AQUA

Water Infrastructure, Ecosystems and Society

AQUA — Water Infrastructure, Ecosystems and Society Vol 71 No 10, 1127 doi: 10.2166/aqua.2022.063

Assimilative capacity and water quality modeling of rivers: a review

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ABSTRACT

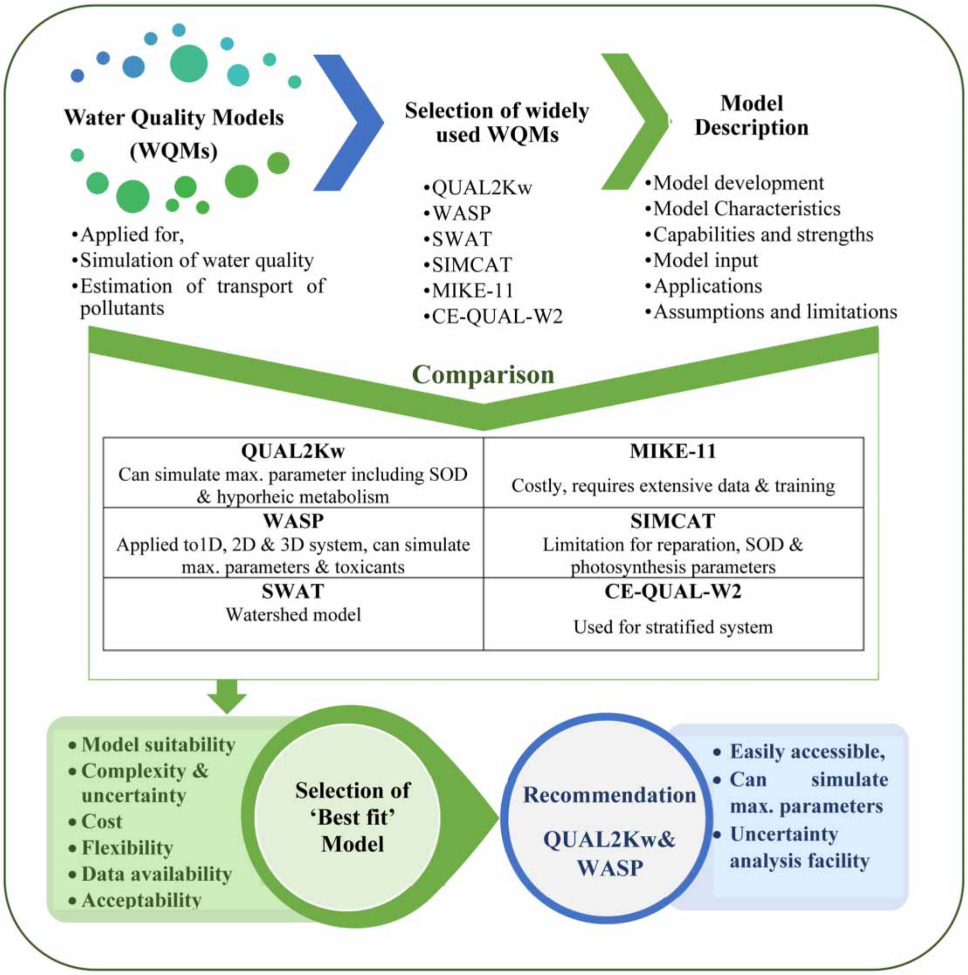
The rivers rejuvenate themselves by traveling over a distance, thereby they assimilate the pollution load and cause their own self-cleansing, also termed 'Self-purification capacity'. To ascertain such assimilative capacity of the river system, various water quality models (WQMs) were studied. Out of numerous WQMs, six models including QUAL2Kw, WASP, SWAT, SIMCAT, MIKE-11, and CE-QUAL-W2 were selected and studied on the basis of their development, characteristics, capabilities and strengths, model input, governing equations, application, assumptions and limitations. A comparison based on such a study showing input variables and data, assumptions and limitations, strengths, and specific characteristics has been carried out and tabulated. While the selection of a model is based on the problem for which the decision-making is to be done. Of all the models, QUAL2Kw and WASP have been found to be advantageous over the rest. For a complex river system, a single model may not work and in such cases, a combination may be tried. A model finally selected for a problem must be calibrated so as to have minimum errors and maximum accuracy.

Key words: pollutant transport, river health, river pollution, self-purification capacity, total maximum daily loads (TMDLs), water quality models (WQMs)

HIGHLIGHTS

- Sustaining river water quality is essential for the entire river ecosystem.
- The assimilative capacity of the rivers defines its limit to absorb pollution load.
- Dissolved oxygen (DO) content is a key indicator of the health of the river.
- Mathematical modeling support in estimation of pollution loads of the river.
- Water quality models serve as an effective tool in Environmental Impact Assessment.

GRAPHICAL ABSTRACT



QUAL2Kw Can simulate max. parameter including SOD & hyporheic metabolism	**MIKE-11** Costly, requires extensive data & training
WASP Applied to1D, 2D & 3D system, can simulate max. parameters & toxicants	**SIMCAT** Limitation for reparation, SOD & photosynthesis parameters
SWAT Watershed model	**CE-QUAL-W2** Used for stratified system

1. INTRODUCTION

The water quality of the river system is a matter of global concern due to escalating urbanization and industrialization. The discharge of huge quantities of untreated wastewater and lack of adequate treatment infrastructure threaten the health of the rivers (CPCB 2021). Depleting river water resources and increased water pollution in rivers remain critical issues in many states of the country (CPCB 2019).

Rivers play an important role in the assimilation of pollution load due to their dynamic characteristic and self-purification capacity (Bennett & Rathbun 1971). Self-purification is the natural process by which the river water quality recovers to its background state after traveling a certain distance. For Indian rivers, especially the River Ganga, the terms *Aviral* (unobstructed flow) and *Nirmal* (pure) have been used many times. While *Aviral* means free flow of water in the river allowing it aeration from the atmosphere, *Nirmal* is related to the self-purification process. The absorption and dissolution of the atmospheric oxygen is a key process in the self-purification process of a river that causes an increase in dissolved oxygen (DO), required for microbial respiration. Hence, DO is considered the most important factor depicting the health of the river (Wen *et al.* 2017; Susilowati *et al.* 2018). It depends on the characteristics of the river such as the velocity of flow, temperature, and depth of flow (Vagnetti *et al.* 2003; Basant *et al.* 2010; Karthiga *et al.* 2017). The organic pollution adversely impacts the DO content of the river (Agunwamba *et al.* 2006; Basant *et al.* 2010). As the organic load in the river increases, the DO starts depleting due to the degradation of biological oxygen demand (BOD). However, the self-purification process allows the river or stream to handle organic loads to a certain extent, which describes its assimilation capacity. Beyond this, as the pollution load increases, it still continues to consume the DO till an anoxic condition of receiving water body is reached, which seriously affects the river ecosystem and its existence (Tian *et al.* 2011; Hanelore 2013). The sustainability of different rivers to carry pollution load depends on various temporal and local factors as well as the type and intensity of the pollutants discharged into the river (Moghimi Nezad *et al.* 2018). Pollution load depends on anthropogenic activities, microbiological reactions, geo-hydrological background, etc. (Ayoko *et al.* 2007).

To limit the pollution load and to maintain the water quality of pristine riverine sources, it is necessary to estimate its assimilative capacity. It enables the assessment of the extent of degradation of water quality. United States Environmental Protection Agency (USEPA) has defined the method for determining the assimilative capacity of the surface water by total maximum daily loads (TMDLs), which determines the maximum allowable pollutant load in water bodies. The method includes the summation of pollutant loads of point source and nonpoint sources with the accountability of seasonal variation as a margin of safety (Wilk *et al.* 2018; USEPA 2021).

$$\mathrm{TMDL} = \Sigma \mathrm{WLAs} + \Sigma \mathrm{LAs} + \mathrm{MOS} \tag{1}$$

where WLAs is the point source loads, LAs is the nonpoint source loads, and MOS is the margin of safety.

The advancement in the field of water quality and for ease of estimating the transport of pollutants resulted in the development of water quality models (WQMs). Mathematical modeling facilitates defining the correlation between assimilative capacity and pollution load and consequently water quality parameters. WQMs act as decision-making tools for determining the extent of dispersion of pollution and its long-term impacts on water quality (Tyagi *et al.* 1999; Bhutiani & Khanna 2007; Singh *et al.* 2009; Mishra *et al.* 2017). It provides the basis for the environmental managers and decision-makers for taking remedial measures for improvement in water quality (Jackson *et al.* 2001; Cassardo & Jones 2011; Wang *et al.* 2013).

The Streeter-Phelps model was the very first WQM that was developed to describe the correlation of DO and BOD and variation in the quality of surface water sources (Alam *et al.* 2007; Dash *et al.* 2020). The model prescribes the DO sag curve that enumerates how DO decreases in a river or stream by degradation of BOD at a certain distance (Streeter & Phelps 1925; Ji 2017). Many studies have utilized the Streeter-Phelps method for the determination of pollution load and self-purification capacity of the river (CPCB 2017; Karthiga *et al.* 2017; Pradana *et al.* 2019). Due to continuous development and a need to analyze specific water quality problems more scientifically, many WQMs have been developed. Wide varieties of WQMs are now available. However, in all such models, the basis is the assimilative capacity of the river system based on the pollution load and self-cleansing velocity of the river. The application of the model requires a thorough understanding of the process, water quality variables, and the parameters of significance that influence water quality. The choice of appropriate model depends on the type and magnitude of the data set, model input requirement, complexity, and limitation of the model. To select a model for a particular water quality problem, it is required to evaluate all existing WQMs.

Several reviews of WQMs are available. Cox (2003) provided a review of six WQMs including SIMCAT, TOMCAT, QUAL2E, QUASAR, MIKE-11, and ISIS. The author examined the capability of each model for the simulation of DO in the lowland river. Sharma & Kansal (2013) compared AQUATOX, BLTM, EPD-RIV1, QUAL2Kw, WASP, and WQRRS models. Each model was described in detail along with the types of errors that occurred during the simulation. Ranjith *et al.* (2019) reviewed models available in the public domain and described six models, WASP7, SIMCAT, QUASAR, TOMCAT, QUAL2Kw, and QUAL2EU. Kannel *et al.* (2011) selected SIMCAT, TOMCAT, QUAL2Kw, QUAL2EU, WASP7, and QUASAR models based on their suitability to simulate the DO content of rivers and streams. Costa *et al.* (2021) evaluated five models, AQUATOX, CE-QUAL-W2, SPARROW, SWAT, and WASP7, and verified the particularities of each model along with its applications. Ejigu (2021) described an overview of water quality modeling with model classification and the selection and highlighted certain WQMs used at the catchment and for water bodies including BASINs, MIKE, Streeter-Phelps, QUAL, AQUATOX, CE-QUAL-RIV1, CE-QUAL-W2, DUFLOW, HSPF, TELEMAC, WASP, HEC-5Q, and EFDC.

The models described above are the physical models and describe the chemical mechanism of water systems. These models compute the linear relationship within variables. The application of these models becomes limited in case of missing data and varying environments, while data-driven models work on artificial intelligence. Artificial neural networks (ANNs) are capable of describing more complicated nonlinear relationships within variables. These models employ a deep learning approach based on a machine learning algorithm. The system of the ANN model includes three distinct layers: input, hidden, and output layers. The hidden layer is comprised of interconnected neurons, where the data introduced through the input layer are processed. A neuron describes the nonlinear function. The results of the model are displayed in the output layer

(Chen *et al.* 2020). Many studies have utilized ANN models for water quality prediction (Krapu & Borsuk 2019; Zhou 2020; Jiang *et al.* 2021; Wu *et al.* 2021; Wu & Wang 2022). The output of the model strongly depends on the quantity of the data. Relatively small data results in poor prediction. In addition, the selection of the algorithm for calibration of the model parameter is an important step for computing complicated relationships between the parameters (Singh *et al.* 2009).

This study includes a review of physically based WQMs. From the review of various research studies and the applicability of existing WQMs in the simulation of river water quality, it was found that certain models are used more. Hence, this study aimed to describe widely used WQMs so as to assist the researchers in the selection of the model as also the significant variables. Six models, including QUAL2Kw, WASP, SWAT, SIMCAT, MIKE-11, and CE-QUAL-W2, have been included in the study. Each model has been described with its development, governing process, applicability, capability to measure different variables, and limitations. The review provides a comparison of the models and a concise summary to support users in the selection of the 'Best fit' model.

2. WATER QUALITY MODELS

The concentration of the pollutants entering the river system may increase or decrease as it undergoes the mass transfer reactions and kinetic processes. WQMs simulate the changes in the concentration of the pollutants as it travels from one place to another. The process of water quality modeling starts with the building of a working hypothesis in the form of a mathematical model. It involves two main stages, analysis of the system and synthesis of the mathematical replica of the system (Wang *et al.* 2013).

WQMs work on the principle of mass transport. The transport in the river is characterized by the phenomena of dispersion and advection. Advective transport is governed by flowing water. Dispersive transport occurs due to differences in concentration. It depends on the physical, chemical, and biological processes and characteristics of the river (Martin *et al.* 2018).

2.1. Model selection criteria

Wide ranges of WQMs are available in the market. WQMs use different algorithms and mathematical equations. The input data requirement, capabilities, complexity, and limitations vary with models. The selection of the model requires a thorough understanding of a specific condition and requirement of a river system. It is necessary to recognize the existing models and their effectiveness to have a reliable output for the management of the water quality of a certain river system.

The selection of a model is the foremost step in the application of modeling. The selection of an appropriate model that matches the objectives of the study is a challenging task and thus there is a need to have criteria for selecting a model.

The criteria for the selection of the WQM are summarized in Figure 1. The model selected should be based on the objectives of the study, data availability, characteristics of the river system, characteristics of the model, and literature review. It should be so selected that it addresses all important aspects of that particular river body. The complexity of a problem leads to complexity in a model. The selection of a very simple model may result in inaccurate and uncertain output, while too complex a model may introduce too many parameters with increased cost of resources. The selected model should be acceptable to the decision-makers of water quality management based on the purpose of its intended use. Every model has its own capability to simulate particular variables. The availability of water quality data for input variables required would be important for model selection through flexibility of the model to update and incorporate more variables for

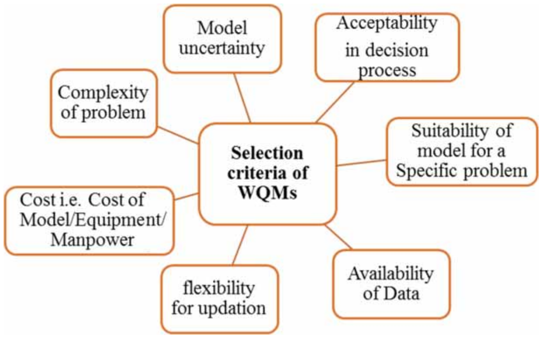


Figure 1 | Model selection criteria.

future requirements should be considered. It is more cost-effective to select a comprehensive model that can simulate present and future needs (Loucks & Van Beek 2017).

The model should be evaluated based on the defined criteria. The Scope-Record-Experience (ScoRE) method can be utilized for the selection of a model in which a set of criteria is defined by the end-users and technical team. The method encompasses the evaluation of the models based on the defined criteria, weightage is assigned based on the criteria, and the model is selected based on the final ranking (Mateus *et al.* 2018).

2.2. Classifications of WQMs

WQMs are broadly classified into two categories: simulation models and optimization models. The optimization model involves a group of mathematical techniques for a particular situation with cost constraint. Simulation models include a set of equations to represent a change in water quality and describe the functioning of the system. A simulation model could either be a physical or a mathematical model. A physical simulation is a scaled representation of a system and obtained results are applied and related to the real system while mathematical models use computer programs to solve the equations for the prediction of changes.

Various mathematical-based WQMs have been developed to represent the water quality change of a water body (Riecken 1995; Sharma & Kansal 2013). Mathematical models can be further classified based on the process, data type, time, and space. Figure 2 illustrates the classifications of WQMs.

- Statistical models use mathematical equations for the analysis of data and establish a fixed relationship between input and output parameters. They are easy to solve. They require an adequate site-specific data set for the prediction of reliable results; otherwise, it leads to uncertainty in the results with large errors. On the other hand, mechanistic models work on theoretical principles. They describe the chemical, mechanical, and biological phenomena of the water system through mathematical equations. Extrapolation from mechanistic models is reliable, though such models themselves may be complex.
- The deterministic model contains no random elements. The relationship between input and output components is determined conclusively and precisely by mathematical equations. The initial condition and parameter values fully define the output of the model, while stochastic models include random elements. The output of the model varies with the same initial condition and parameter value. They are comparatively more complicated.
- Static and dynamic models are classified based on time dependency. Static/steady-state models represent the system that is constant on the time. Dynamic models are time-dependent and the state of variables changes with time.
- Lumped models are zero-dimensional models that describe the homogeneous models and remain uniform in the entire system. Distributed models describe the heterogeneous system that varies with the spatial dimension. Spatial resolution may be one-dimensional, two-dimensional, or three-dimensional based on the spatial characteristics.

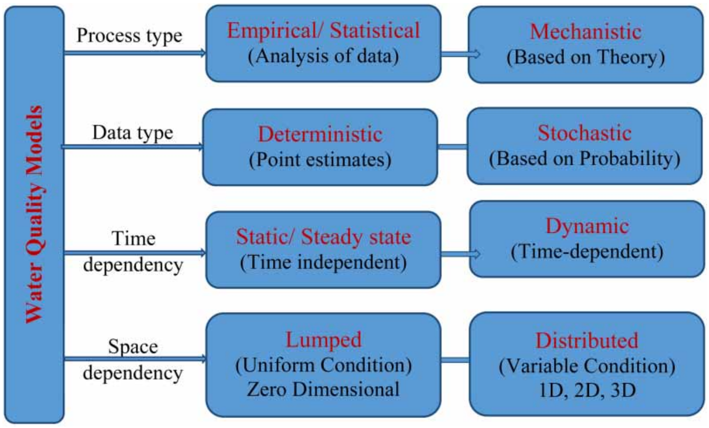


Figure 2 | Classification of water quality models.

3. MODEL REVIEW

The concept of water quality modeling was developed a long time ago. The pioneering work in WQM was done by Streeter and Phelps who developed the first WQM in 1925 for the identification of depletion of DO and pollution scenario of Ohio River (Streeter & Phelps 1925). Subsequently, various WQMs including the steady-state model, dynamic model, and one-, two-, and three-dimensional models have been developed and are used for various water quality aspects.

This section describes QUAL2Kw, WASP, SWAT, SIMCAT, MIKE-11, and CE-QUAL-W2, and widely used river WQMs.

3.1. QUAL2Kw/Q2K

3.1.1. Model development

USEPA developed various QUAL models for water quality modeling of the dendritic river and nonpoint sources of pollution. These are one-dimensional steady-state or dynamic models. A series of models have been developed from QUAL models to QUEL2E series to QUAL2K series models. QUAL2E was amended and established as the QUAL2K model to overcome the limitation of QUAL2E. The modifications include the changes in computer code and the addition of new constituents like algal growth, denitrification, and change in DO by the fixed plant (Park & Lee 2002). QUAL2Kw was an updated version of the QUAL2K model, which was originally developed by Chapra and Pelletier in 2003. QUAL2Kw/Q2K is the modified version of the QUAL2E/Q2E model.

3.1.2. Model characteristics

It is a one-dimensional steady-state model but simulations are in dynamic mode for water quality kinetics and heat budget (Chapra & Pelletier 2003; Turner *et al.* 2009; Ranjith *et al.* 2019).

QUAL2Kw is featured with several new elements: Software is programmed in Microsoft Office with macro and visual basic application and excels as a user interface; river reaches of equal or unequal lengths can be simulated in one system with multiple loadings input option; organic carbon is represented by carbonaceous biochemical oxygen demand (CBOD) in two forms (slow and fast); DO and nutrient fluxes are simulated internally resulting from the interactions of sediment and water; the parameters of bottom algae, alkalinity, total inorganic carbon, pathogens can also be simulated; other parameters like a hyporheic exchange, sediment pore water quality, and light extinction are also included.

The model could be evaluated using sensitivity analysis that helps in the quantification of errors associated with the simulated parameters. The reliability of the model can be obtained by uncertainty analysis. Monte Carlo simulation (A Monte Carlo simulation add-in for Microsoft Excel) calculates the uncertainty of the parameters. Various statistical tests like R^2, Mean Bias Error (MBE), Root Mean Square Error (RMSE), and Standard Deviation Bias Error (SDBE) give better judgment for variations among predicted and observed data (Moghimi Nezad *et al.* 2018).

3.1.3. Capabilities and strengths

It can simulate various constituents including pH, temperature, CBOD, DO, electrical conductivity (EC), organic nitrogen (ON), ammonia-nitrogen (NH_4N), nitrate-nitrogen (NO_3N), organic phosphorus, inorganic phosphorus, phytoplankton, and periphyton. Such simulation also includes both point loads and nonpoint discharge pollutants.

The goodness of the model is that it has an auto-calibration system (Pelletier & Chapra 2008). The model provides a genetic algorithm that is used to determine the optimum value of kinetic rate parameters for the application of the model in good agreement with the observed data. Pelletier Chapra & Tao (2006) provide a framework of QUAL2Kw including a genetic algorithm facilitated by the model for calibration.

The calibrated and validated model provides the results with minimum relative and route square error and is found to be successful in the simulation of water quality data in the effective implementation of the river water quality restoration plan (Sharma *et al.* 2017; Raeisi *et al.* 2022).

3.1.4. Model input

The inputs to the model are general information, simulation and output options flow, concentration of headwater and downstream boundary conditions, reach data, system's hydraulics, dispersion, aeration, weir's height, sediment oxygen demand, flux, reach rate, initial conditions, air temperature, dew point temperature, wind speed, cloud cover, shade, solar radiation, light and heat, model's rate parameters, rate parameters to control genetic algorithm for optional auto-calibration, and water quality parameters (Pelletier & Chapra 2008).

3.1.5. Governing equations

The model uses the following mass balance equation for the analysis of constituents that exist in the water column of respective reach.

$$\frac{dC_i}{dt} = \frac{Q_{i-1}}{Vi}C_{i-1} - \frac{Q_i}{V_i}C_i - \frac{Q_{\mathrm{ab},i}}{V_i}C_i + \frac{E'_{i-1}}{V_i}(C_{i-1} - C_i) + \frac{E'_i}{V_i}(C_{i+1} - C_i) + \frac{W_i}{V_i} + S_i \tag{2}$$

where Q_i is the flow (m^3/d), ab is the abstraction, W_i is the external loading of the constituent to reach i (g/d or mg/d), V_i is the volume (m^3), E'_i is the bulk dispersion coefficient between reaches i and $i+1$ (m^3/d), and S_i is the sources and sink of the constituent due to reactions and mass transfer mechanisms ($g/m^3/d$ or $mg/m^3/d$).

3.1.6. Applications

Ghorbani *et al.* (2022) simulated the water quality of the Dez River (southwest of Iran) by applying the QUAL2Kw model for the parameters of temperature, discharge, BOD, and EC parameters. The model was calibrated and validated for the past data and the critical value of BOD was simulated for the discharge value. The simulation results indicated the critical value of BOD at 40 km from Dez Regulating Dam for the discharge of 190 m^3/s. EC value was found to exceed the permissible limit at a discharge of 50 m^3/s. The reliability of the model checked with RMSE and the percent Bias (PBIAS) coefficient showed the goodness of the model with 95% accuracy. Tran *et al.* (2022) applied the model to Lam Takhong River, Thailand to simulate DO, BOD, nitrate-nitrogen, and ammonia-nitrogen for the critical period and compare it with the designated surface water quality class. The study focused on determining the impairment of DO with the other parameters at different segments of the river. Simulated data of the calibrated and validated model showed that water quality criteria failed to meet at the downstream location showing fourth class water quality with desired DO value >2.0 mg/L and BOD value <4.0 mg/L. The model was found suitable to simulate the future water scenario of Lam Takhong River and would assist resource managers to take appropriate policy measures. Pramaningsih *et al.* (2020) analyzed the pollution load capacity of Karang Mumus River, Samarinda city, and East Kalimantan at four of its different segments using the QUAL2Kw model and land use settlement using Arc GIS. The results showed the exceeding of BOD in all segments and chemical oxygen demand (COD) in three segments. The pollution load was found to have originated due to domestic activities and major land use settlements. Angello *et al.* (2021) used the QUAL2Kw model to determine the impacts of rapid urbanization, lack of pollution management, and sanitation infrastructure facility in the degradation of water quality of Little Akaki River (LAR), Ethiopia. Different scenarios for pollution reduction and water quality improvements were selected. The study concluded that integration of pollution load control strategy, application of best pollution management practices, and application of instream measures such as wastewater treatment at source, control of diffuse source pollution, and the use of cascaded rock ramps could be the best feasible alternative for sustainable development of river catchment. Moghimi Nezad *et al.* (2018) applied the QUAL2Kw model for determining the self-purification of a stretch of the Karun River. The model was calibrated and verified for the past measured data. The results obtained from the model indicated minimum relative and root square error. Park & Lee (2002) applied both QUAL2K and QUAL2E to determine the water quality of Nakdong River, Korea for the parameters including DO, BOD, nitrogen, and phosphorous. The results of these two models showed a significant difference. The author found the results of QUAL2K to be in parity with the results of the field data, which was due to its capability to simulate algal death to BOD, DO, and denitrification.

3.1.7. Assumptions and limitations

The limitation of the model is that it can simulate the main stem of the river system but not its branches (Pelletier & Chapra 2008). The model was found to be highly sensitive to oxidation rate, depth coefficient and moderate to point sources flow, total nitrogen, CBOD, and nitrification rate (Kannel *et al.* 2007; Babamiri *et al.* 2021). Khonok *et al.* (2022) found the model more sensitive for ultimate carbonaceous biochemical oxygen demand (CBODu), EC, and pH compared to DO, total phosphorous, and total nitrogen parameters during both low and high water flow months.

3.2. WASP

3.2.1. Model development

WASP (Water Quality Analysis Simulation Program model) was initially developed in 1970 by Hydro Science, Inc. and was then adapted by the Large Lakes Research Station (LLRS) of the US Environmental Protection Agency for applications to the great lakes (Nikolaidis *et al.* 2006). WASP8 is a modernized version of the earlier 7 versions (Ambrose *et al.* 1991, 2001; Ambrose & Wool 2017). Wool *et al.* (2020) have described the detailed framework of the WASP model from its evolution to the release of the model in 2020, marking 50 years of evolution.

3.2.2. Model characteristics

It is a dynamic model and can be applied to one-, two-, and three-dimensional systems. It is available in the public domain and can be downloaded freely. It can be utilized to assess water quality problems of different water bodies such as rivers, ponds, lakes, streams, reservoirs, coastal waters, and estuaries.

The model can also be connected with sediment transport and hydrodynamic model that provides temperature, depth, flow, velocity, sediment fluxes, and salinity. The model has two submodels within the system; the EUTRO model and TOXI model for aiding simulation of conventional water quality pollution and toxic pollution, respectively.

3.2.3. Capabilities and strengths

The model can simulate various water quality parameters such as BOD, DO, ammonia, organic nitrogen, organic phosphorus, nitrate, phosphate, Phytoplankton, Coliform bacteria, and silica (Melaku Canu *et al.* 2004; Wool *et al.* 2020).

It can be applied to the simulation of water quality of 1D, 2D, and 3D systems. It has been applied extensively for the simulation of organic compounds, polychlorinated biphenyls (PCBs), nutrients, and heavy metals in different water bodies and was found to represent accurate and reliable results of water quality (Mahalakshmi *et al.* 2018; Gordillo *et al.* 2020; Diansyukma *et al.* 2021; Ziemińska-Stolarska & Kempa 2021).

3.2.4. Model input

The inputs to the model are model segmentation, time series flow, point, and nonpoint source loads, initial concentrations, boundary limit output control, kinetic parameters, and constants (Ambrose & Wool 2009).

3.2.5. Governing equations

The simulation is based on a set of equations of transport and transformation phenomena (Ambrose *et al.* 1993; Ambrose & Wool 2009). The model follows the following mass balance equation for simulation (Kuo *et al.* 2006; Yang *et al.* 2007).

$$\frac{\partial C}{\partial t} = -\frac{\partial U_x C}{\partial_x} + \frac{\partial}{\partial_x}\left(E_x \frac{\partial C}{\partial_x}\right) - \frac{\partial U_y C}{\partial_y} + \frac{\partial}{\partial_y}\left(E_y \frac{\partial C}{\partial_y}\right) - \frac{\partial U_z C}{\partial_z} + \frac{\partial}{\partial_z}\left(E_z \frac{\partial C}{\partial_z}\right) + S_L + S_B + S_K \tag{3}$$

where C is the concentration of the water quality constituent (M/L^3); t is the time (T); U_x, U_y, U_z are the longitudinal, lateral and vertical advective velocities (L/T); E_x, E_y, E_z are the longitudinal, lateral and vertical diffusion coefficients (L^2/T); S_L is the direct and diffuse loading rate (M/L^{3}T); S_B is the boundary loading rate (including upstream, downstream, benthic, and atmospheric) (M/L^{3}T); and S_K is the total kinetic transformation rate, positive is source and negative is sink (M/L^{3}T).

3.2.6. Applications

Shabani *et al.* (2021) applied the WASP model and linked it to the Hydrologic Engineering Center-River Analysis System (HEC-RAS) 2D hydrodynamic model to calculate the transportation of arsenic-contaminated sediments due to flood events on Woodbridge Creek, New Jersey. The coupled model was found capable of depicting the transport of surface sediment and arsenic ranging from a net loss of 13.5 cm to a net gain of 11.6 cm, and 16.2 to 2.9 mg/kg, respectively at the end of 48-h flood simulation, per model segment. Obin *et al.* (2021) used the WASP model for the Lushui river to calculate the pollution load using the flux method. The model was calibrated by sensitivity analysis, orthogonal design, and trial and error method. The water quality parameters including COD, ammonia-nitrogen, and total phosphorous parameters were simulated for the normal, wet, and dry seasons. The results were compared with the data given by Zhuzhou Ecological Environment Bureau and found the model quite reliable for water quality prediction and management. Ramos-Ramírez *et al.* (2020) estimated the dispersion of Chrome III (Cr III) pollutants discharged with the process water in the Bogota River. Simulated results showed eight main zones requiring water treatment. Flow, system geometry, and dispersion coefficient were identified as important factors affecting the simulation results. The model was validated by the Index of Agreement (IOA) parameter, which was derived as 0.853, which indicated a good agreement between observed and simulated data. Mbuh *et al.* (2019) applied the model successfully to the Shenandoah River basin to evaluate the influence of nutrient loads and nonpoint sources of pollution on water quality. Yao *et al.* (2015) utilized the model to evaluate the risks of the point source of pollution in the Taipu River. Hosseini *et al.* (2017) found the model effective in determining the impacts on the water quality of the river with the increase in water flow and air temperature. Lai *et al.* (2011) integrated the WASP model with the Integrated Watershed Management Model (IWMM). The model was applied in integration with the watershed model for simulating the water quality of Kaoping River basin, Taiwan for the nonpoint source (NPS) of pollution. The integration showed significant advances in the estimation of the impact of NPS pollutants on river water quality that would be underestimated by the application of only WQM nonpoint sources.

3.2.7. Assumptions and limitations

The model works with the assumption of a completely mixed regime in the river system. The process of sediment transport is based on the user-defined value of temperature and dispersion coefficient. The model has limitations in that it requires extensive training for its effective use, and requires extensive data and time for its calibration and validation. Furthermore, it cannot simulate the parameters of microalgae and periphyton. The effect of mixing zones is not encountered in the model system (Sharma & Kansal 2013; Gao & Li 2014).

3.3. SWAT

3.3.1. Model development

The SWAT (Soil Water and Analysis Tools) model was developed in the early 1990s by the United States Department of Agriculture, Agricultural Research Service (USDA – ARS) in the early 1990s. The model was developed for the prediction of long-term impacts of land management practices on sediment, water, and agricultural chemical yield in large and complex watersheds with the varying conditions of land use and soils. The model was developed with the SWAT94.2 version and upgraded later with the versions of SWAT96.2, SWAT98.1, SWAT99.2, SWAT2000, SWAT2005, SWAT2009, and currently SWAT2012 (Neitsch *et al.* 2005, 2009; Arnold *et al.* 2012a). The algorithm used in SWAT2009 and SWAT2012 is different and hence the model system is nontransferable for nutrient parameters between these two models (Seo *et al.* 2014).

3.3.2. Model characteristics

It is a physical-based model. It can be accessed freely in the public domain. It is used for the simulation of nutrient transport from reservoirs, channels, and groundwater flow transportation. It is a continuous model and helps in understanding long-term impacts (Neitsch *et al.* 2009).

For the simulation process, the model divides the watershed into sub-basins. The sub-basins are further grouped into Hydrologic Response Unit (HRU) and lumped within the sub-basin.

The accuracy of the model depends on the validation and calibration of the model. The performance of the model can be evaluated based on the performance rating of statistics used for the model evaluation (Moriasi *et al.* 2007; Arnold *et al.* 2012b). Arnold *et al.* (2012b) have established the methods for calibration of the model with uncertainty analysis.

3.3.3. Capabilities and strengths

It includes the simulation of water quality parameters such as DO, carbonaceous BOD, and algae. The model allows the simulation of physical processes associated with the transport of nutrients, bacteria, sediments, water, and crop yield directly (Arnold *et al.* 1998).

The model requires minimum data input and can be used for very large and complex basins without extensive cost and time.

3.3.4. Model input

The inputs to the model are watershed general information, precipitation, temperature, solar radiation, wind speed, relative humidity, evapotranspiration, land cover/plant growth, pesticides, nutrient content of fertilizer, water quality, soil characteristics, and point source data (Arnold *et al.* 2012a).

3.3.5. Governing equations

The model simulates the hydrology of a watershed into two divisions. The first division is the land phase which controls the amount of water, nutrient, sediment, and pesticide loadings in each sub-basin of the main channel. The hydrologic cycle is governed by the following water balance equation:

$$\mathrm{SW}_t = \mathrm{SW}_0 + \sum_{i=1}^{t} (R_{\mathrm{day}} - Q_{\mathrm{surf}} - E_a - w_{\mathrm{seep}} - Q_{gw}) \tag{4}$$

where SW_t is the final soil water content (mm H_2O), SW_0 is the initial soil water content on day i (mm H_2O), t is the time (days), R_{day} is the amount of precipitation on day i (mm H_2O), Q_{surf} is the amount of surface runoff on day i (mm H_2O), E_a is the amount of evapotranspiration on day i (mm H_2O), w_{seep} is the amount of water entering the vadose zone from the soil profile on day i (mm H_2O), and Q_{gw} is the amount of return flow on day i (mm H_2O).

The second phase is the water or routine phase that simulates the movement of water, sediments, nutrients, and organic chemicals flowing through the channel. The simulation is governed by a set of equations for the transport of each parameter (Neitsch *et al.* 2009).

3.3.6. Applications

The model has been used worldwide for different applications (Gassman *et al.* 2007). Chen *et al.* (2014) utilized the SWAT model in one of the main tributaries of Xiangjiang River and Zhengshui River to estimate the impacts of different watershed management practices on the transport of nutrients and sediments. The results showed a 10 and 30% increase in nitrate and ammonium nitrogen facilitating implementation of effective measures for improvement in water quality. Malik *et al.* (2022) simulated streamflow of a part of Kashmir valley by the SWAT2012 model and achieved good performance of the model by optimizing parameters through calibration. Epelde *et al.* (2015) applied the model to the watershed area of Alegria to determine the long-term impacts of nitrogen used in agriculture and found trends in nitrogen concentration in groundwater due to its excessive use.

3.3.7. Assumptions and limitations

The limitations of the models are that it is difficult to handle numbers of input files as a large watershed is divided into numbers of the hydrological response unit. It cannot simulate detailed single event flood routing. It does not simulate daily flow occurrences such as storm runoff and changes in DO in a water body. It is difficult to model the impacts of erosion of floodplain and snowmelt (Shoemaker *et al.* 2005).

3.4. SIMCAT

3.4.1. Model development

SIMCAT (Simulation of catchment) was developed by Anglian Water in the United Kingdom (Warn 1987). The model was developed to assess the potential impact of the proposed road drainage outfall on water quality to River Dee Special Area of Conservation (SAC) and some of its tributaries to fulfill the requirement and authorization under Water Environment (Controlled Activities) (Scotland) Regulations 2005 (CAR).

3.4.2. Model characteristics

SIMCAT is a steady-state, one-dimensional, and deterministic model. It is a stochastic model and uses Monte Carlo analysis techniques for simulation. It is used for simulation of fate and transport of pollutants in the river that comes from the point source of pollution (Cox 2003). The impacts of pollutants of conservative and nonconservative nature can be determined by the model (Warn 2007).

In the model system, the river system can be divided into user-defined stretches. The river stretches are considered as continually stirred tank reactors (CSTRs) in series. It considers the complete mixed condition of pollutants for each stretch of the river. It simulates pollutant transport with an assumption of no interactions with sediments (Ranjith *et al.* 2019).

It has been used widely over the years in the United Kingdom and proved to be a cost-effective and practical tool for the management of water quality (Crabtree *et al.* 2009; Warn 2010).

3.4.3. Capabilities and strengths

The model can simulate parameters like DO, ammonia, biochemical oxygen demand, and other user-defined parameters. It is used for the river catchment area to ascertain defined water quality targets and identification of the measures for control of water quality within the defined criteria.

It has an auto-calibration system and hence provides quick and reliable results (Warn 2010). SIMCAT can model up to 600 reaches and can include about 1,400 features such as rivers, weirs, abstractions, discharges, and diffuse pollution (Tsakiris & Alexakis 2012).

3.4.4. Model input

The model can be operated with limited data. The flow of the main river and water quality data are required to enter. The model requires a statistical summary of water quality as it utilizes the Monte Carlo method. The model supports the statistical data in the form of means, standard deviation, and count, statistical distribution data in the form of constant, normal, log-normal, 3 parameters log-normal, nonparametric distributions, and seasonal (monthly) data (Warn 2010).

3.4.5. Governing equations

The mass balance of a particular stretch follows the following equation.

$$C_o = \frac{C_i Q_i + C_t Q_t + C_e Q_e}{Q_r + Q_t + Q_e} \tag{5}$$

where Q is the flow (m^3/min), C is the pollutant concentration (mg/L), O is the outflow, i is the upstream input, t is the tributary input, e is the effluent discharged, and a is the abstractions.

$$v = aQ^b \tag{6}$$

$$t = \frac{L}{v} \tag{7}$$

where v is the flow velocity (m/min), Q is the flow rate (m^3/min), a,b are constants, t is the residence time (min), and L is the length of the reach (m).

The concentration of solute is subjected to the first-order decay, which is used to determine the concentration of pollutants moving to the next reach.

3.4.6. Applications

Crabtree *et al.* (2009) used the SIMCAT model to determine a range of Programmes of Measures (PoMs) to control pollution of phosphate, BOD, and ammonia in River Ribble catchment, North West of England to comply with the water quality standards prescribed in Water Framework Directive (WFD). The results indicated that the daily load of phosphate from all sources would be required to reduce from consented load of 744 to 82 kg/day by 90%. Compliance levels were not achieved for BOD and ammonia. The study suggested reducing the load from wastewater treatment works to achieve compliance. The model has been reported as the best tool to support decision-making in the planning and management of river water quality. Crabtree *et al.* (2006) used the model for an integrated planning study for river catchments of Ehen, Derwent, Kent, and Eden Rivers, England that fails to meet prescribed water quality criteria for the ecosystems under candidate Special Areas of Conservation (cSAC). The results recommended providing controls on effluent discharges and pollution from other sources to meet the defined criteria. Jacobs UK Limited (2007) applied the model to the Dee River to determine the potential impact on the water quality of the river and its tributaries due to the proposed road drainage. Hankin *et al.* (2016) mentioned the limited applicability of the model as a model does not provide a clear mechanism to allow uncertainty parameters.

3.4.7. Assumptions and limitations

The limitation of the model is that it does not simulate a few parameters associated with DO and hence cannot produce reliable results for DO factors. Its application is limited to the parameters of sediment oxygen demand, photosynthesis, respiration factor, and reaeration rate. It does not include the temporal changes and is hence not suitable for complex water systems (Ranjith *et al.* 2019).

3.5. MIKE-11

3.5.1. Model development

It was developed by the Danish Hydraulic Institute, Nederland initially in 1972 (DHI 1993). A series of models have been developed including MMIKE-11, MIKE-21, MIKE-3, MIKE SHE, Mouse, and MIKE Basin models (DHI 1996b, 1996a).

3.5.2. Model characteristics

It is a deterministic model and can be used to simulate unsteady-state flow in a river system. It can be applied to simple as well as complex river systems. It can be used as a WQM to determine the impacts of discharges on river water quality. Also, it can be used as a hydraulic model for flood analysis. The model is integrated with a set of modules including rainfall-runoff, advection-dispersion, and hydrodynamic.

The model is widely used in the United Kingdom (UK) for the management of urban pollution. It has been adopted by the Environment Protection Agency to examine the pollution load of receiving water bodies resulting from a discharge of wastewater (DHI 2017, 2022).

3.5.3. Capabilities and strengths

It can simulate the water quality parameters including BOD, DO, nitrate, ammonia, heavy metals, and coliform bacteria.

3.5.4. Model input

The inputs to the model are water quality; hydrodynamic, advection, and dispersion parameters; cross-section; boundary conditions specifying tributaries, discharges, and abstractions. The data are linked to a time series of flow and water quality entered in an editor interface (DHI 2017).

3.5.5. Governing equations

The hydrodynamic model of MIKE-11 uses Saint-Venant equations for the simulation of one-dimension dynamic flows in the rivers as follows.

$$\frac{\partial Q}{\partial x}+\frac{\partial A}{\partial t}=q \tag{8}$$

$$\frac{\partial Q}{\partial t}+\frac{\partial}{\partial x}\left(\alpha\frac{Q^2}{A}\right)+gA\frac{\partial h}{\partial x}+\frac{n^2gQ|Q|}{AR^{\frac{4}{3}}}=0 \tag{9}$$

where Q is the discharge (m^3/s), A is the cross-section (flow) area (m^2), q is the lateral inflow (m^2/s), h is the water level above a reference datum (m), x is the downstream direction (m), t is the time (s), n is the Manning's resistance coefficient ($s/m^{1/3}$), R is the hydraulic or resistance radius (m), g is the acceleration due to gravity (m^2/s), α is the momentum distribution coefficient introduced to account for the nonuniform vertical distribution of velocity in a given section.

3.5.6. Applications

Minh *et al.* (2022) utilized the MIKE-11 model for the complex river network of the Mekong delta area in Vietnam to analyze spatial and temporal variation in BOD, DO, and temperature parameters. The simulated data obtained from the model revealed the pollution scenario of the study area with the need to take adequate measures to reduce the impact of harmful pollutants. Doan *et al.* (2013) and Kumar *et al.* (2021) adopted the MIKE BASIN model to simulate different scenarios affecting the water availability of the Nhue River of Vietnam and Shipra River, respectively. Dehkordi & Kashkuli (2015) applied the MIKE 11 model for control of total dissolved solids (TDS) entering the Hendijan River from the adjoining drain and Zohreh River and Kheirabad River. The simulated data showed that control of TDS to Hendijan River was achieved through constant TDS and discharge from drains and Zohreh River and increase of discharge from Kheirabad River. The simulated results from the model were found to be important in decision-making in water management. Kamel (2008) applied the MIKE-11 HD model for simulation of unsteady flow along the stream reaching the Euphrates River in Iraq. The model provided satisfactory simulated data that assists the decision-making in the prevention of floods in the Euphrates River.

3.5.7. Assumptions and limitations

The model requires extensive data for its operation without which simulation is difficult for some constituents. A skilled person is required for model set-up. The model can be applied to complex water systems but it does not include the denitrification process. The cross-sections of channels are required to reach boundaries and hence make the simulation lengthy (Cox 2003; Olowe & Kumarasamy 2018).

3.6. CE-QUAL-W2

3.6.1. Model development

The US Army Corps of Engineers (USACE) waterways experiment station developed the CE-QUAL-W2 (Corps of Engineers-Quality-Width Averaged) model. It is a two-dimensional (longitudinal and vertical) water quality and hydrodynamic model. The model was developed originally as an LARM (Laterally Averaged Reservoir Model) and applied to a reservoir without branches (Edinger & Buchak 1975). It was amended subsequently with a water quality algorithm (EHL 1986). A series of versions have been developed and version 4.5 is the latest model upgraded with several new features.

3.6.2. Model characteristics

The model is suitable mainly for rivers, lakes, reservoirs, estuaries, and entire river basins with multiple segments. It is freely available and can be downloaded from www.ce.pdx.edu/w2 (Cole & Wells 2018).

3.6.3. Capabilities and strengths

The model can compute hydrodynamic parameters such as water levels, vertical and horizontal velocities, temperature, and 52 water quality parameters such as pH, DO, nutrients, algae, organic matter, bacteria, and sediment parameters. From the state variables above 60 variables can be derived internally from the state variables such as pH, turbidity, organic carbon, organic nitrogen, total phosphorous, total nitrogen, ammonia in unionized form, and Secchi disk depth (Wells 2021a, 2021b).

3.6.4. Model input

The inputs to the model are topographic map and/or sediment range survey; project volume-area-elevation table; initial conditions of time, temp., inflow and outflow, water body type; boundary conditions; hydraulic and kinetic parameters; calibration data (Wells 2021a).

3.6.5. Governing equations

The model works with the following concentration change equation (Gao & Li 2014).

$$\frac{\partial BC}{\partial t}+\frac{\partial UBC}{\partial x}+\frac{\partial WBC}{\partial z}-\frac{\partial\left(BD_x\frac{\partial C}{\partial x}\right)}{\partial x}-\frac{\partial\left(BD_z\frac{\partial C}{\partial z}\right)}{\partial x}=C_qB+SB \tag{10}$$

where B is the layer of time-space change, C is the horizontal component of the average concentration, U and W are the lateral average velocities in the x-direction and y-direction, respectively, D_x and D_z are the diffusion coefficients of temperature and composition, respectively, C_q is the components of input and output flow of material flow rate, and S is the sources and sinks.

3.6.6. Applications

Al-Murib & Wells (2019) utilized the CE-QUAL-W2 model to calculate the impacts of TDS in the downstream stretch of the Tigris River basin by changes in water flow as the TDS level in downstream areas exceeds the standards of drinking and irrigation water quality. The study revealed that increasing river flow by 15% in the upstream stretch resulted in a decrease in TDS content by 5%. Deus *et al.* (2013) assessed the impact of pisciculture on the water quality of the largest flooded area of Tucurui Reservoir, Brazil by the application of the CE-QUAL-W2 model. The model was calibrated with field data of about 5 years for the parameters of temperature, DO, total suspended solids, ammonia, chlorophyll-*a*, and nitrate. The model was able to reproduce vertical and horizontal gradients with their spatial and temporal variability. The results showed that chlorophyll-*a* is a vital indicator to define the trophic status of the system. The model was found capable of simulating many water quality management scenarios by changes in the reservoir management system. Park *et al.* (2014) applied the W2 model for estimating nutrient loads discharged from a parallel-connected three reservoirs into the ocean considering the different flow scenarios. The simulated data showed that under an optimal flow scenario and by controlling chlorophyll-*a* content in the reservoir the loading of total nitrogen and total phosphorous could be reduced by 27.2 and 6.6%, respectively.

3.6.7. Assumptions and limitations

The limitations of the model are that the governing equations are averaged layer and laterally; lateral variations in temperature, velocities, and water quality constituents are not accounted for; it is a complex model and its operation is time-consuming; the complexity of the model limits the data required for its operation; vertical momentum is not included, which might not give an accurate outcome in the case of significant acceleration (Wells 2021a).

4. DISCUSSION

WQMs are very useful in identifying the extent of pollution contaminants in water quality and forecasting their long-term impacts. The Streeter-Phelps model was the very first model to describe the DO sag over the transport of pollutants along with the waterways. A wide range of WQMs has been developed and used for simulating different pollution scenarios of river water quality. The WQMs have gained much importance because of their application in the projects of river water quality management and its restoration. However, choosing a particular model for a specific type of water quality problem is a challenging task and varies with the different applications. Rivers are complex water systems. Alterations in the water quality of river water depend on the characteristics of the water body, seasonal variations, pollutant sources, and the predominance of pollutants. The data requirement of each WQM varies and each model has some limitations due to its governing mathematical equations and the type of software used. The selection of a WQM depends on various factors such as the water body type, availability of data set, the objective of the user, and availability of resources. A list of criteria have been attempted at the selection of the model. The level of complexity and output from the model are the governing criteria in the selection of a WQM. Table 1 represents the summary of selected WQMs widely used for the simulation of river water quality. Based on the summary of selected WQMs, an appropriate model may be chosen and applied.

From the review and summary of the selected model, the following can be inferred:

- MIKE-11 is not available in the public domain and also needs substantial training for its operation.
- The requirement of data input is quite extensive in the case of CE-QUAL-W2, WASP, and MIKE-11.
- SIMCAT, though a simple model, has a limitation on simulation of respiration, sediment oxygen demand, and photosynthesis and may be used when modeling using these parameters is not essential.
- As far as considering flow and state conditions are concerned, WASP and MIKE-11 can be applied to the unsteady-state flow condition.
- WASP can be applied for the simulation of one-, two-, and three-dimensional water quality of river systems but it works with an assumption of a completely mixed regime in a water column.
- SWAT is the watershed hydrological model and can be applied for simulation of nutrient transport from reservoirs, channels, and groundwater flow transportation.
- If simulation of maximum numbers of parameters is to be done, QUAL2Kw and WASP may be more useful. WASP is also capable of simulation of toxicants. QUAL2Kw can simulate sediment oxygen demand and hyporheic metabolism as well. It has certain advantages including easy accessibility, an auto-calibration system, etc.
- CE-QUAL-W2 is widely used in stratified water bodies such as lakes, estuaries, etc.
- For a complex river water quality scenario, a single model may not be able to simulate all the required parameters. Such models in combination can solve the problem of simulating desired parameters associated with the single model.

5. CONCLUSION

WQMs have been widely adopted as decision-making tools in water quality management for determining the transport and fate of pollutants. The review describes a few widely used river WQMs with their data requirement, capability to simulate variables, limitations, and criteria for selection of the model. The applicability and complexity of the models have also been compared. Looking at the comparison of six selected models, QUAL2Kw and WASP were found to be advantageous over the others when compared in terms of ease of accessibility, the capability of simulating maximum numbers of parameters and facilitating the computation of uncertainty analysis. These models have been applied widely to river rejuvenation projects in the country like India. However, the choice of model is influenced by the objectives of modeling, availability of data, and

Table 1 | Summary of selected water quality models

Model	Origin and type	Whether in Public domain?	Type of Waterbody	Variables incorporated in the model	Input data requirements	Assumption and limitation	Strengths and specific characteristics
QUAL2Kw	USEPA; 1D, steady-state	Yes	Rivers, Tributaries, lakes	pH, Temperature, DO, Conductivity, SS, Alkalinity, CBOD, Total carbon (Organic, inorganic), ON, NH_3, NO_2, NO_3, OP, PO_4, Bottom algae, Detritus, Phytoplankton	• Headwater flow and concentration • Discharges and withdrawals • Reach lengths and elevations • Meteorological data • Hydraulic data • Kinetic rates and constants	• Flow is assumed to be a steady-state • Cannot simulate branches	• Includes multiple loadings and abstractions • Includes an in-built automatic calibration system • Allows simulation of unequal river spaces • Can simulate even the bottom algae
WASP	USEPA; 1D, 2D, 3D	Yes	Rivers, Streams, Lakes, Ponds, Estuaries, and Coastal waters	pH, Temperature, DO, NO_2, NO_3, OP, PO_4, Phytoplankton, Periphyton, CBOD, Bottom algae, Detritus, Salinity, Coliform Bacteria, Silica, Sediments, Metals, Toxics	• Output control • Initial concentrations • Boundary limit • Model segmentation • Point and nonpoint source loads • Kinetic parameters and constants • Time series flow	• Does not consider mixing zone • Requires extensive data for calibration and verification • Enables simulation of periphyton or microalgae • Dispersion coefficient and temperature are included as a user-defined parameter	• Flexible model and can simulate 1D, 2D, and 3D systems • It addresses the process of the water column and underlying sediments • Used to simulate a wide range of organic compounds, nutrients, heavy metals, PCBs
SWAT	USDA - ARS; 1D, Continuous-time work	Yes	Groundwater flow, sediments, and nutrients transported in channels and reservoir	Sediments, NH_3, NO_2, NO_3, OP, PO_4, DO, BOD	• Precipitation • Temperature • Solar radiation • Wind speed • Relative humidity • Evapotranspiration • Land cover/Plant growth • Pesticides • Nutrient content of fertilizer • Water quality • Soil characteristics • Point source data	• Difficult to handle numbers of input files due to division of large watershed into numbers of units • Cannot simulate storm runoff and changes in dissolved oxygen	• A watershed hydrological model • Used to predict long-term impacts in rural and land management practices and complex watershed • Can be applied for simulation of nutrient transport from reservoirs, channels, and groundwater flow transportation
SIMCAT	United Kingdom (UK); 1D, Steady-state	Yes	Rivers	DO, CBOD, PO_4, NH_3, User-defined parameters	• Discharge and water quality data in the form of statistical distribution	• Changes in reaeration rate and temporal changes are not considered	• Auto-calibration • Can be operated with limited data • No specific training required

(*Continued.*)

Table 1 | Continued

Model	Origin and type	Whether in Public domain?	Type of Waterbody	Variables incorporated in the model	Input data requirements	Assumption and limitation	Strengths and specific characteristics
MIKE-11	Danish Hydraulic Institute, Nederland; 1D, unsteady flow	No	River, Lakes, Estuaries, and Tidal wetlands	DO, BOD, Nitrate, NH_3, Heavy metals, Coliform bacteria	• Water quality • Hydrodynamic, advection and dispersion parameters • Cross-section • Boundary conditions specifying tributaries, discharges, and abstractions are linked to a time series of flow • Water quality to enter in an editor interface	• Requires extensive data for its operation • Need expertise for the operation of the model • Simulation is lengthy as it requires cross-sections of the channel to reach boundaries • Not freely available and may be costly to use	• Can simulate complex river water systems with branches • Capable of simulating dynamic movements of river water in addition to water quality parameters
CE-QUAL-W2	US Army Corps of Engineers; 2D, longitudinal/vertical	Yes	Rivers, Lakes, Estuaries	pH, Temperature, DO, Alkalinity ON, NH_3, NO_2, NO_3, OP, PO_4, CBOD, Bottom algae, Detritus, Phytoplankton	• Topographic map and/or sediment range survey • Project volume-area-elevation table • Initial conditions of time • Temperature • Inflow and outflow • Water body type • Boundary conditions • Hydraulic and kinetic parameters • Calibration data	• Assumes a well-mixed condition in the lateral direction • Lateral variations and vertical momentum are not included • Complex and time-consuming model • Requires a significant amount of data	• Can simulate the eutrophication process and sediment relationship • Best suited for the long and narrow water body

1D, one-dimensional; 2D, two-dimensional; 3D, three-dimensional; DO, dissolved oxygen; SS, suspended solids; CBOD, carbonaceous biochemical oxygen demand; ON, organic nitrogen; OP, organic phosphorous; BOD, biochemical oxygen demand.

resources. The user would thus have to understand the assumptions of the model and the suitability of the model for a defined problem. An appropriately selected model can simulate the actual scenario of a given water system and would reflect the reliable output. A model must be calibrated before its application to a specific problem. The goodness of the model can be defined by uncertainty analysis. The calibrated and validated model provides the 'Best fit' results to conclude a problem.

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.

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First received 2 May 2022; accepted in revised form 6 September 2022. Available online 17 September 2022