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Choosing an appropriate water quality model—a review

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Abstract Water quality models are quite complex to use even for scientists, requiring knowledge in different areas such as biology, chemistry, physics, and engineering. Hence, the use of these models by a non-specialist is quite complicated, demanding considerable time and research, particularly to choose which model is the most appropriate for a given situation. In this study, a comparative guide is suggested, which can help users select the appropriate water quality model for certain systems and variables. Five models were considered as follows: AQUATOX, CE-QUAL-W2, Spatially Referenced Regression Model on Watershed Attributes (SPARROW), Soil and Water Assessment Tool (SWAT), and Water Quality Analysis Simulation Program 7 (WASP7), which have been widely used during the last 5 years. All of these selected models are free and easily available. It was verified that each model has its particularities and applications; however, the AQUATOX model has several advantages compared with the other models analyzed. In addition, to illustrate the availability of the proposed comparative guide, a case study was carried out to demonstrating the selection process of the selected models.

Keywords Comparative guide · AQUATOX · CE-QUAL-W2 · SPARROW · SWAT · WASP7

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Introduction

Sustainable management of freshwater is a major concern throughout the world. However, the constant process of environmental degradation has resulted in several problems related to water contamination that contaminates other parts of the ecosystem. Moreover, water once contaminated is quite complex to restore, requiring time and a significant economic investment, which makes the restoration of water resources unfeasible in most cases. Therefore, to avoid future major problems, the most effective means is investing in water quality control and maintenance. In this context, water quality models have emerged as an effective tool to assist in the control, prevention, and remediation of water resources contamination. Water quality models are essential in predicting how catchments may respond to the pressures of pollutant sources, from the headwaters to the river network, in the present and the future.

Water quality modeling is considered as an element in supporting water quality management decisions, not only determining the requirements for meeting water quality standards, but also calculating the effectiveness of actions in limiting pollutant sources for a designated use (Xue et al. 2015). This modeling helps in understanding hydrological processes and how they affect water quality and the management of water bodies by analyzing different scenarios for different management actions (Slaughter et al. 2017). However, the models are only useful if they capture the correct processes, otherwise, there is the risk of management decisions being based on unreliable information (Jackson-Blake et al.

2017). To the authors, there is a growing awareness that many water quality models used today are too complex, making it difficult, time-consuming, and expensive to set them up and reducing the reliability of their predictions. According to Slaughter et al. (2017), among the drawbacks in using water quality management models when compared with quantitative models is that water quality models are more complex and less developed because it is a relatively young science.

Cox (2003) reviewed six models currently in use for describing water quality in freshwater river systems: SIMCAT, TOMCAT, QUAL2E, QUASAR, MIKE-11, and ISIS. The author also examined the potential for each model in relation to the issue of simulating dissolved oxygen (DO) in lowland rivers. Costa et al. (2019) reviewed seven models for water quality simulations that have been widely applied around the world for 21 years (1997–2017): AQUATOX, CE-QUAL-W2, EFDC, QUALs, Soil and Water Assessment Tool (SWAT), Spatially Referenced Regression Model on Watershed Attributes (SPARROW), and WASP. The authors also listed the countries that most frequently applying water quality models and collated the themes of interest and the most simulated parameters for the seven countries that most frequently employed the seven water quality models studied. Today, there are several quality models available and research of their applications in certain case studies. However, articles that aid in choosing a suitable water quality model by non-specialists remain scarce. Furthermore, in the few articles found in the literature that have performed a review or that have conducted a methodology of choosing among models, the authors selected models that no longer have wide application in scientific research during recent years.

Mateus et al. (2018) proposed a method to assist in the selection of a particular model from a set of apparently similar models, for that the authors selected eight water quality models: CE-QUAL-W2, MIKE HYDRO River, MOHID Water, SIMCAT, SisBaHIA, TOMCAT, QUAL2Kw, and WASP7. Chinyama et al. (2014) developed a simple framework for selecting water quality models to aid non-specialists through the review of five models, but four of these models (SELECT, DYSREM, MINLAKE, and BATHTUB) have hardly been used in scientific research during the last 5 years. Sharma and Kansal (2013) compared six river quality models based on their conceptualization, processes, strengths, and limitations and provided broad criteria for the choosing of a suitable model. Among the models reviewed, three (BLTM, EPD-RIV1, WQRRS) have not been widely applied in scientific research during recent years. The same occurred in the study of Kannel et al. (2011), who reviewed six water quality models for rivers and flows, three of which (SIMCAT, QUASAR, QUAL2EU) have been sparingly employed in recent scientific research. Thus, this study was different in performing a review of water quality models that have been widely used in scientific research during the last 5 years.

The objective of the study is to describe the main models of water quality currently applied in studies and discuss their characteristics to assist researchers in the selection of which model to use. In this study, a comparative guide is suggested, which can help beginners in choosing the appropriate quality model systems and variables. The models analyzed were as follows: AQUATOX, CE-QUAL-W2, SPARROW, SWAT, and WASP7. All of the selected models are free and easily available.

Model review

The models reviewed in this article were selected according to three criteria: they are freely available, have been widely implemented in scientific journals with a high impact factor during the last 5 years, and offer a wide variety of resources available as technical and manual documents (Fig. 1). This last requirement was adopted for a more complete comparison of the models, rather than a simplified comparison based only on their use in articles. Therefore, according to these criteria, five models were considered the most relevant as follows: AQUATOX, CE-QUAL-W2, SPARROW, SWAT, and WASP7. The SWIM model, despite meeting all the of the aforementioned criteria, was not selected because its dissemination is restricted to project collaboration partners and experienced modelers, and this study was intended for beginning researchers in water quality modeling. The prioritization of the study being aimed at beginning researchers is due to the fact that expert researchers already have previous knowledge about the use of the model, so beginners usually need more reading in various formats, often with specific terms that are difficult to understand for beginners. However, this methodology of choice can be adopted by both experts and beginners, seeking to be practical and easy to understand. Although the study is focused on the 5 models chosen, it can be adopted for several others, observing based on the comparison of these models what are the main points to be considered when choosing the appropriate model for the studied situation and providing a sequential step by step.

In addition, models commonly used for water quality were selected. In this way, models that are widely used for other purposes such as Montecarlo were not selected. Another criterion adopted in the selection of the models was to check in the Springerlink database the models that were most present in articles of water quality modeling.

All the models selected, except for SPARROW, contain a user-friendly Windows-based interface, and SWAT also includes Geographic Information System (GIS) interfaces to link land use/land cover maps to model plant types. Schwarz et al. (2006) stated that the SPARROW model has a unique infrastructure that consists of a detailed stream reach network with digital elevation model (DEM)–delineated watersheds, including monitoring stations and spatially referenced GIS data.

AQUATOX

AQUATOX is an ecosystem model that simulates pollutants (nutrients and sediments) and several trophic levels (attached and planktonic algae, aquatic vegetation, invertebrates, and fish). Furthermore, it is among the few models that expresses the environmental fate of chemicals in aquatic ecosystems and their effects on resident organisms. It may be applied to experimental tanks, ponds and pond enclosures, streams, small rivers, linked river segments, lakes, reservoirs, linked reservoir segments, and estuaries. Moreover, according to Park and Clough (2014), it can be executed as a simple model, for example, to simulate an abiotic flask or used as a complex food web model.

Applicability

Grechi et al. (2016) applied the model to quantitatively describe the food web and, consequently, understand ecosystem functioning in the Po River, Italy. Moreover, Scholz-Starke et al. (2013) applied the model to predict the fate of pollutants (pesticides or nutrients) and represent the potential accumulation within the food webs of the Three Gorges Reservoir along the Yangtze River, China. Furthermore, Akkoyunlu and Karaaslan (2015) applied the model to predict a water quality scenario at Mogan Lake, USA.

Limitations

According to Park and Clough (2014), the AQUATOX model is quite complex, requires considerable data, and like any box-type model, its interactions are not completely understood. In addition, non-living organic matter and associated decomposers are modeled together under the term “detritus.”

CE-QUAL-W2

CE-QUAL-W2 is a distributed spatial and temporal analysis model capable of simulating any complex river–reservoir system (Masoumi et al. 2016). The US Army Corps of Engineers’ Waterways Experiment Station developed this model for modeling hydrodynamics and water quality in two dimensions. The model assumes lateral homogeneity; therefore, it is suitable for long and narrow waterbodies exhibiting longitudinal and vertical water quality gradients. Moreover, as outlined by Cole and Wells (2017), it may be applied to modeling rivers, lakes, reservoirs, estuaries, and river basins, with reservoirs and river segments.

Applicability

CE-QUAL-W2 linked with particle swarm optimization (PSO), an effective single and/or multiple optimization algorithm, showed good results when evaluating scenarios of eutrophication in the Karkheh River Reservoir, Iran, to maximize the waste loading capacity of a river–reservoir system (Masoumi et al. 2016). Another scenario analysis was performed by Jeznach et al. (2016) in the Wachusett Reservoir, EUA, to investigate the impact of sewage overflow, with hypothetical fecal coliform, and an accidental railway spill of ammonium nitrate on water quality. Moreover, Sadeghian et al. (2018) improved the algal simulations of CE-QUAL-W2 by implementing variable chlorophyll a/algal biomass ratios in a study of Lake Diefenbaker, Canada.

In addition, the model has proven to be quite efficient when coupled with SWAT. Yazdi and Moridi (2017) applied both models to simulate water quality variables in a watershed-reservoir system in Iran. The SWAT model was used for runoff and pollutant transportation modeling in the watershed, while CE-QUAL-W2 was

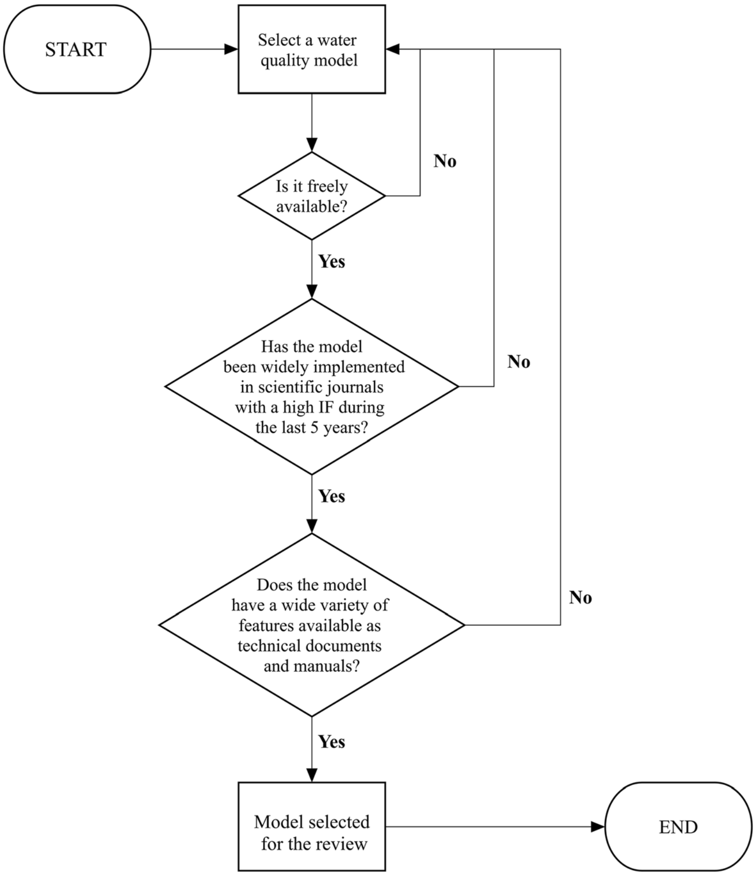

Fig. 1 Flowchart of the process applied by the authors to select the models

used for reservoir water quality simulation. Another utilization of these models linked was realized at a lake in North Dakota, USA, where both models were used to simulate water balance and sulfate concentrations. SWAT was chosen to evaluate snow accumulation and melting and to estimate the impact of natural and human activities on the hydrology and water quality. The CE-QUAL-W2 model was selected because the model is well-suited to a narrow and long lake, and it simulates the dynamics of water constituents in reservoirs. In addition, according to Shabani et al. (2017), this model can be used for different types of artificial outflows such as pumps, withdrawals, and spillways.

Limitations

The governing hydrodynamics and transport equations are laterally averaged; thus, variations in velocities, temperatures, and constituents are negligible, which may be inappropriate for large waterbodies with relevant lateral variations in water quality. In addition, Cole and Wells (2017) stated that if vertical momentum is not included, then the model may provide inaccurate results where there is significant vertical acceleration. However, the selective withdrawal algorithms compensate for this in the vicinity withdrawals. Moreover, according to Sadeghian et al. (2018), the process descriptions of algal growth mechanisms are oversimplified which compromises the quality of the algal simulations.

SPARROW

Spatially Referenced Regression Model on Watershed Attributes (SPARROW) is a hybrid statistical/mechanistic watershed and surface water modeling technique. The model has a simple mathematical structure: it associates the data of a network of monitoring stations to the watershed. Moreover, it understands the processes that affect contaminant transport.

Applicability

The model was coupled to the optimized genetic algorithm (GA) solution sets to acquire the mean annual *Escherichia coli* flux, an indicator of fecal contamination, in the Guadalupe and San Antonio River Basins of Texas, USA (Puri et al. 2017). The effects of conservation practices on water quality have been quantified using SPARROW, verifying the statistical correlation between conservation intensity and nutrient loads in the Mississippi River Basin, USA (García et al. 2016). Moreover, the model has been applied to evaluate the spatial distribution of total nitrogen (TN) sources (Saleh and Domagalski 2015) and baseflow (Miller et al. 2016).

Limitations

SPARROW is a “black box” model, and thus, the process description is too limited and the statistical results are difficult to interpret. Moreover, the model is only suitable for long-term water-quality records (multi-year to decadal periods). The model demands a sufficiently large number of water-quality monitoring stations for modeling. Although the methodology and program code do not restrict its application to variables that are expressed as mass flow, very few research studies have been performed for variables that are not expressed as mass flow.

SWAT

The Soil and Water Assessment Tool (SWAT) is a semi-distributed hydrology and water quality model developed by United States Department of Agriculture–Agriculture Research Service (USDA–ARS) for the prediction of management technique impacts on rural and agricultural environments (water, sediment, and agricultural chemical yields). The model is capable of simulating in daily, monthly, and annual periods, and it has been widely used in watersheds and large river basins (Arnold et al. 1998). Furthermore, SWAT can simulate a watershed and its sub-units: sub-basins, reach/main channel segments, impoundments on the main channel network, and point sources. The first level of the sub-unit is the sub-basin that contains at least one hydrologic response unit (HRU), a tributary channel, and a main channel or range, or it may be characterized by containing two types of dams, a pond, and/or wetlands. Sub-basin delineations may be obtained from grid cells and sub-watershed boundaries, which are more appropriate because they maintain routing reaches and topographic flow passages. The aforementioned HRU is a part of the sub-basin that possesses unique land use/management/soil attributes. Moreover, according to Arnold et al. (2012), the water bodies of the stream network of the watershed are modeled as reservoirs, which in this case do not mean that they are anthropogenic.

Applicability

Qi et al. (2016) improved the SWAT model to predict soil temperature in the Black Brook Watershed, Atlantic Canada; thus, the model could be used in cold-climate regions of the world. Xu et al. (2016) identified non-point source pollution in critical source areas based on nutrient loads (TN and total phosphorus) along the Xiangxi River, a tributary of Three Gorges Reservoir, China. Costa et al. (2019) points out that the model can be applied from hydrographic basins to the continental scale, being able to obtain a successful calibration even under scarcity of data. In addition, the model was used to predict streamflow, sediment, and pesticide diuron loading in the San Joaquin Watershed, CA, USA (Chen et al. 2017). SWAT was used in a study in Europe to model sediment fluxes of the Danube Basin (Vigiak et al. 2017). Golmohammadi et al. (2017) conducted a study that indicated the possibility of SWAT being used to predict temporal variations in potential contributing area, improving the runoff generation modeling.

Limitations

SWAT shows significant errors in predicting soil temperature, baseflow discharge, sediment, and soluble-phosphorous and nitrate loadings when applied to regions with significant snow cover during winter (Ahmad et al. 2011; Qi et al. 2016). Simulations of alternating bacterial growth are not included in SWAT oversimplifying soil and in-stream bacterial modules (Cho et al. 2016). In addition, it is not well-suited to simulate forest dynamics (Yang and Zhang 2016).

WASP

The Water Quality Analysis Simulation Program (WASP) is a surface water quality model that was developed by the US Environmental Protection Agency (EPA) for water quality modeling in one (1-D), two (2-D), and three (3-D) dimensions. The latest version of the model (WASP7) includes two general kinetic modules to simulate conventional pollution (dissolved oxygen, biochemical oxygen demand, nutrients, and eutrophication) and toxic pollution (organic chemicals, metals, and sediment) (Ambrose et al. 2001).

Applicability

WASP may be applied to several water bodies such as ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters (Ambrose et al. 2001). The model has been applied to model current and future water quality of the upper Qu'Appelle River, Canada (Hosseini et al. 2017a). In addition, the model has been applied to analyze and quantify the destination and transport of naphthenic acids. The goal was to investigate the potential impact of oil sand processed water on the Athabasca River, Canada (Kannel and Gan 2013). Moreover, a sensitivity analysis framework for water quality modeling and monitoring of rivers during two seasons, ice-covered and ice-free, were performed using WASP7 by Hosseini et al. (2017b). It was found that the sensitivity of some parameters during the ice-covered season was as high as that during the ice-free season.

Limitations

WASP is not able to simulate mixing zones or near-field effects and it does not manipulate sinkable/floatable materials (Kannel et al. 2011). In addition, periphyton or macroalgae are not simulated and the sediment flux calculation is oversimplified. In addition, flow files for solving advection are not provided by the model; this is required a hydrodynamic model. Moreover, according to Sharma and Kansal (2013), it applies a 1st-order UPWIND difference in space, which may induce relevant numerical diffusion.

Method of selection of the water quality models

Chinyama et al. (2014) proposed the following criteria for selecting water quality models: (1) select the type of water body to investigate, (2) choose the important parts of the water body to be simulated, (3) choose the processes to be simulated (i.e., mechanistic and empirical), (4) choose the expected outputs (i.e., deterministic and stochastic), (5) select the important parameters, (6) identify the available resources, (7) identify the available data (i.e., monthly, weekly, daily, and hourly and of what parameters), and (8) establish the user type.

In this review, the models were compared according to the aforementioned criteria to facilitate the choice among the models that are today widely used in the literature, proving its applicability throughout the world (Fig. 2). The water of the system that was analyzed was considered the important part in criteria two. Criteria eight was not considered when comparing because it is a particular part of each study. However, the models were compared in terms of the degree of complexity, which indicates the ease of use for each user type.

The first step was to determine the type of system to be modeled. The operating capacity of the models in the most used systems, considering application articles, manuals, and the technical documentation previously cited, are shown in Table 1. Channels, rivers, and streams are similar systems. They are fast-moving water bodies; however, rivers are larger, deeper, and longer than streams. In addition, channels are usually the confinement of a river that is narrow because of the relief by which it is surrounded. Coastal is a water body near the sea or ocean, while estuaries form a transition zone between fluvial and marine environments. Lakes and ponds are slow-moving water bodies on land; the difference is that lakes are larger and deeper than ponds. Enclosures, reservoirs, and tanks are formed by dams or locks to store water, and, generally, they are used for a particular purpose. River basin systems and watersheds are rainwater catchment areas that flow through the drainage network. The wetlands include freshwater, brackish, or saltwater, characterized by the biodiversity of the fauna and flora.

Then, according to criteria three and four, the types of processes and output data to be simulated may be identified (Table 2). Mathematical models use mathematical equations to simulate natural phenomena; thus, the system information is represented by mathematical languages. Mathematical models can be further classified as empirical or mechanistic and deterministic or stochastic. The mechanistic and empirical models, also termed black box or statistical, are differentiated by the adjustment of the simulated data to the observed data. If physical processes are involved, the model will be mechanistic; otherwise, it will be empirical. Deterministic models perform predetermined system results based on the input data, while stochastic models perform

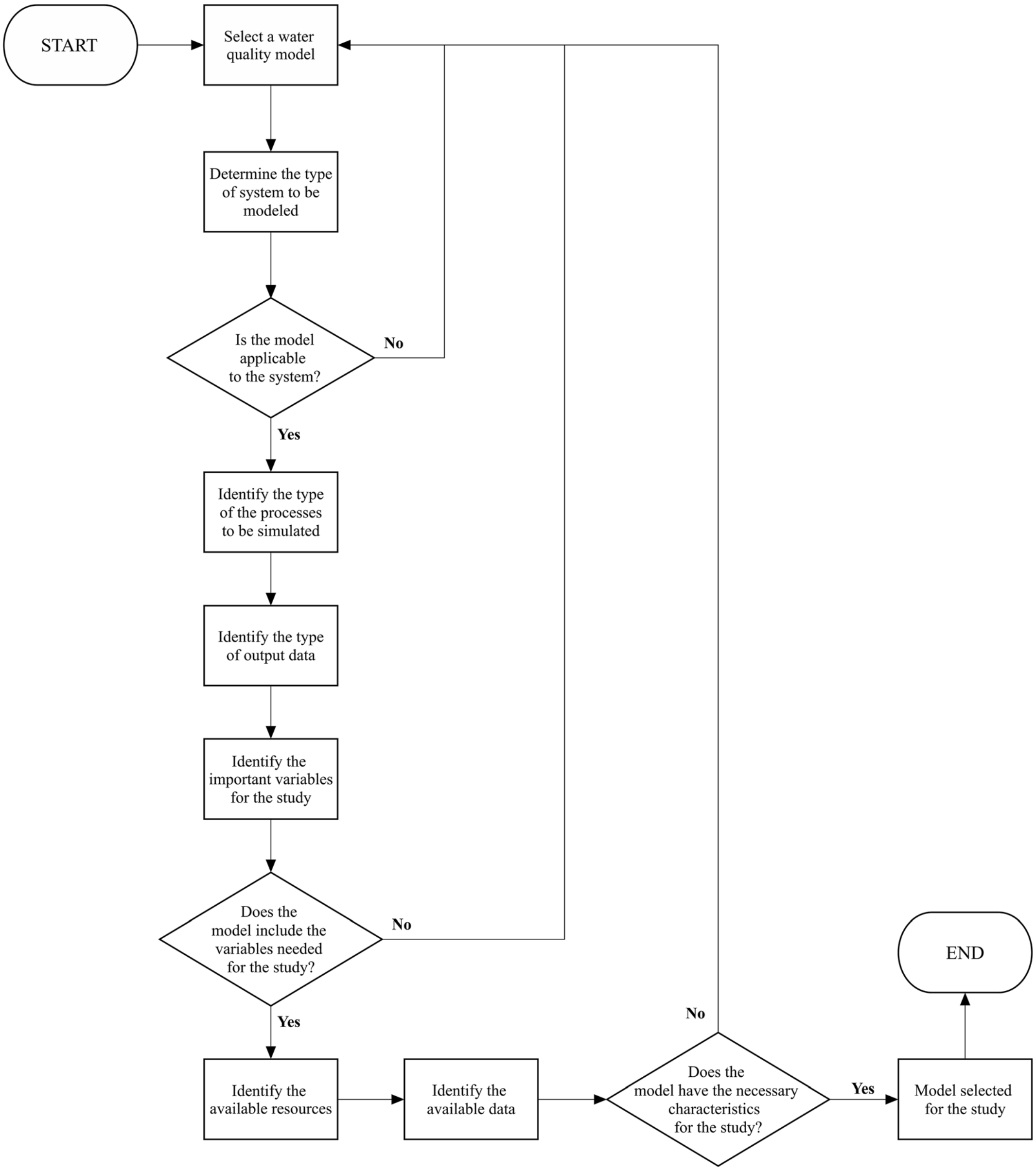

Fig. 2 Flowchart of a comparative guide to help beginners in choosing an appropriate water quality model

system output that depends not only on input data, but also on other, usually random, factors requiring a probabilistic approach.

The third step consists of identifying the important variables for the study; the most relevant variables of water quality are shown in Table 3. The AQUATOX model has similar codes for state variables and driving variables, providing more flexibility to the system. The model may be applied to simulate nutrients, animals, plants, organic toxicants, sediments, and organic matter. Additionally, when the sediment diagenesis model is enabled (and one driving variable), 21 state variables are added as follows: ammonia, nitrate, orthophosphate, methane, sulfide, biogenic and dissolved silica, chemical oxygen demand (COD) and three components of particulate organic matter (POM), particulate organic carbon (POC), particulate organic nitrate (PON), and particulate organic phosphate (POP).

The CE-QUAL-W2 model has more than 40 water quality state variables, including nutrients, temperature,

Table 1 Type of system simulated by the five models

Simulated system	AQUATOX	CE-QUAL-W2	SPARROW	SWAT	WASP
Chanel/river/stream	X	X	X	X	X
Coastal					X
Enclosure/experimental tanks	X				
Estuary	X	X	X		X
Lake	X	X			X
Linked reservoir segments	X				
Linked river segments	X	X			
Pond	X			X	X
Reservoir	X	X	X	X	
Wetland				X	
Total	8	6	4	5	5

sediments, algae, Periphyton, and Phytoplankton. Moreover, more than 60 derived variables can be internally computed from the state variables and output by comparison with the measured data, including pH, algal production, total suspended solids (TSS), and turbidity. The SPARROW model is more applicable to simulate contaminants in water bodies using dependent variables expressed as mass units or by percentage of total contaminant flux to the reach, because the modeling is expressed in the form of a mass balance. In addition, the model technical documentation does not present a list of variables; therefore, for the elaboration of Table 3, the data used were the technical documentation in addition to the articles of application already mentioned. SWAT models are applied to several variables such as climate change, including snow and runoff processes, hydrological cycles, sediments, and phosphorus and nitrogen cycles. The WASP model simulates conventional water quality variables and toxicants.

Therefore, a detailed analysis of the available resources and data for modeling is required. Although they are personal parts of each study, some characteristics of the models help to identify the most suitable for these factors. For example, the dimensions of each model provide information regarding its level of complexity; the larger the dimension, the greater the complexity. Moreover, simplified models are shown for data scarcity; then, the dimensions and temporal resolutions of each model selected are indicated (Table 4). The models can be classified by complexity level considering the following criteria: number of analyzed variables, dimensions, types of processes, and types of outputs. Sharma and Kansal (2013) classified SWAT as an intermediate level of complexity and AQUATOX as a higher level. Chinyama et al. (2014) describes 3-D models as too complex; thus, the WASP as AQUATOX can be considered a model of high complexity. According to Schwarz et al. (2006), in general, purely statistical models tend to be simpler. In addition, SPARROW is described as simpler than SWAT, which indicates that SPARROW can be classified as a lower level of complexity. CE-QUAL-W2 is a 2-D and deterministic

Table 2 Types of processes and output data

	System information			
	Mechanistic	Empirical	Deterministic	Stochastic
AQUATOX	X		X	X
CE-QUAL-W2	X		X	
SPARROW	X	X		X
SWAT	X		X	
WASP	X		X	

Table 3 Modeled water quality constituents

Water quality constituents and processes		AQUATOX	CE-QUAL-W2	SPARROW*	SWAT	WASP7
Nutrients	Ammonia	X	X			X
	Ammonium	X			X	
	Nitrate	X	X	X	X	X
	Nitrite	X	X	X	X	X
	Nitrogen			X	X	
	Orthophosphate		X			X
	Phosphorus				X	X
Water properties	Temperature		X	X	X	X
	Salinity	X	X			X
	Alkalinity		X			
	pH	X	X			
	CBOD		X		X	X
	Dissolved oxygen (DO)	X	X		X	X
Parts of the ecosystem	Algae	X	X		X	X
	Bacteria (coliform)		X	X	X	X
	Fish	X				
	Invertebrates	X				
	Macrophytes	X	X			
	Periphyton	X	X			X
	Phytoplankton	X	X			X
	Zooplankton	X				
	Zoobenthos	X				
Organic toxicant in	Sediments	X				X
	Stratified sediments	X				X
	Phytoplankton/periphyton	X				
	Macrophytes	X				
	Zooplankton/zoobenthos	X				
	Fish/birds/other animals	X				
	Ecotoxicity	X				
	Linked segments	X	X			X
Organic/sediment matter	Labile dissolved organic matter (DOM)	X	X			
	Refractory DOM	X	X			
	Labile particulate organic matter (POM)	X	X			
	Refractory POM	X	X			
	Refractory sediment organic matter (SOM)		X			
	Labile SOM		X			
Agricultural pollutants	Land cover			X	X	
	Pesticide			X	X	
	Human and animal wastes			X		
Dissolved solids	Detritus	X	X			X
	Sand, silt, clay or (TSS)	X	X		X	X
	Sediment diagenesis	X	X			X
Hydrologic cycle	Evapotranspiration				X	
	Runoff				X	
	Time of concentration				X	
	Groundwater				X	
Total		30	25	8	17	19

Table 3 lists the variables that the model has simulated in the literature (from reviewed technical documentation and articles)

*The SPARROW model may be applied to simulate any variables expressed as mass units or by percentage of total contaminant flux to the reach.

model as well as SWAT; thus, by similarity, CE-QUAL-W2 can be considered an intermediate complexity model. Therefore, the models are classified as of lower complexity (SPARROW), intermediate complexity (CE-QUAL-W2 and SWAT), and higher complexity (AQUATOX and WASP).

Case study: Cuiabá River sub-basin

The Cuiabá River Basin is in Mato Grosso State, Brazil. The length of the river is approximately 980 km, with a drainage area of approximately 102,750 km^2. For this study, a 3,645-km-long stretch of the middle river was selected (Fig. 3). Boundaries of the study basin were extracted using the Quantum Geographic Information System (QGIS) and based on a digital elevation model (DEM) (Fig. 4a). Five major types of land use can be found in the sub-basin. The largest land-use area is agriculture, followed by diverse uses, planted pastures, urban, and forests and grassland (Fig. 4b).

The Cuiabá River has strategic importance for its state of origin. More than a third of the population of the state of Cuiabá resides in the drainage area of the river and 46% of the sources of water intake for domestic consumption in several municipalities that make up the basin come from this body of water. The river is also part of the plain of Pantanal, flooding fields and ponds during the flood season. In this way, the river contributes to form one of the largest continuous wetlands and also one of the reference areas for biodiversity in the world (FEMA/MT 2002). The last water quality analysis report made by the State Secretariat for the Environment was carried out in 2005, indicating the importance of current studies in the region.

In this section, a case study is adopted, with a purely didactic purpose in order to facilitate the understanding of the proposed model choice methodology. Considering for this particular study, only the five models were selected in this review.

The first step to identify the most appropriate model for this case was to identify the type of system that is being analyzed, in this case a river basin system (Table 1). Three models (SPARROW, CE-QUAL-W2 and SWAT) were indicated. The influence of land use and occupation on water quality involves physical processes; thus, the model can be mechanistic. The model also may be deterministic or stochastic; thus, all three models can still be used (Table 2). According to the modeled water quality constituents (Table 3), the SWAT and SPARROW models were the most indicated in a study of water pollution by agriculture, because they allow for an analysis of the land use and occupation, nutrients and pesticides. Meanwhile, CE-QUAL-W2 only performs analysis of nutrients, which are sources of agricultural pollution. Finally, it was necessary to check the available data and the desired complexity of the model. For this study, the data was obtained from a site of the National Water Agency (ANA 2020). ANA (2020) provides water quality data; however, the analysis was not continuous. The data were provided at intervals ranging from 4 to 8 months during the years 2011 to 2014 for the study region. Therefore, SPARROW was not indicated because this model demands a sufficiently large number of water-quality monitoring stations and it is a statistical model indicated for long-term water-quality records (multi-year to decadal periods). Some of the parameters monitored in the basin are the following: nitrogen, nitrate, nitrite, temperature, BOD, DO, and TSS. All parameters can be modeled by the SWAT model as shown in Table 3. In this manner, considering only the five models that were selected in this review, the SWAT model was chosen as the most suitable for the study area.

Discussion and conclusion

According to Chinyama et al. (2014), modeling skills are not reserved only for specialists; other researchers and non-specialists also need to acquire modeling skills because of the importance of mathematical modeling to water quality management. Currently, several water quality models are available; however, each model has its particularity. Therefore, the models should not be applied without a previous study of their capacities and limitations for the phenomenon that has been analyzed. In this study, five water quality models currently widely applied were selected and compared with facilitate decision-making regarding which model should be used. The wide applicability of these models during the last 5 years proves their effectiveness in applications worldwide.

The correct choice of a model is part of the management planning work that is among the most important stages of a study. Choosing a model requires a detailed previous study, which takes time; thus, this article seeks to assist in this process. In addition, the choice of an

Table 4 Dimensions and temporal resolution

	AQUATOX	CE-QUAL-W2	SPARROW	SWAT	WASP
Dimension	1-D, 2-D, or 3-D	2-D	2-D	2-D	1-D, 2-D, or 3-D
Temporal resolution	Hours, days, and years	Seconds, hours, days, and years.	Decades, years, and centuries	Hours, days, and years	Seconds, minutes, hours, and days

inadequate model can cause several negative impacts for researchers, such as having to return to the planning stage, or wasting time and resources, particularly if the project has already begun. Moreover, projects must seek their realization in an efficient manner, to select a model with the maximum capacity to model the phenomena involved in the study, according to the availability of resources. Furthermore, the choice of models with considerable technical collection, including manuals and technical documents, facilitates research regarding the functionalities of the models and their manner of application, reducing the invested time.

The studied models were classified as lower complexity (SPARROW), intermediate complexity (CE-QUAL-W2 and SWAT), and higher complexity (AQUATOX and WASP). The SPARROW model was indicated for simple statistical modeling, because it has a simple mathematical structure and is readily built. Moreover, it was indicated for scarce data availability. In addition, SPARROW may be applied to simulate any variables expressed as mass units or by percentage of total contaminant flux in a reach. It is among the few models that has modeled agricultural pollutants such as land cover, pesticides, and human and animal wastes. This model is suitable for modeling long periods of many years up to centuries.

The CE-QUAL-W2 model is relatively simple and has a short model run time, compared with a 3-D model. It was indicated when a fine temporal resolution (seconds) is required. The SWAT model is able to predict the impact of land management practices on water, sediment, and agricultural chemical yields in large complex watersheds with varying soils, land use, and management conditions over long time periods. Also, the model has the advantage of performing the modeling of hydrologic cycle variables, such as evapotranspiration, runoff, concentration time, and groundwater. Moreover, it also includes GIS interfaces to link land use/land cover maps to model plant types, favoring the visualization of the spatial relationship between sub-basins.

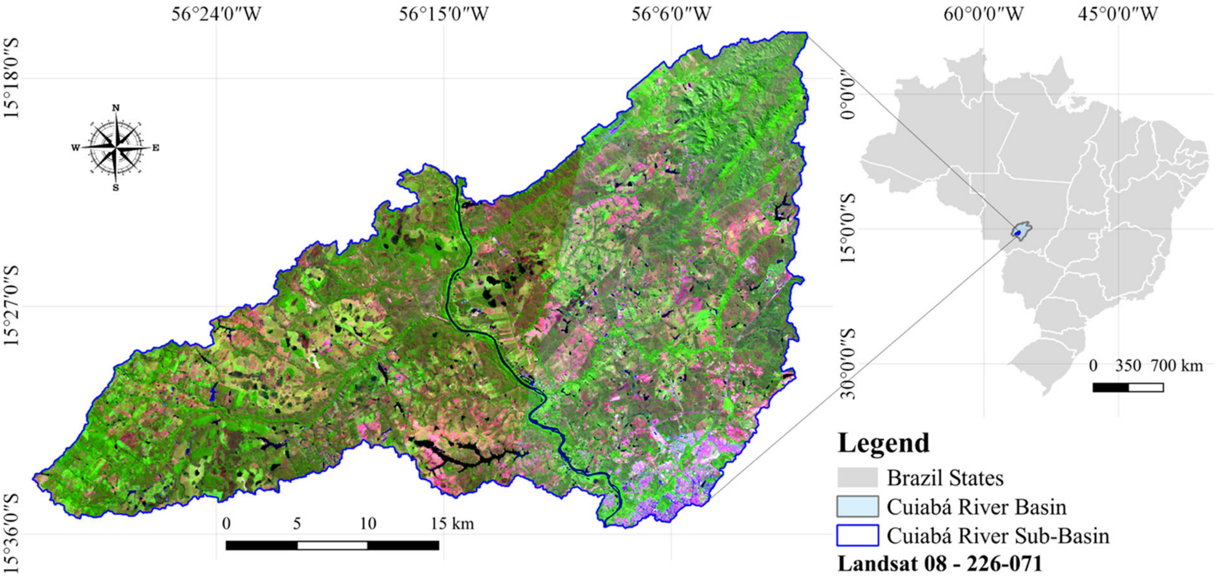

Fig. 3 Location map of the study area

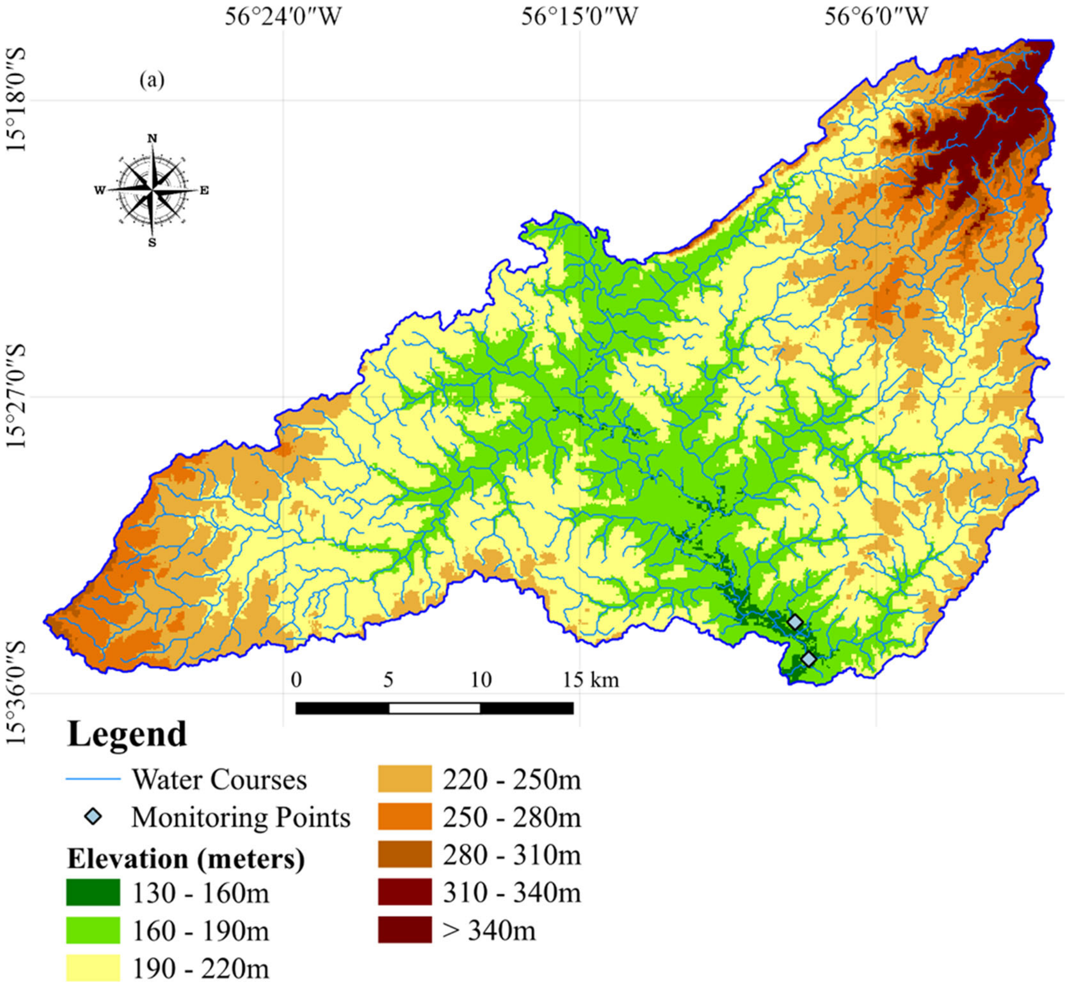

Fig. 4a Elevation of the study area

SWAT was indicated in the exemplified case study of the article when compared with the other models. However, several factors can influence the good calibration of the model, so in each case, the effectiveness of the model must be validated. Thus, the article does not have the objective of choosing the best model among the others studied, because this would not be possible, each model must be analyzed in the specific case.

Sharma and Kansal (2013) state that WASP presents a number of advantages in comparison with the other models AQUATOX, EPD-Riv1, and BLTM. However, most of these advantages are the same as those of the AQUATOX model as follows: public domain; 1-D, 2-D, and 3-D; graphical user interface; and uncertainty analysis. Moreover, although the AQUATOX model is more complex, it has several advantages over the other models. AQUATOX models the largest number of water quality variables, including organic toxicants in several components of the water system, providing a far more detailed ecotoxicological analysis than that of the others. In addition, the model can be implemented in more systems than the others and has the advantage of being able to perform both statistical and deterministic analyses. The model has been widely used for simple studies to complexes such as food webs in 1-D, 2-D, and 3-D. According to Kannel et al. (2011), the WASP7 model is very complex and it is difficult to justify its required time and cost. The WASP model performs ecotoxicological analyses, but in a much more simplified manner than those of AQUATOX, analyzing only the presence of toxicants in sediments, stratified sediments, and linked segments. However, the temporal resolution of the model is

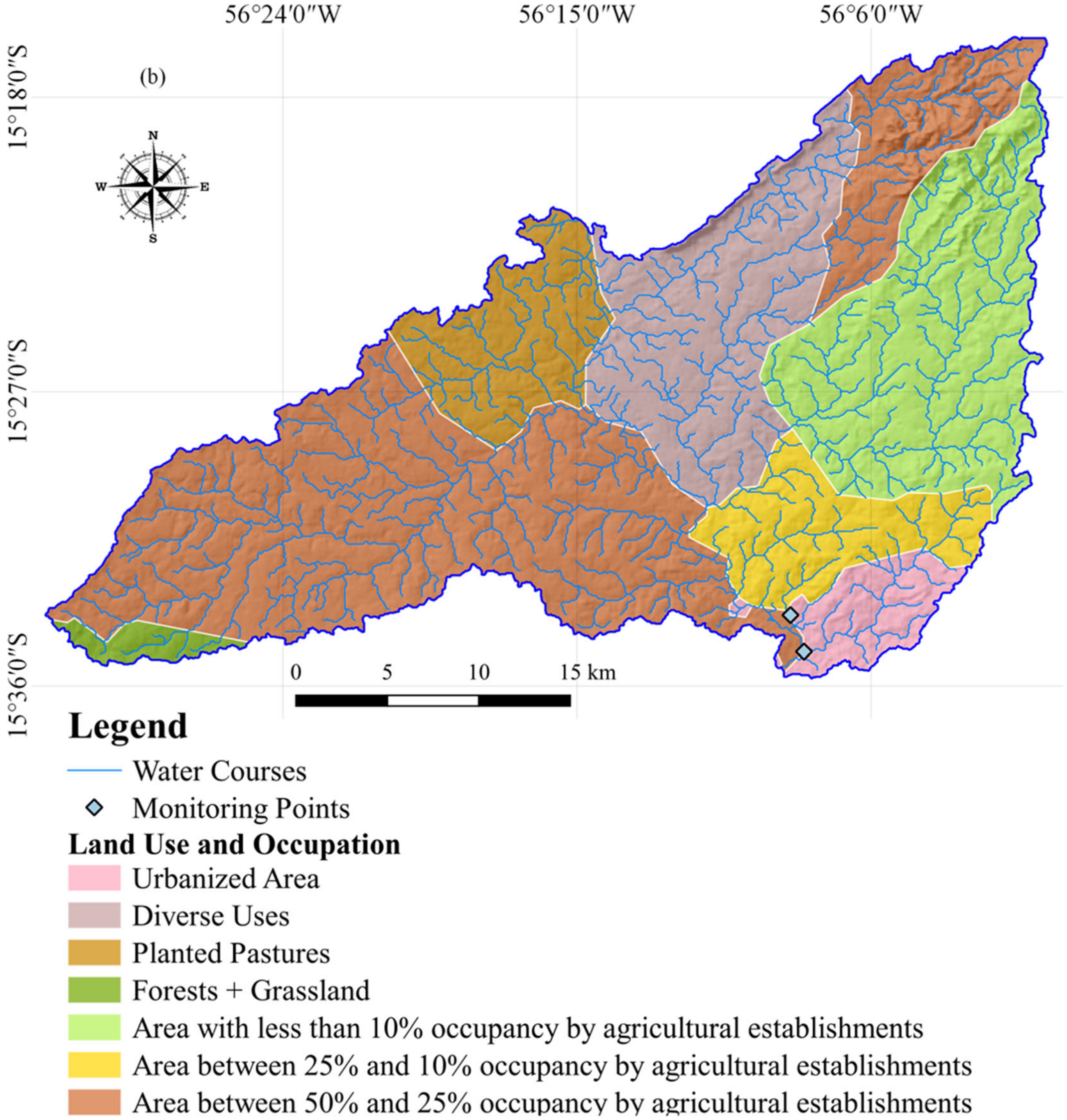

Fig. 4b Land use and occupation of the study area

among its greatest attractions, generating outputs in seconds, minutes, hours, and days.

Therefore, in this study, a comparative guide was proposed to help beginners in choosing an appropriate water quality model. It is useful to save time during the selection stage of the modeling exercise; however, researchers should invest time in identifying the goals of the modeling exercise and the potential consequences of the model results. Moreover, the choice of a model is personal; therefore, other factors must be considered, such as available financial resources, degree of affinity with the models, knowledge of the user, and study objectives.

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