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Advantages, disadvantages and methods of applying mathematical models to evaluate water quality in reservoirs: a systematic review

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ABSTRACT

Human activities are affecting reservoir water quality; consequently, methods are necessary to verify those impacts. Mathematical modeling improves the understanding of the anthropic impact on water quality, changes in limnological data, and helps formulate management strategies. However, it is necessary to consider the (dis)advantages as well as the methods used for water-quality assessment in reservoirs. This study conducted a systematic review in four databases: (i) PubMed/Medline; (ii) Scopus; (iii) Web of Science; and (iv) Wiley Online Library. We combined Boolean operators and words aiming to identify papers linked to the scope. Rayyan software allowed the initial screening of the found papers. Peer-reviewed papers and the use of mathematical models to assess reservoir water quality were the inclusion criteria. Exclusion criteria included articles in languages other than English, grey literature, and inaccessible articles. Our research found 169 articles, of which 39 were selected and only 13 were included in the review. Mathematical modeling has many benefits related to real-world problems, but the main disadvantages are process simplification, specific rules of the model, and lack of information or data monitoring. Kinetic equations, regression models, Monte Carlo analysis, finite segment models, modeling tools, zero-order rate equations, partial differential algebraic equations, and predictive analysis are the methods observed in mathematical modeling. This review provides information for unfamiliar managers who intend to use mathematical models to assess the water quality of reservoirs.

Keywords: limnologic tool, model inventory, water management.

Vantagens, desvantagens e métodos dos modelos matemáticos aplicados para avaliação da qualidade da água em reservatórios: uma revisão sistemática

RESUMO

As atividades humanas afetam a qualidade da água dos reservatórios, portanto, métodos são necessários para verificar esses impactos. A modelagem matemática auxilia no entendimento do impacto antrópico na qualidade da água, variações nos dados limnológicos e auxilia na formulação de estratégias de manejo. Entretanto, é preciso considerar as (des)vantagens, bem como os métodos utilizados para avaliação da qualidade da água em reservatórios. Este estudo conduziu uma revisão sistemática em quatro bases de dados: (i) PubMed/Medline; (ii) Scopus; (iii) Web of Science e (iv) Wiley Online Library. Foram combinamos operadores booleanos e palavras para encontrar os artigos ligados ao escopo. O *software* Rayyan permitiu a triagem inicial dos artigos encontrados. Artigos *peer-reviewed* e o uso de modelos matemáticos para avaliar a qualidade da água em reservatórios foram critérios de inclusão. Os critérios de exclusão foram artigos não publicados em inglês, literatura cinzenta e artigos inacessíveis. Foram encontrados 169 artigos, dos quais 39 foram selecionados e apenas 13 foram incluídos na revisão. A modelagem matemática tem muitos benefícios relacionados à problemas do mundo real, mas as principais desvantagens são a simplificação do processo, regras específicas e a falta de informações ou monitoramento de dados. Equações cinéticas, modelos de regressão, análise de Monte Carlo, modelos de segmento finito, ferramentas de modelagem, equações de taxa de ordem zero, equações algébricas diferenciais parciais e análise preditiva são os métodos observados. Esta revisão fornece informações para gestores não familiarizados que almejam o uso de modelos matemáticos para avaliar a qualidade da água de reservatórios.

Palavras-chave: ferramenta limnológica, inventário de modelo, manejo da água.

1. INTRODUCTION

Considering water-quality loss in reservoirs, approaches are commonly adopted for assessment and management action proposals (e.g. Dippong *et al.*, 2017; 2018; Bianchini Jr. and Cunha-Santino, 2018). Mathematical modeling greatly improves the understanding of these systems. This tool aims to construct a model that can verify changes in water quality, considering the initial conditions, the dependence of simulations/phenomena, and the final impact (Ziemińska-Stolarska and Skrzypski, 2012).

Previous research recognized the use of mathematical models for the assessment of reservoir water quality (Ward and Linch, 1996; Xu *et al.*, 2017, Crespo *et al.*, 2018, Bianchini Jr. *et al.*, 2019; Chen *et al.*, 2019; Absalon *et al.*, 2020). As demonstrated, this tool seems to be a robust way to verify the impact of human activities on the reservoir, mainly water quality loss, and the main drivers of change in the limnological variables.

Taking into account the results of mathematical modeling, actions can be formulated aiming to reduce the human interference on water quality, due to the identification of priority areas for restoration and action plans formulation (Anderson *et al.*, 1998; Westphal *et al.*, 2004; Zhou *et al.*, 2016). In addition, factors such as potential economic benefits, storage capacity, the impact of climate change, and the dynamics of biogeochemical variables in the reservoir can be verified (Nover *et al.* 2019; Siniscalchi *et al.*, 2020).

Many regions are facing problems because of water scarcity and the negative impacts on agriculture and public water supply (Rosa *et al.*, 2020). Reservoirs play an important role for society, since they provide benefits as supporting services due to the mineralization process (Chen *et al.*, 2019) and water provision for multiple purposes. However, due to alterations in hydrological conditions and changes in metabolism, human activities (urbanization, agriculture, etc.) have adversely affected the reservoirs (Shi *et al.*, 2021).

Mathematical modeling emerges as an alternative to reservoir management. This tool helps to understand the processes taking place in the reservoir, it provides the basis for the strategy, and strengthens water quality restoration (Thibodeaux and Aguilar, 2005; Siniscalchi *et al.*, 2020). However, there is a need to verify the benefits, disadvantages, and methodologies primarily used in the assessment of water quality in reservoirs. Such information helps to understand the tool and may provide information for unfamiliar managers and scientists.

In this study, we conducted a systematic review of the literature, considered primary research, and examined the (dis)advantages of the mathematical models applied to assess the reservoir's water quality. Furthermore, we verified the adopted methodologies in the studies.

2. MATERIAL AND METHODS

The present research was conducted following the guidelines from Collaboration for Environmental Evidence (2018), considering seven steps: (i) planning the systematic review; (ii) conducting the search; (iii) eligibility screening; (iv) data coding and extraction; (v) critical appraisal of study validity; (vi) data synthesis and (vii) interpreting findings. The RepOrting standards for Systematic Evidence Synthesis (ROSES) were also followed. Eventual derivations from the guidelines were detailed below. The primary research question was "What are the benefits and the disadvantages of the mathematical model(s)/approach(es) for the water quality assessment of freshwater reservoirs?". Furthermore, a secondary question was proposed: "Which research methodologies have primarily been used for water quality assessment and management of those freshwater reservoirs?". We based the main research question on the PICO strategy (Population, Intervention, Comparator, Outcomes), Table 1 describes each element of the strategy and the research expression.

Table 1. PICO strategy for the research question.

Description	Abbreviation	Components
Population	P	Freshwater reservoir
Intervention	I	Mathematical model/approach
Comparator	C	Not applicable
Outcomes	O	Water quality

A literature search was conducted between February and April of 2021, in four databases without data limits: (i) PubMed/Medline; (ii) Scopus; (iii) Web of Science; and (iv) Wiley Online Library. Using search terms and Boolean operators, the following expression was employed: ("mathematic* model*" OR "mathematic* approach*" OR "mathematical modeling" OR "modeling approach" OR "mathematical modelling" OR "modelling approach" OR "math model") AND ("freshwater reservoir*" OR "water reservoir*" OR "man-made lake*" OR "man-made reservoir*") AND ("water quality" OR "drinking-water quality" OR "water physicochemical parameters" OR "water biological parameters" OR "limnological parameters" OR "limnological variables" OR "water variables").

Zotero was the chosen bibliographic management software. The studies were screened based on inclusion criteria by two independent researchers (FLS and ATF) using the software Rayyan, verifying the title and abstract. Rayyan (http://rayyan.qcri.org) is a free web app developed by Ouzzani *et al.* (2016), destined to conduct an initial screening of titles and abstracts by a semi-automatic process. The independent reviewers were unaware of each other's decision, in case of disagreement between the two independent researchers (FLS and ATF), a third independent reviewer (MBCS) would solve the disagreements. The full textual analysis of the screened articles was operated by a single reviewer (FLS); however, two reviewers validated the information considering the full text. In the cases of exclusion, the reviewers left a comment specifying the reason for the no inclusion.

Inclusion criteria involved: (i) peer-reviewed articles published in English and (ii) articles that employed mathematical models/approaches to assess the water quality/parameters of reservoirs. On other hand, exclusion criteria were: (i) duplicated articles; (ii) articles in other languages than English; (iii) articles that did not meet the research objective (i.e. reviews, articles that not employed mathematical modeling to verify water quality in freshwater reservoirs); (iv) grey literature and (v) articles not available in full form or with restricting access. The validity level was attributed according to Martins and Carmo Júnior (2018), the study adequacy was verified (full or partial coverage) to the research question, a situation double-checked.

Regarding the critical appraisals of the included articles, we have adopted modified elements pointed out by Haddaway *et al.* (2014), similar to Cresswell *et al.* (2018). Two reviewers (IBJ and MBCS) verified the quality analysis of the papers, the following elements were considered: replication ('possible' or 'no possible'); level of methodological details ('high', 'moderate' or 'low'); results discussion ('consistent' or 'no consistent'); potential bias ('none evident' or 'evident'). Concerning replication (possible or not), it is important to note that, for the evaluation of this criterion, only the degree of data complexity (i.e., quantity and accessibility) was considered for the application (or benchmarking) of the model. Thus, the integrity of the model is not being evaluated, as the articles were previously peer-reviewed. We minimize the bias of this study opting for no temporal delimitation, conducting the process with independent reviewers, and including positive and negative results. The strategy adopted for data extraction and coding was narrative synthesis due to the lack of standardization of the studies. In the end, the findings were interpreted.

3. RESULTS

As shown in the flow chart (Figure 1), 169 articles were recovered from the selected publication databases. Initially, 39 articles were excluded based on repeated results. Conducting an initial review of the title and abstract, we excluded 99 articles. Furthermore, After the criteria adoption and the full reading, 13 articles were included in the review. These studies enabled us to answer the proposed questions.

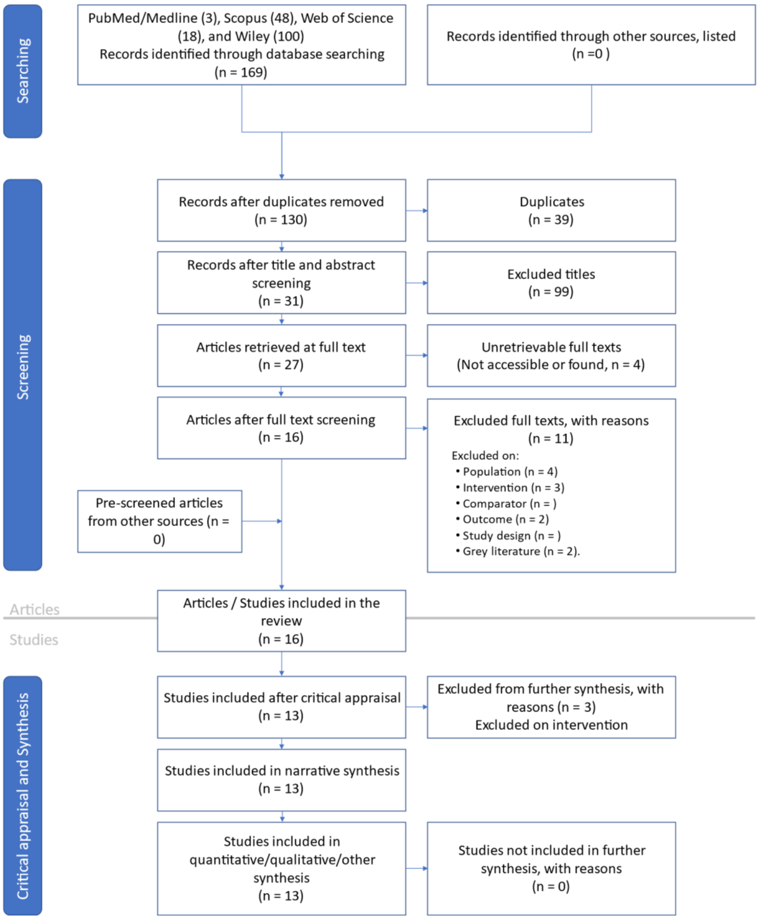

Figure 1. ROSE Flow diagram of the study selection.
Source: Haddaway *et al.* (2018)

Regarding the finds, the articles were published in 11 journals: (i) Water Air Soil Pollution (n=1); (ii) Water Research (n = 1); (iii) Journal of American Water Resources Association (n = 1); (iv) Journal of Water Science (n = 1); (v) Chemosphere (n = 2); (vi) Environmental Monitoring and Assessment (n = 2); (vii) Journal of Hydrology (n = 1); (viii) Science of Total Environment (n = 1); (ix) Computer Aided Chemical Engineering (n = 1); (x) Lake and Reservoir Management (n = 1) and (xi) Sensors (n = 1).

Considering the temporal distribution, the finds cover a period from 1998 to 2020 (Table 2). A single study was published in 1998, 2004, 2005, 2013 and 2016. Regarding the number of publications in the remaining years (2017, 2018, 2019 and 2020), two papers were found in each year. Relatively, the studies are concentrated in the last five years (from 2016 to 2020), because of the number of records (ca. 69%). The mathematical modeling studies were carried out in or the authors were from the United States of America - USA (n = 4), China (n = 3), Brazil (n = 2), Argentina (n = 2), France (n = 1), and Poland (n = 1). Most of the studies focused on temperate zones, followed by the subtropical ones. The critical appraisal can be verified in Table 2.

Table 2. Authors of studies, study area or study conditions, the country of the study, adequacy to the proposed questions and critical appraisal.

Authors (year)	Study area or study conditions	Country	Adequacy	Replication
Anderson *et al.* (1998)	Eastside Reservoir	USA	Total	Not Possible
Westphal *et al.* (2004)	Wachusett Reservoir	USA	Total	Possible
Thibodeaux and Aguilar (2005)	Hypothetical	USA	Partial	Possible
Cunha-Santino *et al.* (2013)	Laboratory conditions	Brazil	Partial	Possible
Zhou *et al.* (2016)	Yuqiao reservoir	China	Partial	Not Possible
Harris and Graham (2017)	Cheney Reservoir	USA	Partial	Possible
Xu *et al.* (2017)	Qingcaosha Reservoir	China	Total	Possible
Crespo *et al.* (2018)	January Lake	France	Partial	Not Possible
Siniscalchi *et al.* (2018)	Chasicó Lake/Paso de las Piedras	Argentina	Partial	Not Possible
Bianchini Jr. *et al.* (2019)	Piraju Reservoir	Brazil	Partial	Possible
Chen *et al.* (2019)	SY Reservoir (referred name)	China	Total	Possible
Absalon *et al.* (2020)	Paprocany Reservoir	Poland	Partial	Not Possible
Siniscalchi *et al.* (2020)	Paso de las Piedras Reservoir	Argentina	Partial	Not Possible

	Level of methodological details	Results discussion	Potential bias
Anderson *et al.* (1998)	Moderate	Consistent	Evident
Westphal *et al.* (2004)	High	Consistent	Evident
Thibodeaux and Aguilar (2005)	Moderate	No Consistent	Not Evident
Cunha-Santino *et al.* (2013)	Moderate	Consistent	Not Evident
Zhou *et al.* (2016)	High	Consistent	Not Evident
Harris and Graham (2017)	Moderate	Consistent	Evident
Xu *et al.* (2017)	High	Consistent	Not Evident
Crespo *et al.* (2018)	Moderate	Consistent	Evident
Siniscalchi *et al.* (2018)	Low	Not Consistent	Not Evident
Bianchini Jr. *et al.* (2019)	Moderate	Consistent	Not Evident
Chen *et al.* (2019)	High	Consistent	Not Evident
Absalon *et al.* (2020)	High	Consistent	Not Evident
Siniscalchi *et al.* (2020)	High	Consistent	Not Evident

3.1. Benefits and the disadvantages of the mathematical model(s)/approach(es) for the water quality assessment of freshwater reservoirs

Mathematical modeling allows the determination of pathogen concentrations (e.g., *Cryptosporidium*, *Giardia* spp, rotavirus, and poliovirus) in the epilimnetic and hypolimnetic region of the water reservoir, and the number of contaminated people because of recreation activities, considering the annual data values and the intensity of recreational activities

(Anderson *et al.*, 1998). This situation was proven in the East End Reservoir (USA) of Anderson *et al.* (1998), besides the benefits (comparison of results with available monitoring data, peak events, eventual risks for population), the lack of mechanistic information, the requirement of sampling data, the assumption simplification, limited information related to impacts of major water exposure, the assumptions involving the decomposition of fecal material and the dispersion of pathogens constitute limitations.

The mathematical model generated information about the diffusion or advection of total organic carbon (TOC) in the Wachusett Reservoir, but Westphal *et al.* (2004) pointed out that model calibration requires a large amount of data and the deviation caused by observational data to improve model performance. In addition, the authors point out that considering some relationships between light and nutrients, model refinement is possible, and it is necessary to obtain water samples to evaluate the effects of proposed plans and actions.

Through mathematical modeling, Thibodeaux and Aguilar (2005) quantified the dissolved organic carbon (DOC) in the bed and water column based on transport, bed sediment, and microbial production. It is worth mentioning that the use of algebraic expressions and differential equations enabled the authors to obtain the necessary empirical evidence, and the generated algorithm predicted the DOC in the hypothetical reservoir.

Mathematical modeling allows to verify the temporal mass changes of course particulate organic matter detritus (CPOM) in the case of new reservoirs and the oxygen consumption, a situation that can reflect on water quality and on the release of greenhouse gases in the short and long time (Cunha-Santino *et al.*, 2013). The authors strengthened the impact, including the risk of eutrophication, oxidation of debris, and increased biochemical oxygen demand (BOD).

Zhou *et al.* (2016) based on the Dyna-CLUE (Land Use Conversion and Its Impact in a Small Area) model and Grey Relational Analysis (GRA), verified the land use changes of the Yuqiao Reservoir (China). The use of GRA allows the development of solutions to real-world problems because of the consideration of changes in development scenarios. In view of the correlation with land use/land cover and land use change, it is possible to verify the restoration of the area near the reservoir, the impact of resettlement and the activities of agribusiness, and generate useful information about the loss of phosphorus (P) in the soil. The authors reinforce that actions based on the model enhance the reduction of P concentrations in the reservoir and how the management actions can reduce the P concentration (36-45%).

In Cheney Reservoir (USA), a comparison of 12 linear and nonlinear regression modeling techniques, aiming the prediction of cyanobacterial abundance and metabolites (microcystin and geosmin) using water quality data from 2004 to 2015, was conducted by Harris and Graham (2017). The authors reinforce that the models had a poor prediction to verify the maxima concentrations, a situation attributed to drought and rainfall events; the models predict cyanobacterial using seasonally variation and do not differ the formation conditions and years. It is highlighted that Cubist modeling has a unique structure, and its creation is based on a tree-based modeling method, a set of rules and terminal node data.

Xu *et al.* (2017) stand out that mathematical modeling has advantages in scenario simulation and identification of mitigation actions aimed at ensuring safe drinking water and managing emerging pollutants, such as atrazine and bisphenol in Qingcaosha Reservoir (China). The researchers verified that the employed model enhances the determination and exchange of atrazine in the reservoir, however, important variations can be ignored due to the long interval of the data input or rainfall events, some simulation bias in the winter, generation of uncertain because of the low frequency of observed data and information about the practical operation.

Crespo *et al.* (2018) verified the pollutant's distribution and optimal strategies for refilling water in January Lake (France) using mathematical modeling. It was possible to determine the localities with adequate water quality for recreation and water intake, considering the constant volume of the lake, the wind influence, water currents, and the water quality evolution.

Using mechanistic models and optimal control problem models, Siniscalchi *et al.* (2018) evaluated the salt concentration considering the humid climate scenario and the variables that affect the phytoplankton in the reservoir, aiming at a recovery strategy. Due to the numerical results, the authors believe that modeling is a useful tool for planning and verifying the impact on water bodies.

Bianchini Jr. *et al.* (2019) showed that the mathematical model used to verify the material mass balance in the Piraju Reservoir (Brazil) is a feasible method to assist in the water quality monitoring of watersheds. In addition, the authors emphasize that since freshwater ecosystem services can be inferred, the model can be used in water quality plans and scenarios involving aquatic bodies.

The carbon dynamics, climatic conditions and nutrient scenarios, algal blooms and systemic carbon conversion of SY Reservoir (China) were simulated by Chen *et al.* (2019). The benefits involved the slight tendency to underestimate the level of the water because of a tributary negation, and a negative bias of surface carbon dioxide in the function of an overestimation in SY reservoir.

Absalon *et al.* (2020) used a three-dimensional hydrodynamic and ecosystem model, in Paprocrany Reservoir (Poland), considering the following data from 1995 to 2014: temperature, dissolved oxygen, pH, total suspended solids, DOC, dissolved inorganic carbon, dissolved (in)organic nitrogen, particulate organic nitrogen, ammonia nitrogen, dissolved organic phosphorus, particulate organic phosphorus, phosphate organic phosphorus, silica, bacteria, phytoplankton, and zooplankton. The researchers have increased the demand for available data, and monitoring of watershed areas is necessary for assessment and scenario formulation. The analysis is helpful to verify the impact on water quality and changes in limnological variables in the reservoir area, analysis of mitigation options, and maintenance/improvement of water quality related to climate change (Absalon *et al.*, 2020).

Artificial wetlands models associated to a mechanistic reservoir model demonstrated potential as a remediation tool, the mathematical modeling study carried out in Paso de las Piedras Reservoir (Argentina) enhanced the comparison of different scenarios and opportunities to the obtainment of improvements strategies formulation to reduce nutrients loading and favor the water quality recovery in eutrophic systems (Siniscalchi *et al.*, 2020). Due to the information about gradients, differential algebra, and variable optimization, the authors considered this method an advantage, which is conducive to the planning and design of water supply systems.

3.2. Research methodologies for water quality assessment and management of freshwater reservoirs

In the case of Eastside Reservoir (USA), it was observed that the Monte Carlo technique was transformed into a finite-segment model (hybrid Monte Carlo finite-segment method). Multiple simulations occurred based on parameters (pathogen content, feces mass, inaction rate, infection rate, feces shed, reservoir segmentation, depth, volume variation assumptions, water body filling in the climatic seasons), which allowed verifying the dispersive transport, and the pathogen inputs, based on available data (Anderson *et al.*, 1998).

Westphal *et al.* (2004) adopted a quasi-mechanistic approach to verify the advection, settling, and diffusion of TOC in Wachusett Reservoir; a situation that resulted in a simple mass balance model with equations which considered the longitudinal reservoir division, the bathymetric information, two-dimensional structures, flow, volume, time step, diffusion component, and mixing component.

A two-step DOC release model inferred in a previous study, in the tea bag equation and continuous microorganisms' production was employed by Thibodeaux and Aguilar (2005), considering a hypothetical reservoir. These authors assumed that the readily quantification of DOC, the microbial production and transport of DOC (steady-state model and mass balance), boundary condition with to Fick's first law, the inter-phase transport, the water column DOC accumulation model, and a zero-order rate equation that was based on DOC kinetics. The following variables were considered: soil porosity, the concentration of carbon (mg/L), DOC concentration in the pore-water, the distance from the interface into the bed, DOC production rate, the DOC diffusivity, mass-transfer coefficient. In addition, there is a model for quantifying DOC in water bodies and DOC productivity based on bed depth (Thibodeaux and Aguilar, 2005).

Cunha-Santino *et al.* (2013) used a set of equations to verify the mineralization of CPOM under experimental conditions. These equations are based on the parameterization of the time evolution of elements (particulate organic carbon - POC, total inorganic carbon – TIC, TOC) and nonlinear regression calculations using the Levenberg-Marquardt algorithm. It took into account: POC mass loss, formation and mineralization of DOC, the formation of gases and inorganic substances, and the kinetics of the dissolved oxygen consumption during the mineralization process.

It is possible to verify the use of GRA to check problems that are based on a situation without information (black), with complete information (white), and with intermediary information (grey) (Zhou *et al.*, 2016). Data are necessary to calibrate the model and compare the simulated scenarios, multiple linear regression models are adopted to verify the model validation. Zhou *et al.* (2016) based the simulated scenarios of land-use change and adopted driving forces (e.g., P sources, agricultural practices) on the grey model and multiple linear regression analysis, using differential equations, and the grey relational grade to estimate the lack of data, as well as the Conversion of Land Use and Its Effects at Small Regional Extent model.

Harris and Graham (2017) use a predictive model combined with the use of training functions and random data selection. Each model has five repetitions and 10-fold cross-validation. The authors compared the 12 models according to the root mean square error (RMSE), linear and nonlinear regression models were included, and the comparison occurred with the observed response (variables concentrations). The authors verified the temporal variation patterns and the abundance of cyanobacteria and the metabolites, using cubist models (support vector machines, random forest, bagged trees), due to the predictive roles of water variables (chlorophyll a, nutrients, temperature, time of the year, iron, oxygen).

Xu *et al.* (2017) used a 3D-emerging model in the Qingcaosha Reservoir; this item is a numerical hydrodynamic model that counts with an orthogonal curvilinear coordinate which simulates transport, flow, and water temperature. The foundation of modeling is based on a grid and sounding method. Such models considered meteorological data, processes as degradation, and rainfall, diffusion, and reaction equations allowed the modulation of atrazine and bisphenol.

The description of water quality evolution (generic pollutant) in a reservoir, using numerical simulations and regarding the optimization problem based on an algorithm and the refilling process was possible in Jaunay Lake (France). In the mathematical modeling, Crespo *et al.* (2018) represented the lake surface geometry, denoted the pollutant concentration, the mensuration of the pollutant volume per area, the time for the model process, as well the influence of four effects (diffusion of pollutant, the wind, the water currents and spill/removal of pollutant). Based on the listed factors and the space-time, the formulated equation considered: the diffusion coefficient of pollutant, the wind velocity, the water velocity, the lake geometry, and the river velocity.

Siniscalchi *et al.* (2018) evaluated the salt reservoirs in Argentina (Chasicó Lake and Paso de las Piedras Reservoir) using eco-hydrological models, including the mass balance of variables, evaporation and kinetic equations in the algebraic equation system. The hydrological model shows the dynamic water mass balance based on an equation that takes into account the total mass of the lake (kg), water density, volume, precipitation, flow velocity of tributary rivers, flow velocity of groundwater, and evaporation.

Salt reservoirs (Chasicó Lake and Paso de las Piedras Reservoir) in Argentina were evaluated with ecohydrological models, Siniscalchi *et al.* (2018) included the mass balance of variables, evaporation, and kinetic equations in algebraic equations systems. Evaporation was calculated according to the radiation effects, the net radiation, wind, and vapor saturation deficit. The salt concentration was obtained by algebraic equations that considered water column height, rainfall, and flow rate. Regarding water quality, for this purpose, the authors included the mass balance of the reservoir' trophic chain (nutrients, phytoplankton, zooplankton, zoo planktivorous and piscivorous fishes) and forcing functions (solar radiation, temperature, contributor river's inflows, nutrients concentrations, ecological state). Also, the authors employed a differential-algebraic equation (DAE) to the optimal control of the problems.

In Piraju Reservoir (Brazil), the description of the mass balance of substances used a sampling campaign from 2003 to 2007 and two equations that englobe an assimilation factor (alpha), the first-order reaction rate constant, hydraulic flushing, the volume of the reservoir, the daily load of substance, the upstream flow rate, and the time needed to reach the equilibrium of the concentration (Bianchini Jr. *et al.*, 2019). The authors assumed that the reservoir is in a steady state, represented by a continuous stirred tank reactor. In addition, the researchers emphasized that the reservoir is a hybrid system with a step input; the change in the alpha coefficient indicates the retention or release of the substance being evaluated.

Tools such as Delft3D are used as modeling ones. In the case of SY Reservoir, modules (WAQ, FLOW) and the hydrodynamic model were employed to verify the dispersive/advective fluxes, furthermore, orthogonal curvilinear grid and the k-epsilon model were employed, using data from meteorological data, as air temperature, solar radiation, cloud cover, etc. (Chen *et al.*, 2019). The ecological Delft3D-WAQ model used by the researchers takes into account key processes (inorganic carbon balance, nutrient cycling, phytoplankton dynamics) and ecological aspects (species competition, limiting nutrients, light, temperature), the modulation was based on separate variables and occurred the simulation in the hydrodynamic/ecological models, the calibration occurred considering a trial-and-error method and the performance analysis was based on root mean square error, Nash-Sutcliffe efficiency, and root mean square difference.

The Aquatic Ecosystem 3D Model (AEM3D) was employed to verify the variability of water quality and flow, the effects of the increase related to water supply, the effects of a barrier that limits the water supply, and the climate change impacts. In the modeling simulation, Absalon *et al.* (2020) included the water flow (direction and velocity), retention time, transport of a virtual marker, temperature changes, and the variations in the concentration of nutrients and plankton. The authors used the Reynolds averaged Navier-Stokes and Reynolds average kinematic boundary to simulate the heat exchange, phytoplankton and zooplankton dynamics in the reservoir.

In the case of Paso de las Piedras Reservoir, the mathematical model was based on the dynamic of the limnological variables mass balance (zooplankton groups, phytoplankton groups, nitrogen species, phosphorus species, organic carbon, and dissolved oxygen), and considered the sediment resuspension, a partial differential equation system, and the inflows and outflows of water in the system (Siniscalchi *et al.*, 2020). This model was based on partial differential-algebraic equations that are transformed in an algebraic equation system; the integrated model aims to adopt a vector parameterization approach to an optimal control problem, verified by an optimization algorithm. In this sense, the authors adopted a mass balance, forcing functions and kinetic equations for wetlands construction, with the intent to restore water quality. It was considered that macrophytes, orthophosphate, organic phosphorus, nitrate, ammonium, organic nitrogen, POC, DOC, dissolved oxygen, the input from tributaries, the factor relative with the tributary diverted fraction into wetlands, generation/consumption (rate equations - respiration, natural death and organism growth) in wetlands, and output flow rate (Siniscalchi *et al.*, 2020).

3.3. Finds synthesis

Figure 2 shows a synthesis of the benefits, disadvantages, methods and the data necessary for the modeling models applied to the analysis of water quality in reservoirs. Considering all the included papers in this review, it is clear that many methods support the analysis, and a variety of water quality parameters and scenarios can be evaluated. However, data from monitoring campaigns are essential for the model application, as well as validation. The need to simplify ecological processes or assumptions, the frequency of data monitoring, the lack of data, and the limited information on the object of analysis are the most common designated shortcomings. In Table 3, the main information of the selected articles is pointed out.

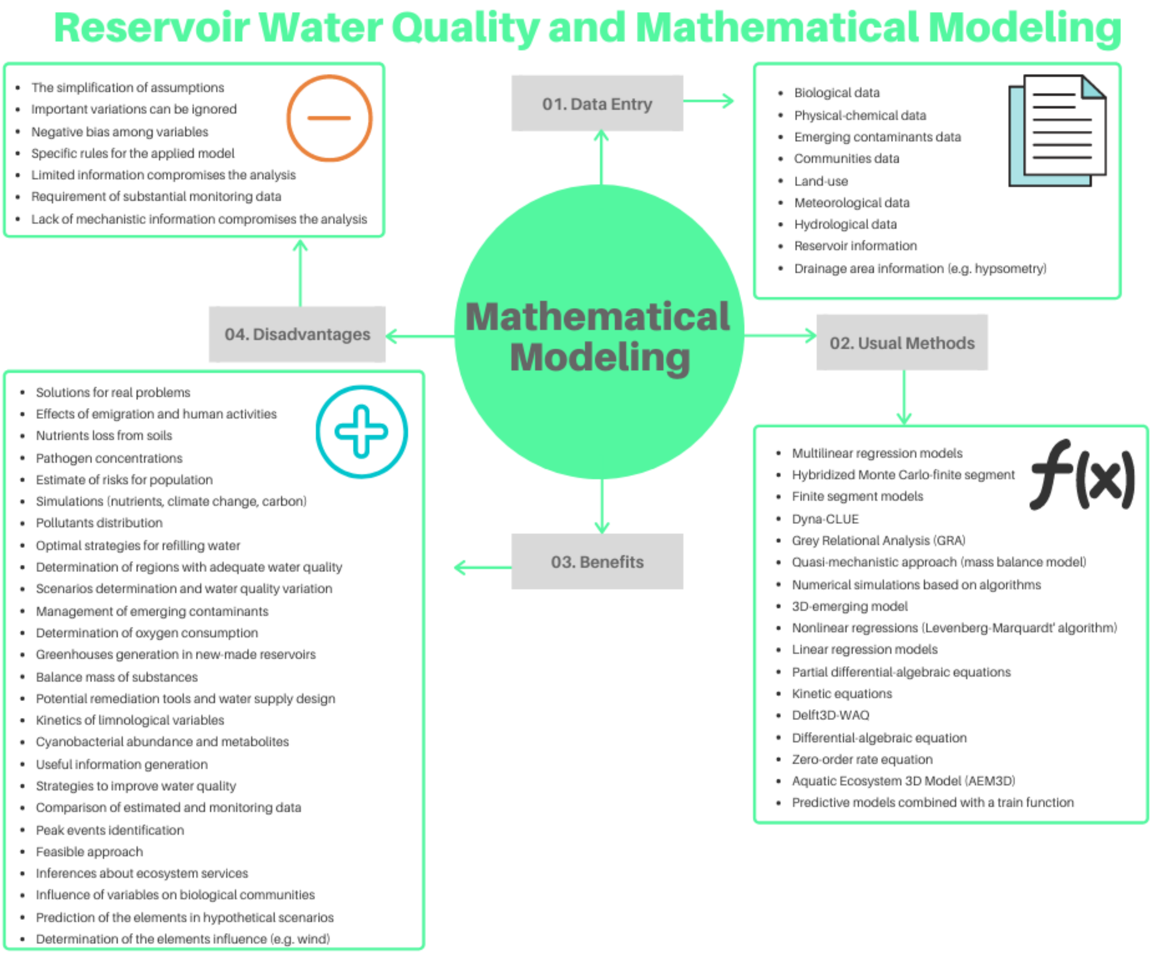

Figure 2. Mathematical modeling in reservoirs: data entry, usual methods, benefits, and disadvantages. Based on: Absalon *et al.* (2020); Anderson *et al.* (1998), Bianchini Jr. *et al.* (2019), Chen *et al.* (2019), Crespo *et al.* (2018), Cunha-Santino *et al.* (2013), Harris and Graham (2017), Siniscalchi *et al.* (2018; 2020), Thibodeaux and Aguilar (2005), Westphal *et al.* (2004), Xu *et al.* (2017), Zhou *et al.* (2016).

4. DISCUSSION

Considering the importance of aquatic ecosystems and the water quality loss the mathematical modeling plays an important role due to strategy formulation (e.g., limitation of human activities around the reservoir), the pollution influence on water, the limnological variables patterns, and the guideline attendance (Kerachian and Karamouz, 2007; Dippong *et al.*, 2018). Mathematical modeling subsidizes the improvement of water quality and the proper management of reservoirs, because of the contribution related to the new made systems and the optimization of the existing ones (Bianhini Jr. and Cunha-Santino, 2018).

Table 3. Synthesis of the selected studies.

Authors	Methods	Advantages	Disadvantages/Limitations
Anderson *et al.* (1998)	Use of a Hybridized Monte Carlo finite segment model to predict the pathogen concentration in the Eastside Reservoir, considering the spatial and temporal variability.	Assessment of the recreational activities impacts on water quality; simulation of pathogen concentration; prediction of annual mean values, considering acceptable levels and treatment practices; comparison of the results with available sampling data; peak events identification.	Requirement of sampling data to identify peak events; lack of mechanistic information; simplification of assumptions.
Westphal *et al.* (2004)	Quasi-mechanistic approach that resulted in a mass balance model with equations to simulate TOC.	Use of historical input series for calibration; simulation of mechanistic elements (e.g. diffusion); the predictive strength can be improved using updated data; credibility to be extended into long planning and operational strategies; characterization of thermal/seasonal structure.	Calibration demands large amounts of data to improve the accuracy; simplification of elements; underprediction/overprediction due to TOC sources; eventual multivariate dependencies in the variables.
Thibodeaux and Aguilar (2005)	Quantification of the DOC in the bed and water column based on a mathematical model, using differential equations, algebraic expressions and transport kinetics in laboratory conditions.	It was possible to obtain an algorithm that predicts the DOC in a hypothetical reservoir. The steps led to the understanding of DOC release, considering basic mechanisms and resulting in the generalization of results.	Assumptions related to temperature are necessary. Also, uncertain intervals need to be considered. Sufficient data are necessary for the modeling. Differential equations are necessary to describe microbial processes.
Cunha-Santino *et al.* (2013)	The CPOM mineralization was described by equations and non-linear regression with an iterative algorithm (Levenberg-Marquardt). The oxygen consumption was described using a first-order kinetics model.	The mathematical model of decomposition kinetics allowed us to verify the half-life of CPOM and the effects on water quality from short to long-term, including oxygen consumption and implications to eutrophication.	Not clear in the text.

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Zhou *et al.* (2016)	Use of Dyna-CLUE model, grey relational analysis (GRA), and grey model (GM) to simulate P levels	Prediction of P concentration changes associated with land use; identification of the ecological and environmental effects of changes in land use. Less data requirement.	There is a need to adapt the modeling approach for other watersheds.
Harris and Graham (2017)	Use of training functions and random data to verify the temporal variation patterns and the abundance of cyanobacteria. The predictive model included (non)linear regression and five repetitions.	Prediction of cyanobacterial, geosmin, and microcystin abundance. It was possible to verify important predictor variables. Also, the model demanded fewer explanatory variables. Improvements are possible adjusting the models.	The cubist model was more robust in the cases of larger cyanobacterial abundances or geosmin concentrations. The maxima concentration was not predicted due to seasonal changes (environmental variation was not captured). The models do not distinguish inter-annual/intra-annual differences. Long-term data are necessary.
Xu *et al.* (2017)	A 3D-emerging model (Delft3D-FLOW/Delft3D-WAQ) was used, the numerical hydrodynamic simulates some parameters (transport, flow, water temperature) and counts with an orthogonal curvilinear coordinate	The modeling was capable of describing the patterns of water temperature, salinity and emerging contaminants over time and space. It was possible to verify the transport and biodegradation of the contaminants, insight into risk of contaminants and base for decision-making. Observational data was employed to adjust the model.	The complications of the water quality model demand different criteria of goodness-of-fit. May high input data and long intervals ignore important variations. Low observed that it can generate uncertainty in prediction.
Crespo *et al.* (2018)	A mathematical model was performed considering numerical simulations and the problem optimization, based on an algorithm and refiling process.	Optimal strategies were obtained for refilling water, and optimal locations were identified ensuring water quality. The generic pollutant distribution associated with refilling location was obtained, as well as prospective refilling.	The model assumes that water volume is constant, the pollutant remains at the water surface, and its distribution is influenced by wind and water currents.
Siniscalchi *et al.* (2018)	Differential algebraic equations (Kinect, mass balance, evaporation) represented the ecohydrological models. A dataset (10 years) was used for calibration.	Optimal control problems were possible; the modeling addressed salinity and flooding issues. Also, eutrophication problems were considered, as well as restoration profiles, biomanipulation processes, and useful elements for decision-making were generated.	The entire model has 110 algebraic equations, as well as 42 differential equations.
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Bianchini Jr. *et al.* (2019)	Description of limnological mass balance from, using two equations.	The model allowed us to verify the retention capacity of the reservoir, showing the numbers of retentions and inferences about the physical processes, using an alpha parameter. It is a feasible approach in water monitoring.	The model had some premises: the reservoir is a completely mixed system; the system can be represented by a zero-dimensional model and is in a steady state.
Chen *et al.* (2019)	A three-dimensional ecological model was employed to simulate the carbon dynamics, the climate conditions, nutrients scenarios, algal blooms, and the systematic carbon transformations.	Scenarios were evaluated, considering climate and nutrients, including the systematic carbon transformations. The model allowed us to verify changes in the trophic state associated with CO2 and water volume. Simulations (algal blooms, carbon dynamics) were possible. The model can be coupled with other models (e.g. watersheds).	A negative bias of surface CO_2 was verified; but the model was validated. Simulated CO_2 concentrations were obtained using derived data from semiempirical equations, so uncertain and potential sources of error can be verified. The atmospheric contribution was not considered. The parameters in the Wanninkhof equation have 20% of uncertainty.
Absalon *et al.* (2020)	The Aquatic Ecosystem 3D Model (AEM3D) was used to assess variability in water quality and flow, considering many parameters (water flow, retention time, transport, temperature, plankton, and nutrients concentration).	Impacts on water quality, flow and limnological variables over time were verified based on the model, including scenarios formulation related to pollutants, climate change and algal bloom. Actions formulation was possible. Also, the main source of problems was identified.	The hydrodynamics and thermodynamics of the reservoir were represented by > 100 equations that represent the system processes. No sufficient available data for 2016 compromised the parameterization of water quality and inflows.
Siniscalchi *et al.* (2020)	It involves an integration of mechanistic models and partial differential-algebraic equations. The analysis considered water variables, mass balance of biogeochemical variables (including taxonomic groups), inflows and outflows.	The approach provided temporal profiles for biogeochemical variables, contributing to planning and restoration measures. Experimental data calibrated the model. Furthermore, optimal control and problem design were considered. The study showed as advantage the information on gradients and the variables optimization.	Not clear in the text.

Previous research showed how mathematical modeling is useful for water quality assessment. Ward and Linch (1996) focused on the use of mathematical modeling for recreational benefits with biological variables and environmental changes; the results reinforce the possibility of water quality improvements allowed by models. Guzman *et al.* (2017) evaluated the influence of landscape cover change, sediment loads, water infiltration and a long-data period, favoring the elaboration of rehabilitation projects. Using mathematical modeling, Cid *et al.* (2011) identified the most polluted areas and the main pollution sources of a reservoir in Argentina, using limnological data and tridimensional models.

In this study we verified such possibilities; many situations linked to water quality and the reservoir drainage area can be explored using mathematical modeling. However, mathematical modeling has many assumptions, and factors such as strategy and system complexity need to be considered (Nover *et al.* 2019). Also, it is necessary that the attainment of optimal operation rules, the adjustment of algorithms, use of hybrid methods, the need of input data (observational data) for the verification of hydro-environmental processes, robustness, acceptable performance, prediction, accuracy, deal with the limitation of models, and the determination of parameters (Bezsonnyi *et al.*, 2017; Karami *et al.*, 2019, Latif *et al.*, 2022).

Reservoirs have several impacts associated with the damming that impact directly the water quality and ecological processes (Winton *et al.*, 2019). A model can be applied to similar systems, sometimes it is not necessary to use specific programs (Bezsonnyi *et al.*, 2017). According to Zieminska-Stolarska and Skrzypski (2012), the most common issues evaluated for mathematical modeling (physical, analytical, or numerical) are related to water quality compromising, basically the models can be divided into: (i) one-dimensional models - common to verify changes in parameters; (ii) two-dimensional models - usual in reservoirs due to longitudinal and depth profile; and (iii) three-dimensional models (3D) - considers the spatial distribution.

In the 1970s and 1980s, the need to assess water quality in reservoirs inspired mathematical modeling. Scientists tried to integrate ecological processes, water quality, and hydrodynamics based on assumptions and dimensional representations (e.g. 1D, 2D, 3D, or more) (Orlob, 1992). Nowadays, we can see that the found results provide evidence about advances in mathematical modeling and yet water quality, ecological processes, the reservoir hydrodynamic, and dimensional representations are elements present in the analysis, the benefits enhance decision-making, but limitations and the resources for the modeling process need to be considered.

Indeed, the model's selection by users demands verification of the complexity, the temporal scales, needful data, personal knowledge, the project, and calibration (Yuan *et al.*, 2020). The model can have many assumptions; it is important to emphasize the need to consider factors that do not exist in the model, especially political and system complexity (Nover *et al.* 2019). Criteria can be adopted for mathematical models' selections, evaluation can be auxiliaries in the selection of the most appropriate model (e.g. Chinyama *et al.*, 2014).

Hundreds of mathematical models can be found for water quality assessment; the guidance of developed countries supports the standardization of model use, but this is not the case in emerging countries (Wang *et al.*, 2013). Mathematical modeling is a feasible tool that saves resources and time for water quality assessment in reservoirs (Heidarzadeh *et al.*, 2021). In view of the achievements and contributions to management, this study points out the tools used for reservoir water quality monitoring and decision-making.

Considering future research involving mathematical modeling and water quality in reservoirs, there is a need to solve the main disadvantages (e.g. bias, specific rules, simplifications, etc.) and maintain the assessment of the system complexity, including the main processes. The advantages can be considered in the selection of the appropriate model for reservoir analysis; however, data availability and mechanistic information compromise the analysis.

It is worth mentioning that the limitation of this study is related to the standards of attendance and the small number of articles included in the review. In addition, the sample supports the obtained composition related to the subject. In future studies, we recommend a review to verify the advantages and disadvantages of the mathematical modeling methods that are mainly used to assess the water quality of reservoirs.

5. FINAL CONSIDERATIONS

This review provides information on the role of mathematical modeling in the assessment of reservoir water quality. The advantages, disadvantages, primarily used methodologies and data required for calibration and analysis of mathematical modeling for water quality assessment in reservoirs are pointed out. The study found that the benefits of mathematical modeling are diverse, and most models allow verification of limnological variable models and the formulation of management actions. Some disadvantages, mainly limited data and simplifications, can compromise mathematical modeling. Regression, mechanical methods and algebraic equations are the most commonly used methods.

Benefits from mathematical modeling are the analysis of real problems involving population growth, climate changes and human activities' development; the nutrients and pollutant's dynamics and contributions from the reservoir area; optimal strategies; determination of areas with adequate quality water; the mass balance of substances; the kinetics of limnological variables; inference about ecosystem services as the supporting ones; the influence of physical-chemical variables on biological communities; and prediction about hypothetical scenarios (e.g., new made reservoirs).

The main found disadvantages are the necessity of simply process and real world situations; important variations can be ignored due to monitoring interval and the modeling conditions; the analyzed variables can demonstrate bias because the causality of variables in some cases; models have specific rules, given the structure and the analytical components; the lack of information or limitations about some themes can compromise the mathematical modeling (e.g., contaminated people due to water contact, lack of mechanistic information related to the reservoir as flow and volume); and the inexistence of a large base of monitoring data can compromise the analysis and the determination of patterns.

Data input requires information from the monitoring program; it is necessary that data be input from communities (phytoplankton, zooplankton, cyanobacterial abundance), limnological data (nutrients, heavy metals, solids, temperature, etc.), biologic data (chlorophyll-a, pathogens), landscape cover in the reservoir area, meteorological data (temperature, wind, precipitation, air humidity), reservoir characteristics (volume, area, retention time, river flow, etc.), new compounds (such as pesticides).

The research methodologies primarily used for water quality assessment of reservoirs include: kinetic equations, multilinear/linear regression models, hybridized Monte-Carlo analysis, finite segment models, GRA, mass balance models, modeling tools (Delft3D WAQ, 3D-emerging, AEM3D, Dyna-CLUE), zero order rate equation, partial differential-algebraic equations, and predictive analysis allied to train function. Further research should evaluate the pros and cons of the research methods that have been identified.

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