80%, which reaches 100% a little downstream, as is the case of Caieiros, Ressaquinha, Amparo, Tanque Grande and Pirapetinga Streams. Even in this scenario, some watercourses showed a low probability of compliance, right downstream of the joining point of Loures (sewage from Alfredo Vasconcelos), Maracanã (sewage from Oliveira) and Algodão (sewage from São Bento do Abate), indicating the need to increase the efficiencies proposed in Table 10 or the implementation of treated sewage outfalls, aiming to carry out the discharge further downstream, where the dilution ratio would be higher.

An interesting situation occurs with the Quilombo Stream, which receives discharges from the urban center of Resende Costa. In Scenario 3, the results for water quality are worse than in Scenarios 1 and 2. We see that, with 90% of sewage collection and treatment, the necessary distance for a 50% probability of meeting the framework is 14.8 km, against 7.7 and 9.2 km in the first two scenarios. This is due to the fact that, in the first two scenarios, there is only 39.4% of sewage collection and the rest is disposed of in sump/sinkhole systems, not being discharged directly into the stream. In Scenario 3, 90% of the collection is considered.

In general, the probabilistic results came to confirm the deterministic model, also showing the precarious current quality of the water, in terms of thermotolerant coliforms, as well as the ineffectiveness of the New Legal Sanitation Framework (Brasil 2020) in meeting the framework of the courses of water in the basin, which will only be achieved with tertiary treatment, with disinfection, in the vast majority of municipalities.

3.3. Analysis of the impact of the framework within environmental licensing

It was found that the current condition of the basin (C-01), as well as Scenarios 2 and 3, present water quality, in terms of thermotolerant coliforms, in disagreement with the proposed framework (CBH-GD2 2018), in the vast majority of modeled stretches. These stretches are problematic for the environmental licensing of enterprises that generate liquid effluents and the State Environmental Agency does not authorize new discharges until compliance with the framework is established.

This is a very delicate issue, as the legislation (Brasil 2005; Minas Gerais 2008) establishes that effluent releases cannot give the receiving body characteristics that are adverse to the class in which it was classified. However, there is no indication of how to proceed when the class is already violated upstream of the release point. The understanding, for the vast majority of analysts of the Environmental Agency, is that under these conditions, new releases of effluents cannot be authorized. This fact brings several inconveniences to undertakings that generate liquid effluents located close to watercourses in this situation.

3.4. Sensitivity analysis

Sensitivity analysis was performed for all model simulations, showing slightly different results for each watercourse studied. As an example, Table 12 presents the results for River Elvas.

Sensitivity analysis was performed for all watercourses studied and in general, the model was sensitive to the variables.

- Flow and thermotolerant coliforms in raw sewage;
- River velocity and temperature;
- Bacterial decay rate – K_b.

Due to the high concentration of thermotolerant coliforms in raw sewage, it was already expected that the model would be very sensitive to this variable, as well as to the discharge flow (De Paoli & Von Sperling 2013; Von Sperling 2014b). The flow velocity of the receiving body also plays an important role, as it is conditioned by the distance at which the necessary decomposition of microorganisms will occur. The temperature, together with the bacterial decay rate – K_b, conditions the velocity with which the decay kinetics will occur (Batista & Harari 2016; Silva *et al.* 2021).

Based on the sensitivity analysis, it is concluded that systematic monitoring of the basin is extremely important, mainly for the quantitative and qualitative characterization of raw sewage. Research is also important in order to reduce the uncertainty in the definition of the coefficient K_b.

Table 12 | Sensitivity analysis for modeling the Elvas River

Variable	Symbol	'p' Value	Important
Sanitary sewage released			
Flow rate	Q e	4.14×10^{-4}	Yes
Thermotolerant coliforms	Coli e	7.54×10^{-3}	Yes
Receiving body upstream of the sewage discharge			
River discharge	Q r	0.105	No
Thermotolerant coliforms	Coli r	0.122	No
Along the receiving body			
Velocity	V r	3.19×10^{-3}	Yes
Temperature	T r	3.86×10^{-54}	Yes
Model coefficient			
Bacterial decay rate	K_b	3.09×10^{-7}	Yes

4. CONCLUSION

Based on the results obtained, it can be concluded that:

- The joint analysis of the deterministic and probabilistic model adopted proved to be an applicable tool for the management of watersheds, especially in Brazil and other developing countries, where the universalization of the collection and treatment of sanitary sewage is not yet a reality, due to its relative simplicity of application.
- The current situation of the basin, in terms of thermotolerant coliforms, is worrying, since almost all of the modeled watercourses, in most of their extensions, are out of their framework class. This has very serious health implications since the current and future uses of the basin's waters are compromised, due to the risk of waterborne diseases. The projection for the year 2033, without forecasting interventions in the basin, further aggravates the scenario, due to population growth.
- The actions proposed in the sanitation legal framework (Brasil 2020), which, despite providing for the obligation of 90% of sewage collection and treatment for all municipalities, are not sufficient to ensure compliance with the framework. This study showed that compliance with the framework, for the variable thermotolerant coliforms, will only be reached with the implementation of tertiary treatment, with disinfection, in the overwhelming majority of municipalities, which is not explicitly provided for in the legislation.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

CONFLICT OF INTEREST

The authors declare there is no conflict.

REFERENCES

Alegbeleye, O. O., Opeolu, B. O. & Jackson, V. A. 2016 Investigation into the bacterial pollution levels at various sites along the Diep and Plankenburg River systems, 3 Western Cape, South Africa. *Water Science and Technology* **73** (11), 2590–2599.

Almeida, F. A. 1979 Estudo de decaimento bacteriano em lagunas do Estado do Rio de Janeiro. 10 Congresso Brasileiro de Engenharia Sanitária – Manaus. Anais. FEEMA, Rio de Janeiro, Brazil.

Amâncio, D. V., Coelho, G., Marques, R. F., de, P. V., Viola, M. R. & De Mello, C. R. 2018 Qualidade da água nas sub-bacias hidrográficas dos rios Capivari e Mortes, Minas Gerais. *Scientia Agraria* **19** (1), 75.

ANA 2009 *Implementação do enquadramento em bacias hidrográficas no Brasil; Sistema nacional de informações sobre recursos hídricos – Snirh no Brasil: arquitetura computacional e istêmica*. Caderno De Recursos Hídricos 6 – Agência Nacional De Águas – ANA, Brasília, Brazil.

ANA – Agência Nacional Das Águas – Ana 2022 Sistema Nacional de Informações de Recursos Hídricos – SNIRH. Disponível Em: https://www.snirh.gov.br/hidroweb/serieshistoricas (Acesso Em 3 January 2022).

Andersson, K., Otoo, M. & Nolasco, M. 2018 Innovative sanitation approaches could address multiple development challenges. *Water Science and Technology* **77** (4), 855–858.

Arceivala, S. J. 1981 *Wastewater Treatment and Disposal. Engineering and Ecology in Pollution Control*. Marcel Dekker, New York, NY, USA.

Ashouri, M. J. & Rafei, M. 2018 Analysis of asymmetries in air pollution with water resources, and energy consumption in Iran. *Environmental Science and Pollution Research* **25** (18), 17590–17601.

Batista, S. S. & Harari, J. 2016 Modelagem da dispersão de coliformes termotolerantes e enterococos em duas enseadas na região costeira de Ubatuba (SP), Brasil. *Engenharia Sanitaria e Ambiental* **22** (2), 403–413.

Beck, M. B. 1987 Water quality modeling: a review of the analysis of uncertainty. *Water Resources Research* **23** (8), 1393–1442.

Bello, A.-A. D. & Haniffah, M. R. M. 2021 Modelling the effects of urbanization on nutrients pollution for prospective management of a tropical watershed: a case study of Skudai River watershed. *Ecological Modelling* **459**, 109721.

Brasil 2005 *Resolução CONAMA no 357, de 17 de março de 2005 - classificação dos corpos de água e diretrizes ambientais para o seu enquadramento*. Diário Oficial Da União, Brasil.

Brasil 2020 *Lei No 14.026, de 15 de julho de 2020 – marco legal do saneamento básico*. Diário Oficial Da União, Brasília.

Brown, L. & Barnwell, T. 1987 *The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and User Manual*. US Environmental Protection Agency. Office of Research and Development. Environmental Research Laboratory, Athens, GA, USA.

Brum, M., Fan, F. M., Salla, M. R. & von Sperling, M. 2022 Analysis of a probabilistic approach for modelling and assessment of the water quality of rivers. *Journal of Hydroinformatics* **24** (4), 783–797.

Bui, H. H., Ha, N. H., Nguyen, T. N. D., Nguyen, A. T., Pham, T. T. H., Kandasamy, J. & Nguyen, T. V. 2019 Integration of SWAT and QUAL2K for water quality modeling in a data scarce basin of Cau River Basin in Vietnam. *Ecohydrology & Hydrobiology* **19** (2), 210–223.

CBH-GD2. 2018 *Deliberação Normativa CBH GD2 No 22, de 13 de agosto de 2018. Enquadramento dos corpos de água da Bacia Hidrográfica do Rio das Mortes – UPGRH GD2*. Comitê Da Bacia Hidrográfica Do Rio Das Mortes, São João Del Rei, Brasil.

Collischonn, W. 2001 Simulação hidrológica de grandes bacias. [S.L.] Tese (Doutorado Em Recursos Hídricos e Saneamento Ambiental) – Universidade Federal Do Rio Grande Do Sul.

Costa, D. 2021 De A. O enquadramento de recursos hídricos como estratégia para melhoria da qualidade da água: o caso do rio piabanha/RJ. [s.l.] Tese (Doutorado em Planejamento Estratégico) – Universidade Federal do Rio de Janeiro (COPPE/UFRJ), Brasil.

Costa, D. J. L. & Teixeira, D. 2011 Análise de incerteza em um modelo matemático de qualidade da água aplicado ao Ribeirão do Ouro, Araraquara, SP, Brasil. *Ambiente e Agua – An Interdisciplinary Journal of Applied Science* **6** (2), 232–245.

De Menezes, J. P. C., De Oliveira, L. F. C. & Salla, M. R. 2016 Incertezas sobre a modelagem matemática de qualidade da água em curso de água Urbano. *Ciencia Y Engenharia/Science and Engineering Journal* **25** (2), 1–8.

De Oliveira Filho, A. A. & Lima Neto, I. E. 2018 Modelagem da qualidade da água do rio poti em teresina (PI). *Engenharia Sanitaria e Ambiental* **23** (1), 3–14.

De Paoli, A. C. & Von Sperling, M. 2013 Avaliação das condições hidrodinâmicas de wetlands de escoamento horizontal subsuperficial (unidades plantada e não plantada). *Revista Eletrônica De Gestão e Tecnologias Ambientais* **1** (2), 213–222.

EPA, U. S. E. P. A. 1985 *Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling*, 2nd edn. United States Environmental Protection Agency, Athens, GA, USA.

Fan, C., Wang, W. & Liu, K. F. 2012 Sensitivity analysis and water quality modeling of a tidal river using a modified Streeter-Phelps equation with HEC-RAS-calculated hydraulic characteristics. *Environ Model Assess* **17**, 639–651.

Ferreira, M. M., Fiore, F. A., Saron, A. & da Silva, G. H. R. 2021 Systematic review of the last 20 years of research on decentralized domestic wastewater treatment in Brazil: state of the art and potentials. *Water Science and Technology* **84** (12), 3469–3488.

Gomes, S. H. R., Guedes, H. A. S., Siqueira, T. M., Corrêa, L. B., Andreazza, R. & Hüffner, A. N. 2018 Modelagem sazonal da qualidade da água do Rio dos Sinos/RS utilizando o modelo QUAL-UFMG. *Engenharia Sanitaria e Ambiental* **23** (2), 275–285.

IBGE – Instituto Brasileiro De Geografia e Estatística 2022 Censos Demográficos Dos Anos De 2000 **e** 2010. Available from: https://www.ibge.gov.br (Acesso Em: 3 January 2022).

IGAM, I. M. De G. Das Á. 2013 *Plano Diretor de Recursos Hídricos da Bacia do Rio das Mortes*. IGAM, Belo Horizonte, Brasil.

IGAM, I. M. De G. Das Á. 2022 Monitoramento de Qualidade das Águas Superficiais. Available from: http://repositorioigam.meioambiente.mg.gov.br/handle/123456789/416 (Acesso Em: 3 January 2022).

Kaufman, D. E., Shenk, G. W., Bhatt, G., Asplen, K. W., Devereux, O. H., Rigelman, J. R., Ellis, J. H., Hobbs, B. F., Bosch, D. J., Van Houtven, G. L., McGarity, A. E., Linker, L. C. & Ball, W. P. 2021 Supporting cost-effective watershed management strategies for Chesapeake Bay using a modeling and optimization framework. *Environmental Modelling and Software* **144** (July), 105141.

Khorashadi Zadeh, F., Nossent, J., Woldegiorgis, B. T., Bauwens, W. & Van Griensven, A. 2022 A fast and effective parameterization of water quality models. *Environmental Modelling and Software* **149** (January), 105331.

Koo, H., Chen, M., Jakeman, A. J. & Zhang, F. 2020 A global sensitivity analysis approach for identifying critical sources of uncertainty in non-identifiable, spatially distributed environmental models: a holistic analysis applied to SWAT for input datasets and model parameters. *Environmental Modelling & Software* **127**, 104676.

Kroese, D. P., Brereton, T., Taimre, T. & Botev, Z. I. 2014 Why the Monte Carlo method is so important today. *Wires Computational Statistics* **6** (6), 386–392.

Lima, B. P., Mamede, G. L. & Lima Neto, I. E. 2018 Monitoring and modeling of water quality in a semiarid watershed. *Engenharia Sanitaria e Ambiental* **23** (1), 125–135.
Lindenschmidt, K. E. & Fleischbein, K. 2007 Structural uncertainty in a river water quality modelling system. *Ecological Modelling* **204**, 289–300.
Liu, L., Zhang, X. & Lyu, Y. 2022 Performance comparison of sewage treatment plants before and after their upgradation using emergy evaluation combined with economic analysis: a case from Southwest China. *Ecological Modelling* **472**, 110077.
Machado, E. S., Knapik, H. G. & Bitencourt, C. D. C. A. 2019 Comments on the water quality classification of water bodies. *Engenharia Sanitaria e Ambiental* **24** (2), 261–269.
Madani, M., Seth, R., Leon, L. F., Valipour, R. & McCrimmon, C. 2021 Microbial modelling of Lake St. Clair: impact of local tributaries on the shoreline water quality. *Ecological Modelling* **458**, 109709.
Mailler, R., Mèche, P. & Rocher, V. 2021 What removals of pathogen indicators can be expected within large-scale wastewater treatment facilities in the context of wastewater reuse in Paris conurbation? *Water Science and Technology* **83** (4), 781–791.
Metcalf, L. & Eddy, H. P. 1991 *Wastewater Engineering: Treatment, Disposal, and Reuse*. McGraw-Hill, New York, NY, USA.
Minas Gerais 2008 *Deliberação Normativa COPAM/CERH-MG N.º 1, de 05 de Maio de 2008. Padrão de Lançamento de efluentes*. Diário Oficial De Minas Gerais, Cap. V, Minas Gerais, Brasil.
Pujol-Vila, F., Giménez-Gómez, P., Santamaria, N., Antúnez, B., Vigués, N., Díaz-González, M., Jiménez-Jorquera, C., Mas, J., Sacristán, J. & Muñoz-Berbel, X. 2016 Portable and miniaturized optofluidic analysis system with ambient light correction for fast in situ determination of environmental pollution. *Sensors and Actuators B: Chemical* **222**, 55–62.
Quijano, J. C., Zhu, Z., Morales, V., Landry, B. J. & Garcia, M. H. 2017 Three-dimensional model to capture the fate and transport of combined sewer overflow discharges: a case study in the Chicago area waterway system. *Science of the Total Environment* **576**, 362–373.
Saltelli, A., Jakeman, A., Razavi, S. & Wu, Q. 2021 Sensitivity analysis: a discipline coming of age. *Environmental Modelling and Software* **146** (October), 105226.
Silva, S. C., Ramos, M. L. G. & Bernardes, R. S. 2021 Wetlands Construídos Com Meio Suporte De Solo Na Remoção De Coliformes Termotolerantes De Esgotos Domésticos. *Revista Eletrônica De Gestão e Tecnologias Ambientais* **9** (1), 32.
Snis 2021 Diagnóstico Temático Serviços De Água e Esgoto – Visão Geral Ano De Referência 2020. *Sistema Nacional De Informações Sobre Saneamento – Snis* 1–91.
Soares, L. M. V. & Calijuri, M. C. 2021 Sensitivity and identifiability analyses of parameters for water quality modeling of subtropical reservoirs. *Ecological Modelling* **458**, 109720.
Spear, R. 1980 Eutrophication in peel inlet – II. Identification of critical uncertainties via generalized sensitivity analysis. *Water Research* **14** (1), 43–49.
Srikrishnan, V. & Keller, K. 2021 Small increases in agent-based model complexity can result in large increases in required calibration data. *Environmental Modelling and Software* **138** (February), 104978.
Teodoro, A., Ide, C. N., Ribeiro, M. L., Broch, S. A. O. & da Silva, J. B. 2013 Implementação do conceito capacidade de diluição de efluentes no modelo de qualidade da água QUAL-UFMG: Estudo de caso no Rio Taquarizinho. *Engenharia Sanitaria e Ambiental* **18** (3), 275–288.
Thomann, R. V. & Mueller, J. A. 1987 *Principles of Surface Water Quality Modeling and Control*. [S.L.] Harper & Row Publishers, New York, NY, USA.
Universidade Federal De Viçosa – UFV 2009 Hidrotec. Available from: http://www.hidrotec.ufv.br/ (acesso Em 9 Maio. 2022).
Von Sperling, M. 2014a *Princípios Do Tratamento Biológico De Águas Residuárias: Estudos e Modelagem Da qualidade Da Água De Rios*, 4th edn. Ufmg, Belo Horizonte, Brasil.
Von Sperling, M. 2014b *Princípios Do Tratamento Biológico De Águas Residuárias: Estudos e Modelagem Da Qualidade Da Água De Rios*, 2nd edn. Ufmg, Belo Horizonte, Brasil.
Von Sperling, M. & Von Sperling, E. 2013 Challenges for bathing in rivers in terms of compliance with coliform standards. Case study in a large urbanized basin (Das Velhas River, Brazil). *Water Science and Technology* **67** (11), 2534–2542.
White, J. T., Hemmings, B., Fienen, M. N. & Knowling, M. J. 2021 Towards improved environmental modeling outcomes: enabling low-cost access to high-dimensional, geostatistical-based decision-support analyses. *Environmental Modelling & Software* **139**, 105022.

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