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WATER QUALITY MODELS: A COMPREHENSIVE REVIEW

Madhuben Sharma

Sustainability Cluster, University of Petroleum and Energy Studies, Bidholi, Energy Acres, Dehradun, Uttarakhand 248007, India, amadhubensharma06@gmail.com

Abstract

Models of water quality are the instruments that help in in simulating and envisaging the distributions of pollutants, their concentrations, and the associated risks in water bodies. Results of these water quality models provide a platform to figure out how different types of pollution affect water quality. This leads to the development of solutions to overcome the risks. In the present study four water quality models (WQMs) are reviewed viz. QUAL 2K, MIKE, WASP and QUASAR that have been widely used all over the world. All WQMs have window based graphical interface and are freely available except MIKE 11. They are dynamic in nature and also data intensive except QUAL2K model. Each parameter has a default value in every models. The study highlights the usage of these models by different researchers, globally. Key words: Water quality, Water quality models, QUAL, MIKE, QUASAR, WASP

1.0 Introduction

Water is an indispensable natural resource on which all life forms depend. Natural water resources can be grouped into two types: surface water and groundwater. Surface water resources comprise rivers, lakes, ponds, and oceans. Out of all, rivers are an important component of the natural environment, and its water quality needs to be protected from pollution as human survival depends on their sustainable use. Water quality is the degree to which water meets the needs of one or more biotic organisms and/or any human need or purpose Shah[1]. Natural phenomena (climate and geology) and anthropogenic sources (mining, agriculture, forestry, cattle farming, and urbanization) are the major sources of river water pollution. Anthropogenic sources consist of point and diffuse sources of pollutants, which lead to two important water problems—eutrophication and bio magnification. As per World Health organization (WHO), contaminated water can spread diseases like typhoid, polio, dysentery, diarrhea and cholera. It is predicted that each year 485 000 diarrheal deaths are due to consumption of contaminated drinking water [2]. For development of a nation, water plays a key role, as safe water access is under basic human rights. Hence, water pollution control and water quality management strategies have gained prime importance in the wake of serious environmental scenarios such as depletion of resource, shifting of climate, population explosion, increased public awareness. For effective management of water more emphasis should be given to quality than quantity to meet various demands of public. In order to create and implement better management plans, researchers are focusing on the forecast of water quality, the threat posed by contaminants, and their categorization. One of the severe challenge with the study of water quality data is the non-linearity, dynamic and vague properties due to the uncontrolled and non-traceable causes of contamination. The water quality parameters also

interfere with each other making the process more complex. Although efforts are being made by researchers around the world in cooperation with the government, the quality of the world's water is still declining in many regions. It is desirable to build a water quality model that can anticipate water quality based on changes in land use, population growth, effluent discharge, and climate change. The WQMs help us to identify the pollution sources and to perceive different biogeochemical phenomena in the water bodies which otherwise are difficult to be evaluated with field monitoring only. They also assist in predicting the possible future event in given water bodies. The WQMs are cost effective tools that help in simulating the fate and transport of pollutants in the water bodies [3].

In the present paper, development history of WQMs and four popular WQMs are discussed. This review paper will surely help readers to know about these four popular WQMS, their characteristics, strength and weakness in brief

1.1 Water quality model

According to James [4] and Chapra [5], WQM is a series of equations is used to represent the factors and processes that determine the instream concentrations or loads, or the leaching rates if the model is relevant at the plot, field, or sub-catchment scale. Researcher Wang et al. [3] stated that WQMs are effective tools that help in environmental management of surface water quality. Wang et al. [6] found that WQMs are cost effective and help in predicting and simulating pollutant transport in water environment. According to Lacroix et al. [7], models are simple or complex computer programs or spreadsheets depending on the degree of process representation. Globally, numerous WQMs are available for river systems, which are unique in their hydrological characteristics and their own particular pollution problems. With no clear conceptual and consistent worldwide basis for development of WQMs, initially this process took place in phases. Historically, Streeter Phelps (1925) first developed DO sag curve that was further updates by Theriault. [8], Fair. [9], Thomas [10],Dobbins [11], Yu et al. [12].Several authors Wurbs. [13], Tsakiris and Alexakis [14], Wang et al. [3], Gao and Li, [15] reviewed several WQMs are depicted in Figure 1.

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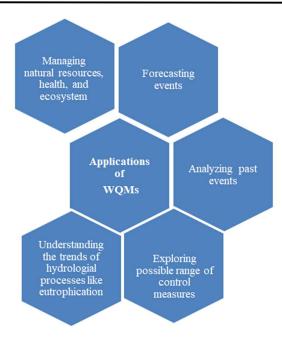


Figure1.1 Applications of WQMs

1.2 Classification of Water Quality models

WQMs can be classified on the basis of environment, purpose, dimension, processes, data type and time variations. Figure 1.2 depicts different subdivision of WQMs.



Figure 1.2 Classification of water quality models

The mechanistic models help in understanding the cause-and-effect relationship of the water quality of a particular stream whereas an empirical model based on past observed empirical relationships relates a water quality parameter to a particular output. In deterministic model, the connection between the user's inputs and the model's outputs is fixed and predetermined. The model always yields the same result regardless of the inputs since its calculations presuppose that the input and output variables are fixed (not subject to mistake). A stochastic/probabilistic model is one that is repeatedly run with different input variables (such as boundary conditions or parameters) chosen from a defined statistical distribution, and then produces results also in the form of a statistical distribution. Cross-sectional models help in understanding the behavior in number of cross sections whereas in a longitudinal model only

Copyright © 2022. Journal of Northeastern University. Licensed under the Creative Commons Attribution Noncommercial No Derivatives (by-nc-nd). Available at https://dbdxxb.cn/ one section of behavior can be understood at a time. Static model is a time-independent model where a behavior of water body will be constant over a period of a time while a dynamic model is a time-dependent model where water quality will vary with time. Lumped parameter model is a zero-dimension model and it represents uniform conditions for the modeled system while a distributed-parameter model helps in understanding the condition of the model in different spatial dimensions (1D, 2D, 3D).

2.0 Evolution history of water quality models

In the year 1925, Streeter and Phelps became the pioneer in the field of river water modelling. They developed DO sag curves which were further advanced by researchers from all over the world. Numerous researchers-Thomann.[16] McBride and Rutherford.[17]; Thomann and Muller [18];Adrian and Sanders [19] have used advance computational methods in modelling complex river systems. Later in 1998, a three tier study was conducted to compare two river quality models series namely – Activated Sludge Models and QUAL2 models developed by International Association on Water Quality (IAWQ) and United State Environmental Pollution Authority (USEPA) as reported by Raunch et al.[20], Shanahan et al.[21], Somlyody et al.[22]. These studies identified numerous significant drawbacks but one of the most significant was poor field data gathering, which make the process of model calibration more difficult.

Researchers (Cox. [23] and Cox [24], Ambrose et al. [25], Kannel et al. [26] also thoroughly examined a variety of water quality models as well as advanced modelling techniques. But, still the amount of research that has been conducted on the application of WQMs and their capacity for prediction is extremely limited. One possible source of this inconsistency is a mismatch between the data collected by water quality surveillance stations and the input data required by WQMs. A further important requirement in modelling is the selection of a model, which is determined by a number of factors including the complexity of model events, the extent of desired output information, the nature of the water body, the assumption used in basic equations, and the scale of interest in either a steady state or a non-steady state condition. In light of the preceding explanation, the following section provides a most recent advances that have been made in the modelling of river water quality. In a river system, intrinsic and extrinsic characteristics affect DO source-sink balance. For example parameters like slope, temperature, width, depth, degree of turbulence influenced the reaeration of DO. Many assumptions initially made for mathematical treatment of the complex phenomenon have been tackled by noteworthy inputs from Velz. [27], Velz. [28], O'Connor and Dobbins. [29], Thomann. [16]. To estimate the "Sinks" for DO a method was developed by Orford and Ingram. [30] and Young and Clark. [31]. There were different schools of thought for order of reaction as Nemerow. [32] relied on second order reaction while Butts and Kothandaram.[33] used first order reaction. Mamedov.[34] used second order BOD reactions for analytical evaluation of the oxygen sag equation. Chen.[35] contributed to the development of nutrient and food chain models for rivers. During 1980's Scavia and Bennett [36] reported that 2D models were developed, in order to overcome the limitations of 1D models. The development of 3D models can be traced back to the 1990s, when eutrophication issues were also included in RQMs. During the same

decade, researchers Adrian et al.[37]; Alshawabkeh and Adrian. [38], Tyagi et al. [39], Kim and Cardone. [40], Lopes et al. [41] included nutrients such as phosphate, nitrogen, phytoplankton, zooplankton, and fishes into RQMs. At the same time optimization and stochastic models were also developed by Demuynck et al. [42], Somlyody et al. [22]. For managing watersheds, there are different computer models for different bodies of water like SWAT and MIKE. Likewise, CE –QUAL-W2 have been developed for lake and reservoir management. In the same way, many models, such as the QUAL series, WASP series, MIKE series and QUASAR have been used to simulate the quality of rivers.

QUAL Series: The United States Environmental Protection Agency (USEPA) has released multiple versions of the QUAL model, including the QUAL2E, QUAL2E-UNCAS, QUAL2K, and QUAL2KW. QUAL series models are a steady-state, one-dimensional (1D) model. These series models are widely used in river simulations. In 1985, QUAL2E was developed which is further improved to QUAL2E-UNCAS and QUAL 2K. Further QUAL2K is upgraded to QUAL2Kw. QUAL2Kw is most advanced and recent version of QUAL series model [43].

MIKE-series: Dansih Hydraulics Institute developed MIKE model. MIKE series have different version models like MIKE 11, MIKE 21, MIKE 3 and MIKE SHE. It is becoming increasingly necessary to have understanding of the water quality as well as the implications of human actions. In many circumstances, numerical modelling is necessary to obtain precise understanding about these complex systems. The high degree of variability that characterizes nature and the complexity of ecological systems necessitates that the modelling software be capable of accounting for these variations. Hence MIKE 21 and MIKE 3 software contains a number of modules that, when combined, essentially cover the entire range of water quality and ecology applications imaginable. These modules were developed to help us solve the aforementioned issues [44]

Water Quality Analysis Simulation Program (WASP): This series models is a well-established three-dimensional deterministic model which provides dynamic compartment-modeling for aquatic systems (Di Toro et al. 1983). The model can reproduce time-varying advection, dispersion, point and diffuse mass loading, and boundary exchange processes [45].

QUAlity Simulation Along River systems (QUASAR) : Researcher [46] developed this model to simulate the river flow and water quality along the Bedford Ouse. Initially this model help in forecasting the river water quality. Data collected from telemetered sources was fed into this model which help in a real-time forecasting at different river abstraction sites [47]

Table 1 summarizes characteristics of typical models such as the QUAL-series, MIKE-series, WASP series and QUASAR. The majority of these models are mechanistic in nature and can be used to simulate the DO and BOD concentrations in river water.

Table 1 Summary of comm	on popular WQMs
Model	QUAL
Model Version	QUAL I;QUAL II;QUAL2E; QUAL2E UNCAS; QUAL 2K
Model Developer	U.S. Environmental Protection Agency's (USEPA)
Popular QUAL model	QUAL 2K
Model Characteristics of	• A steady-state, one-dimensional (1D) model.
QUAL 2K	 QUAL 2K uses unequally spaced reaches and allows multiple loadings and withdrawals per reach. Advective-dispersive mass transport and reaction equations are employed in this model. Dissolved oxygen, temperature, biochemical oxygen demand, organic nitrogen, ammonia nitrogen, nitrate nitrogen, total nitrogen, sediment oxygen demand, organic phosphorus, inorganic phosphorus, total phosphorus, phytoplankton, and algae: all of these can be simulated to improve our
	understanding of water quality.
Region/Country where QUAL 2K model applicable	Malaysia, Vietnam , Iran, India, Kenya, Baghdad, China and Taiwan
References	Kamal [48]; Bui et al. [49], Mustafa et al. [50], Idris et al. [51], Hagdu et al. [52] and Zhang et al. [53]
Model	MIKE
Model Version	MIKE11;MIKE 21;MIKE 3, MIKE -SHE
Model Developer Popular MIKE model	Denmark Hydraulic Institute (DHI) in 1972 MIKE 11
Model Characteristics	• 1D and dynamic model system.
would characteristics	
	• Designed to have an integrated modular structure
	comprising of hydrodynamic, advection-
	dispersion, rainfall-runoff (RR) module, non-
	cohesive sediment transport (ST/GST) module,
	cohesive sediment transport module and water
	quality module with basic computational modules.
	• Simulate
	 solute transport and transformations in complex river systems
	 the hydrodynamics of branched and looped rivers and estuaries.
Region /country where model applicable	Bangladesh, Kenya, Romania, China and India

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References Model Model Version Popular WASP model Model Developer Model Characteristics	 Chowdhury et al. [54], Kanda et al. [55], Andrei et al. [56], Chang and Zhi.[57] and Gedam et al. [58]. Water Quality Simulation Program (WASP) WASP1-7 models WASP-7 U.S. Environmental Protection Agency's (USEPA) widely used three-dimensional WQM. can be applied in 1D,2D, 3D (Wool et al. 2001). Advection, dispersion and kinetic transformation are used to simulated the transport, loading and transport processes. Fourteen state variables transport and transformation can be simulating with WASP 7. Two major water pollution problems-conventional pollutants (DO, BOD, nutrients and eutrophication) and toxic pollutant (organic chemicals, metals and sediments) are simulated by EUTRO and TOXI. Model contain additional sub models namely Periphyton, HEAT and MERCURY. This model is suitable for water quality simulation in rivers, lakes, estuaries, coastal wetlands, and
	reservoirs.
Region /country where	Pakistan, Singapore, Bangladesh, Taiwan and New York
model applicable	
References	Iqbal et al. [59], Angeles.[60], Lin et al. [61] and
Model	Franceschini and Tsai. [62]. QUAlity Simulation Along River systems (QUASAR)
Model versions	QUASAR, HERMES and QUality Evaluation and
	Simulation TOol for River systems (QUESTOR)
Popular Model version	QUASAR
Model Developer	Bedford Ouse
Model Characteristics	• It's a dynamic, stochastic and 1 dimensional
	continually stirred tank reactor (CSTR) based
	model.
	 uses Runge Kutta techniques is for solving ordinary differential equations. consist of 2 modes dynamic and planning. simulate pH, nitrate, ammonium, temperature, E.coli, algae, biochemical oxygen demand (BOD), dissolved oxygen and conservative
	11

pollutant.

Region /country where	• help in modelling large freshwater river systems. India and United Kingdom
model applicable	Lewis et al. [63]; Eatherall et al. [64], Sincock and Lees.
References	[65]

3.0 Conclusion

Most commonly used WOMs are OUAL2K, WASP MIKE 11 and OUASAR. All WOMs have window based graphical interface and are freely available except MIKE 11. All WQMs are dynamic in nature and also data intensive except QUAL2K. For various rate parameters, all models have a set of default values. Maximum number of parameters is simulated by all four models. QUAL2K model performs well even with the limited data. The model incorporates runoff effects and can deal with any backflows or loops in the river system. In comparison with QUAL2K, QUASAR model has advantage of stochastic and deterministic, depending on the data type. However, the model does not incorporate the effects of runoff and any backflows or loops in the river system. MIKE 11 is an advanced model which can simulate hydrodynamics of branched and looped rivers and estuaries. However, it requires large data, which may not available every time. Calibration and evaluation of result in MIKE 11 become tedious when compared with QUAL2K. The MIKE 11 is the only model out of four models which can predict iron and manganese in water. In the WASP model, silica, conservative tracer, pesticides, synthetic organics can be predicted. In terms of model complexity, WASP, MIKE 11 and QUASAR possess a maximum level, whereas QUAL2K has intermediate complexity. The QUAL2K, QUASAR and WASP are easily available and user friendly. Therefore on the basis of the above discussion, it is concluded that all models (QUAL2K, QUASAR and WASP) except MIKE 11 are the most effective tool in modeling river water quality. However, the best model for the study of water quality is selected on the basis of geographical region, watershed type, size of the river, data availability and type of pollutants to be monitored.

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