Rev Environ Sci Biotechnol (2013) 12:285–311
DOI 10.1007/s11157-012-9285-8

REVIEWS

Assessment of river quality models: a review

Deepshikha Sharma · Arun Kansal

Published online: 27 June 2012

Abstract The paper reviews river quality models on the basis of their conceptualization, processes, strengths and limitations. It analyzes advances in basic research and compares river quality models, namely AQUATOX, Branched Lagrangian Transport Model (BLTM), One Dimensional Riverine Hydrodynamic and Water Quality Model (EPD-RIV1), QUAL2Kw, Water Quality Analysis Simulation Program (WASP) and Water Quality for River-Reservoir Systems (WQRRS). All these models are widely used and 'mechanistic' in nature except for BLTM which was selected due its vast 'useage'. In addition, the paper highlights the types of errors which occur during the modelling exercise. The paper also emphasizes on the pivotal role played by water quality models for development and formulation of various river restoration projects worldwide. The present review also suggests broad recommendation for choosing a river quality model.

Keywords River water quality models · QUAL · WASP · WQRRS · BLTM · EPDriv1 · AQUATOX

D. Sharma (✉) · A. Kansal
Department of Natural Resources, TERI University, 10-Institutional Area, Vasant Kunj, Delhi 110070, India
e-mail: deepshikha.k.sharma@gmail.com

A. Kansal
e-mail: akansal@teri.res.in; akansal37@gmail.com

Abbreviations

1,2,3D	1,2,3 Dimension
BOD	Biochemical oxygen demand
BLTM	Branched lagrangian transport model
CBOD	Carbonaceous biochemical oxygen demand
DO	Dissolved oxygen
DYNHYD	Hydrodynamic program
EFDC	Environmental fluid dynamics code
EPD-RIV1	One dimensional riverine hydrodynamic and water quality model
GEMS	Global environment monitoring system
HEC	Hydrology engineering center
IAWQ	International association on water quality
LWDD, FAO	Land and Water Development Division of Food and Agriculture Organization of the United Nations
NCASI	National council for air and stream improvement
SHP	Stream hydraulics package
TMDLs	Total maximum daily loads
USACE	United States army corps of engineers
USEPA	United States Environment Protection Agency
WASP	Water quality analysis simulation program

WEPA	Water environment partnership in Asia
WP: UNDP	Water Portal; United Nations Development Programme
WQRRS	Water quality for river-reservoir systems
WQMs	Water quality models

1 Introduction

Rivers are increasingly getting polluted due to large-scale withdrawal of fresh water and increased discharge of wastewater. Many nations have already initiated resource intensive river quality restoration projects. Planning of these projects and optimal allocation of resources requires application of river quality models. Although these water quality models (WQMs) are generic, the selection of a suitable model requires matching with the physical conditions of the river under study, an understanding of the assumptions and limitations, input data requirements, reliability of default values and uncertainty analysis. In the absence of these, predictive values could be over or under-estimated endangering the entire project objectives.

River system sustains a complex interaction and exchange of mass and energy within its biotic and abiotic components. It offers resilience to change and also recovers itself from the minor changes imposed on it from the polluting surroundings. Growing population, urbanization and industrialization have magnified the amount of total wastewater generated which threatens the health of river ecosystems when discharged into it. Due to long-term ramifications of water pollution, many countries have started investing money to formulate river quality restoration projects primarily focused on pollution reduction. Although zero discharge is often touted as a legislative objective, water resources practitioners understand that a more pragmatic goal is to reduce pollution such that it doesn't exceed its load capacity. The need to predict the fate and impact of a pollutant in the river has led to the development of water quality prediction models. For many decades, WQMs have been developed worldwide in incremental stages without a consistent and clear conceptual basis (Somlyódy et al. 1998). The development and application of models in developed world countries like USA, UK, and some of those members of the EU has resulted in successful river quality restoration projects in these regions as compared to many projects in developing countries where the research and application of WQMs has limited priority (Whitehead 2006).

The pioneering work in the field of river quality modelling was done by Streeter and Phelps (1925) by developing DO sag curves followed by advancement from Theriault (1927), Fair (1939), Thomas (1948), Li (1962, 1972), Camp (1963), Dobbins (1964), Gundelach and Castillo (1976), Van Genuchten and Alves (1982), Bhargava (1983), Ambrose et al. (1996), Jolankai (1997), Yu et al. (1991) and Adrian et al. (1994). The complex river systems were modelled using advances in computational methods (Thomann 1963; McBride and Rutherford 1984; Thomann and Mueller 1987; Koussis et al. 1990; Adrian and Sanders 1998). During the past three decades, substantial contributions have led to the development of user-friendly computer based water quality models which can easily be applied to simulate river quality in 1D, 2D and 3D.

In 1998, a three tier study on the WQMs was done where two models series, namely Activated Sludge Models (ASPs) developed by International Association on Water Quality (IAWQ) and QUAL2 models were compared (Raunch et al. 1998; Shanahan et al. 1998; Somlyódy et al. 1998). Among the various limitations, they highlighted that model calibration is hampered by the inadequacy in field data collection. These constraints negatively impact the simulation ability of a model since the model is unable to capture the marked changes in the river's pollutant load, stream flow, morphometry, or other basic characteristics. The IAWQ task group has proposed the development of improved conversion sub-models for simulating traditional pollutants involving biological, chemical, biochemical, and physical conversion processes. It must serve for research, education, improved communication, knowledge transfer, regulatory applications such as catchment planning, and improved data collection.

The advances in modelling techniques and many WQMs have been reviewed comprehensively by Thomann and Mueller (1987), James (1993), Wurbs (1994), Chapra (1997), Martin and McCutcheon (1999), Cox (2003a, b), Ji (2008), Ambrose et al. (2009) and Kannel et al. (2010), which provide principles on water quality modelling for various parameters and under different conditions. Compared

to the vast literature available on water quality modelling and the development of the models, only a few case-studies are available on their application worldwide. One of the plausible reasons for such a paradox is the mismatch between the data being monitored by water quality surveillance stations and the data required as inputs to WQMs. Often the extent, frequency and detail of the data routinely monitored do not match with the requirements of the model.

The present study compares various models on the basis of their respective capabilities and limitations. These models are available in public domain and have been compared w.r.t. the data requirements, theoretical validity and their applicability. It attempts to bring the objectives of water quality surveillance programs, water quality modelling, and planning of river restoration projects on a common platform of understanding and convergence by discussing the errors accompanied during the modelling process. At the end, study also provides broad criteria for choosing various WQMs.

2 Classification of WQMs

Models have been developed for various pollutants, the nature of source (point or diffuse), and for different river characteristics like morphological, hydraulic and ecological. They estimate changes in contaminant concentrations in a given river stretch integrating the assimilative capacity available from physical, chemical and biological reactions occurring within the system (Cox 2003b; Ji 2008). Depending on the objectives, WQMs can be broadly classified as simulation models (to predict water quality changes due to a pollution source) and optimization models (for optimal allocation of resources) (Bowen and Young 1985; Dudley 1988; Kirchner et al. 1993; Lee and Howitt 1996; Krysanova et al. 1999; Zoppou 2001). Figure 1 illustrates various types of WQMs.

Optimization models can be further divided into linear programming model (Bowen and Young 1985), non-linear programming model (Lee and Howitt 1996) and dynamic programming model (Dudley 1988). A physical simulation model is built to produce a scaled result which can relate back to the real system whereas a mathematical model is based on a set of equations solved numerically to predict the water quality (Ji 2008).

Mathematical models can be further classified on the basis of process description as statistical/empirical or mechanistic; data type as deterministic or

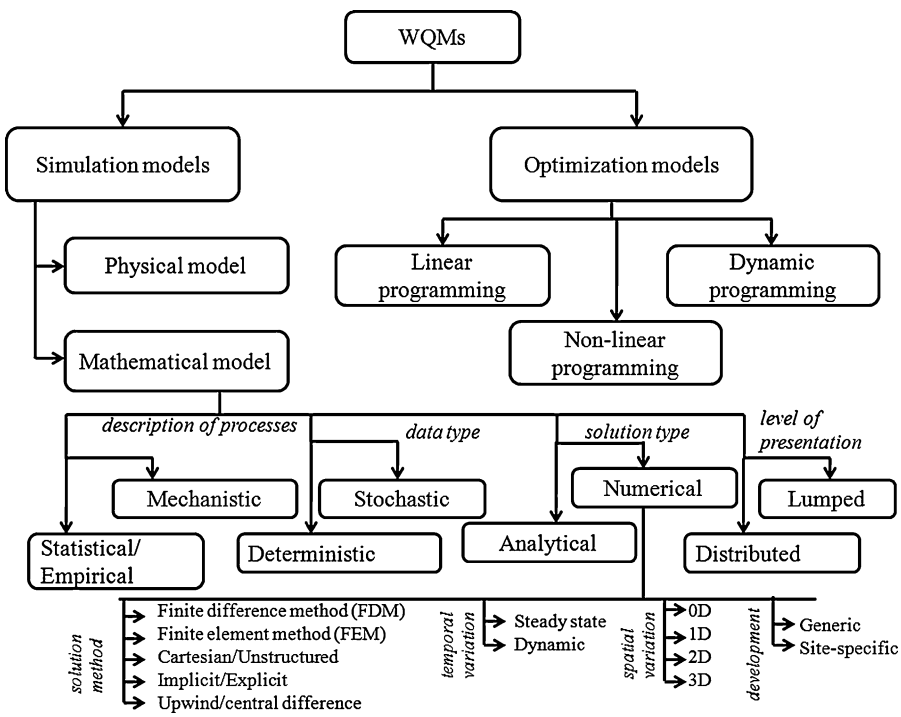

Fig. 1 Types of water quality models. The figure illustrates the classification of water quality models

stochastic; solution types as numerical or analytical; and level of presentation as lumped or distributed.

3 Model review

The present review focus on the following public-domain water quality models: AQUATOX, Branched Lagrangian Transport Model (BLTM), One Dimensional Riverine Hydrodynamic and Water Quality Model (EPD-RIV1), QUAL2kw, Water Quality Analysis Simulation Program 7(WASP 7) series and Water Quality for River-Reservoir Systems (WQRRS) were chosen to be reviewed with a consistent set of criteria: conceptualization, processes, input data, model capability, limitations, model strengths, and their applicability. These models are 'mechanistic' except the BLTM, model system which was chosen due to its wide usage. All these models can be applied successfully to simulate the water quality of river systems especially in terms of DO and BOD.

The section describes the various processes in the WQMs under study. The physical and chemical processes that affect the transport and interaction among the nutrients, phytoplankton, carbonaceous material, sediment, atmosphere and dissolved oxygen in the aquatic environment, for various models are shown in Figs. 2 and 3. A detailed comparison of concepts, assumptions, strengths, limitations, water quality parameters being simulated, dimensions, hydraulic characteristics, pollutant state, process description, method of solution and pollutant transport process are given in Tables 1 and 2.

DO and BOD directly impacts health of a river system and nitrogen and phosphorus describes the level of nutrient loadings to the system. Therefore, the governing equations for these parameters have been illustrated for each WQM. At the end of each model description, a list of few cited applications has also been given.

3.1 AQUATOX

3.1.1 Development

AQUATOX, an ecosystem model can simulate the effect of nutrients, organic chemicals and suspended and bedded sediments on aquatic life. It has incorporated the algorithms from CLEAN model (Park et al. 1974) which is a biological aquatic ecosystem model and the toxic fate model PEST (Park et al. 1982). An additional code was written to integrate the fate and effects of the model with CLEAN, PEST and algorithms from ecotoxicological studies (Park 1990). Park et al. (1995) linked the model to MS windows interface. In 2000, the USPEA release 1 (USEPA 2000a, b, c) followed by Release 1.1 in 2001 (USEPA 2001a, b) with a subsequent Releases 2, 2.1, 2.2 and 3 in 2004, 2005, 2006 and 2008 respectively (Clough 2004; Park and Clough 2004a, b; Clough and Park 2005; Park et al. 2008).

3.1.2 Model system

It simulates the pollutants with spatial and temporal resolutions and represents the average daily conditions for well-mixed and stratified systems, and linked well-mixed segments. The water quality processes are solved by employing 4th and 5th order Runge–Kutta integration method. The model also uses adaptive step method to solve the differential equations. It is a unique model to simulate the impact of pollution on biological life and can be used for stratified lakes, reservoirs, rivers, and estuaries. It can also simulate the transfer of biomass and chemicals from one compartment of the ecosystem to another as it assumes that individual segments are uniformly mixed. Therefore, it can be applied for modelling multiple linked river and reservoir segments. Apart from hydraulic, geometric data, the model also requires data on abiotic and biotic state variables, physical characteristics, biota, remineralization and ecotoxicology. The model can also account for DO fluctuations and toxicity arising from low oxygen and ammonia (Park et al. 1988). The model also computes community similarity indices comparing perturbed and controlled simulations (USEPA 2009).

3.1.3 Governing equations

Basic equation

$$W_{in} = \sum_{u/s} \frac{Wout_{u/s} \cdot V_{u/s} \cdot W_{frac}}{V_{d/s}}, W_{toxcarrier} = \sum_{u/s} \frac{Wout_{u/s} \cdot C_{u/s} \cdot 1e6 \cdot V_{u/s} \cdot Wfrac}{V_{d/s}}$$

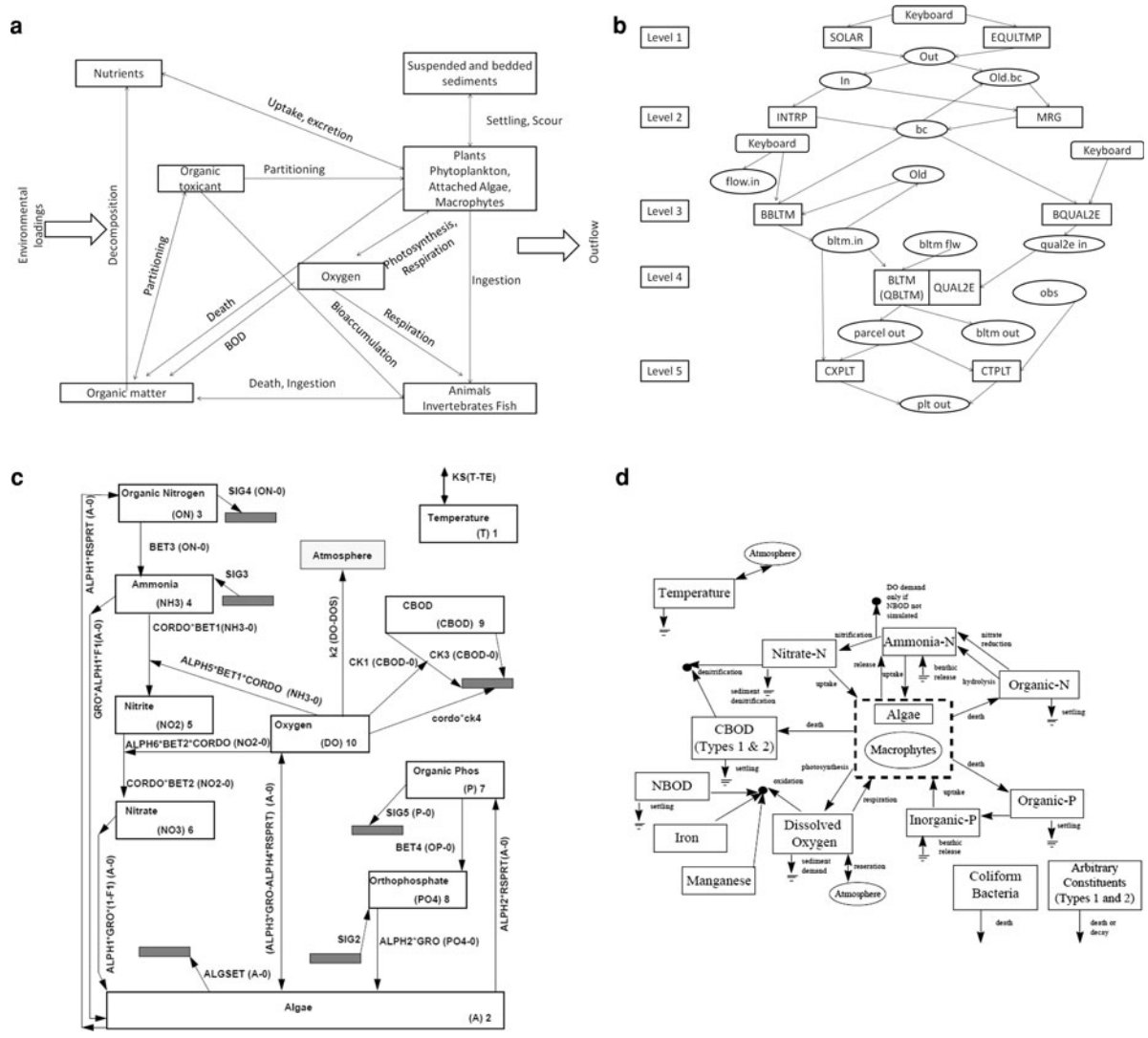

Fig. 2 Conceptual model of **a** AQUATOX; **b** BLTM system; **c** QUAL2E (BLTM Sub Routine); **d** EPd-Riv1

DO

$$\frac{d_{DO}}{dt} = W_{nutrients} + Kreaer(O_{2sat} - O_2) + O_{2photo} \cdot \sum_{plant} Photosynthesis - BOD - \sum (resp20.1045^{(Temp.-20)} \cdot Biomass) - O_2N \cdot Nitrify - W_{out} + W_{in} \pm \frac{Bulkmixcoeff}{V_{epi.hypo}} \cdot (C_{epi.hypo} - C_{hypo.epi}) \pm \frac{Diffcoeff \cdot A}{L_{char}} \cdot (C_1 - C_2)$$

CBODu

$$OM = BOD \cdot \left(\frac{BOD_5 - CBOD_u}{O_2 biomass}\right)$$

Nitrogen

$$\frac{dN_o}{dt} = \alpha_1 \rho A - \beta_3 N_0 - \sigma_4 N_0, \frac{d[NH_4N]}{dt} = \beta_3 N_0 - \beta_1 [NH_4N] + \frac{\sigma_3}{D} - F_1 \alpha_1 \mu A$$

$$\frac{d[NO_2N]}{dt} = \beta_1 [NH_4N] - \beta_2 [NO_2N], \frac{d[NO_3N]}{dt} = \beta_2 [NO_2N] - (1 - F)\alpha_1 \mu A$$

Phosphorus

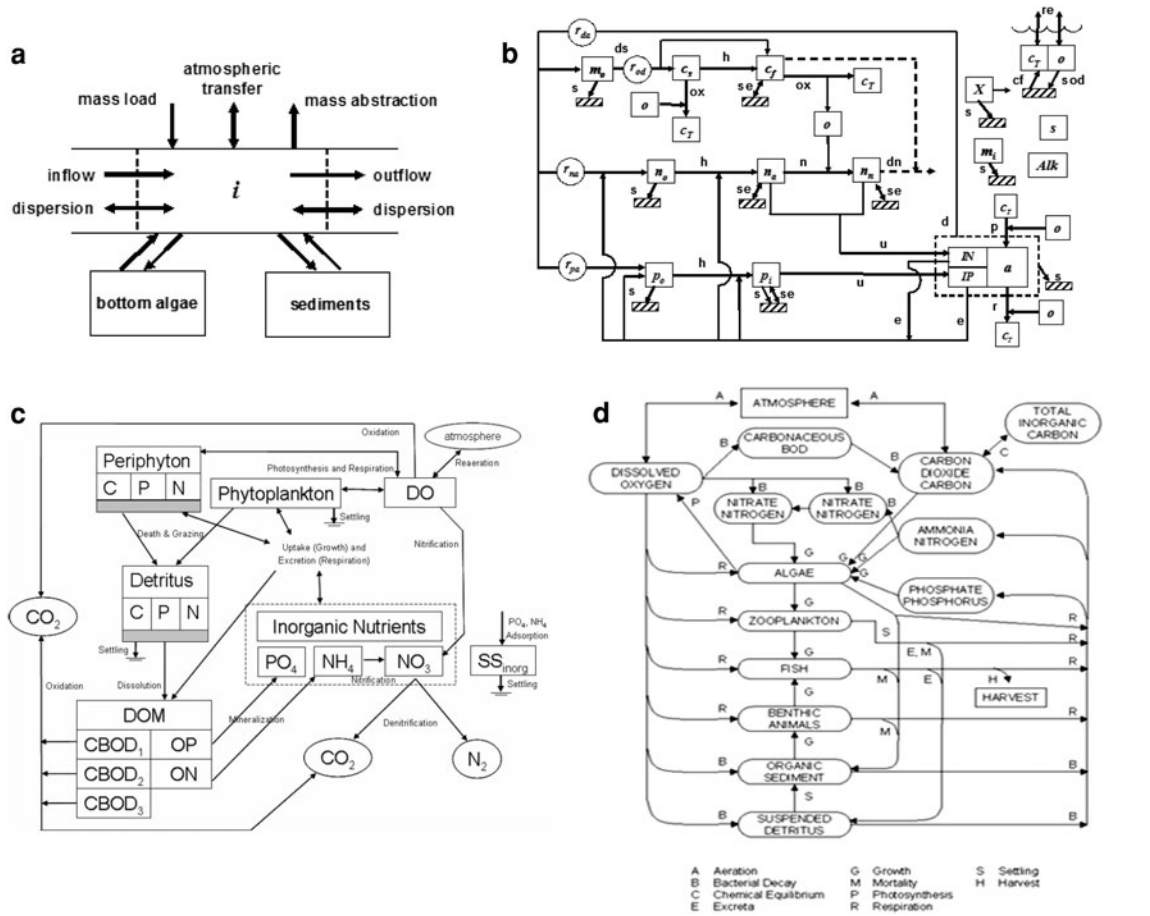

Fig. 3 Conceptual Model of **a** Mass Balance in Reach Segment *i* in QUAL2Kw; **b** QUAL2Kw (ab bottom algae, ap phytoplankton, mo detritus, cs slow CBOD, cf fast CBOD, cT total inorganic carbon, O oxygen, nO organic nitrogen, na ammonia nitrogen,nn nitrite and nitrate nitrogen, po organic phosphorous and pi inorganic phosphorous); **c** WASP7 (Phyto is phytoplankton as carbon, NO3 is nitrate, NH4 is ammonium, PO4 is orthophosphorus, CBOD is carbonaceous biochemical oxygen demand, DO is dissolved oxygen ON is organic nitrogen, OP is organic phosphorous, DOM is dissolved organic matter, SS is inorganic suspended solids); **d** WQRRS The basic concepts, assumptions, input data requirement, limitations and strengths are given in Table 1. Table 2 provides detail of water quality constituents the models can simulate. *Sources* Park et al. (2008), Jobson and Schoellhamer (1987), Environmental Laboratory (1985), Pelletier and Chapra (2005), Ambrose and Wool (2009), USACE-HEC 1978 [revised on 1986])

$$\frac{dP}{dt} = W_{nutrient} + Photo\mathrm{Resp} + Dark\mathrm{Resp} + Animal\mathrm{Resp} + AnimalExcr + DetritalDecomp + Animal\,\mathrm{Pr}\,edation + Nutr\mathrm{Rel}Defecation + Nut\mathrm{Rel}Plant\,\sin k + Nut\mathrm{Rel}Mortality + Nut\mathrm{Rel}GameteLoss + Nut\mathrm{Rel}Colonization + Nut\mathrm{Rel}PeriScour - \sum_{plant} Photosynthesis \cdot Uptake_p - W_{out} - W_{in} \pm \frac{Bulkmixcoeff}{V_{epi.hypo}} \cdot (C_{epi.hypo} - C_{hypo.epi}) \pm z\frac{Diffcoeff \cdot A}{L_{char}} \cdot (C_1 - C_2) - KDPCalcite \cdot Phosphate \cdot CalciteP_{cpt} - 1e-6 + s(f_{d1} \cdot C_1 - C_{watercol}) \cdot H_1$$

Notations Win = inflow load from u/s segment (unit/L d/s day); Wout u/s = washout from u/s segment (unit/Lu/s day); V = volume of given segment (m^3); Wfrac = fraction of u/s segment's outflow that goes to this particular d/s segment (unitless);

Table 1 Comparison of constituents modelled by RWQMs

State variables and processes	AQUATOX	BLTM (Sub-routine QUAL2E)	EPD RIV1	QUAL2Kw	WASP	WQRRS
Hydraulics			√	√	√	√
Conductivity				√		
pH	√			√		
Alkalinity				√		√
Total carbon						√
Total inorganic carbon, Light extinction				√		
Heat budget				√	√	
Temperature		√	√	√	√	
Nutrients	√			√	√	√
NH_4 toxicity	√					
Nitrogen		√	√	√	√	√
Ammonia, nitrate			√	√	√	√
Nitrite						√
Phosphorus		√	√	√	√	√
Orthophosphate				√	√	
Sediment digenesis	√			√	√	
Sand/silt/clay, stratified sediments	√				√	
Sediment effects	√			√		
Organic toxicants in sediments	√				√	√
Cohesive sediments, non-cohesive sediments, Inorganic solids					√	
Inorganic suspended solids				√		
Total dissolved solids						√
Detritus	√			√	√	√
Algae		√	√	√	√	
Bottom algae				√		√
Phytoplankton	√			√	√	√
Periphyton	√				√	
Macrophytes	√		√			
Zooplankton, zoobenthos, fish	√					√
Bird etc.	√					
Bacteria (coliform)		√	√	√	√	√
Pathogens				√		
DO	√	√	√	√	√	√
DO effects on biota	√					
Anoxia				√		
BOD		√	√	√	√	
NBOD			√			
CBOD (slow and fast)			√	√	√	
COD		√	√	√		
SOD				√		
Brines						
Salinity, organic toxicant fate	√				√	
Ecotoxicity	√					
Linked segments	√					
User defined constituent		√	√	√	√	
Silica, conservative tracer, pesticides, synthetic organics					√	
Hyporheic metabolism				√		
Iron, manganese			√			

The table compares WQMs for their capability to simulating various physical, chemical and biological characteristics of water

Table 2 Characteristics of RWQMs

	Dimension	Hydraulic characteristics		Pollutant state		Process description		Nature of data		Pollution transport	Solution method
		Steady	Dynamic	Steady	Dynamic	Empirical	Mechanistic	Deterministic	Stochastic		
AQUATOX	2D	√			√		√	√	√	Mass balance-differential-equation	Numerical
BLTM (subroutine QUAL2E)	1D		√		√	√		√		Convective-diffusion equation	Numerical
EPD RIV1	1D		√		√		√	√		Mass balance/Advective diffusion equation	Numerical
QUAL2kw	1D	√		√			√	√		Mass balance	Numerical
WASP	1D, 2D, 3D	√	√		√		√	√		Mass balance	Numerical
WQRRS	1D	√	√		√		√	√		Advective diffusion equation/Completely mixed reactor	Numerical

The table compares popular WQMs for dimensions, hydraulic characteristics, pollutant state, process description, method of solution and pollutant transport process

Wtoxcarrier = inflow load of toxicant sorbed to a carrier from an u/s segment (μg/Ld/s day); Wout = washout of toxicant carrier from u/s (mg/Lu/s day); C = concentration of toxicant in carrier u/s (μg/kg); 1e-6 = units conversion (kg/mg); Wnutrients = loading of nutrient from inflow (g/m^3 day); KReaer = depth-averaged reaeration coefficient (1/day);O2Sat = saturation concentration of oxygen (g/m3); O2 = concentration of oxygen (g/m^3); O2Photo = ratio of oxygen to photosynthesis (1.6, unitless); BOD = instantaneous biochemical oxygen demand (g/m^3 day); Photosynthesis = rate of photosynthesis (g/m^3 day); Resp20 = user input respiration rate at 20 °C (g/g day); 1.045 =exponential temperature coefficient (°C); Temperature = ambient water temperature (°C); Biomass = plant biomass (g/m^3); O2 N = ratio of oxygen to nitrogen (unitless); Nitrify = nitrification rate (g/m^3 day); Volume = volume of given segment (m^3); C = concentration of given compartment in given zone (g/m^3); Diffcoeff = dispersion coefficient of feedback link, (m^2/day); Area = surface area of the feedback link (m^2); Lchar = characteristic mixing length of the feedback link, (m); OM = organic matter input as required by AQUATOX (gOM/m^3 day); O2Biomass = ratio O2 to organic matter (OM) (unitless); BOD5_CBODu = BOD 5 to ultimate carbonaceous BOD conversion factor, also defined as CBODU:BOD5 ratio; Ammonia = concentration of ammonia (g/m^3); dAmmonia/dt = change in concentration of ammonia with time (g/m^3 day); Denitrify = denitrification (g/m^3 day); Diffusion Seg = gain or loss due to diffusive transport over the feedback link between two segments, (g/m^3 day); dNitrate/dt = change in concentration of nitrate with time (g/m^3 day); KNitri = maximum rate of nitrification (m/day); Loading = loading of nutrient from inflow (g/m^3 day); Nitrify = nitrification rate (g/m^3 day); NitroDemand = oxygen taken up by nitrification (g/m^3 day);PhotoResp = algal excretion of phosphate due to photo-respiration (g/m^3 day); DarkResp = algal excretion of phosphate due to dark respiration (g/m^3 day); AnimalResp = excretion of phosphate due to animal respiration (g/m^3 day); AnimalExcr = animal excretion of excess nutrients to phosphate to maintain constant org. to P ratio as required (g/m^3 day); DetritalDecomp = phosphate release due to detrital decomposition (g/m^3 day); AnimalPredation = change in phosphate content necessitated when an animal consumes prey with a different nutrient content

(g/m^3 day), see discussion in "Mass Balance of Nutrients" below; NutrRelDefecation = phosphate released from animal defecation (g/m^3 day); NutrRelPlantSink = phosphate balance from sinking of plants and conversion to detritus (g/m^3 day); NutrRelMortality = phosphate balance from biota mortality and conversion to detritus (g/m^3 day); NutrRelGameteLoss = phosphate balance from gamete loss and conversion to detritus (g/m^3 day); NutrRelColonization = phosphate balance from colonization of refractory detritus into labile detritus (g/m^3 day); NutrRelPeriScour = phosphate balance when periphyton is scoured and converted to phytoplankton and suspended detritus. (g/m^3 day); KDPCalcite = partition coefficient for phosphorus to calcite (L/kg); Phosphate = concentration of phosphorus in water (mg P/L); 1 e-6 = conversion factor (kg/mg); s = surface diffusive transfer (m/day); fd1 = dissolved fraction in layer 1; C = total concentration of state variable in layer (g/m^3); and H1 = depth of layer 1 (m);

3.1.4 Strengths

The model incorporates ecological effects, Latin hypercube uncertainty analysis, nominal range sensitivity and time-varying process rates analysis. It can simulate up to 20 organic chemicals simultaneously. It is freely available, and forms an integral part of the BASINS system which can be linked to the other watershed models like HSPF and SWAT.

3.1.5 Assumptions and limitations

It is assumed that the linked segments have an identical set of state variables and each segment is well mixed. Linkages between segments are assumed to be either unidirectional or bidirectional. It does not allow dynamic stratification and toxic effects are presumed to be additive. Macrophytes and algae are simulated as steady state; and zooplankton and fish exhibits avoidance behavior. Toxicant exchange via gill membrane is facilitated by same mechanism as the uptake of oxygen. It does not model metals and luxury uptake and limitation by internal nutrients are not represented in algal bioenergetics.

3.1.6 Applicability

A comprehensive review of the model and its application can be found in Park et al. (2008). Lei et al. (2010) have used AQUATOX to simulate toxicity of 2,4-dichlorophenol (2,4-DCP), 2,4,6-trichlorophenol (2,4,6-TCP) and pentachlorophenol (PCP) on the aquatic species existing widely in the Taihu Lake (China).

3.2 BLTM

3.2.1 Development

Jobson and Schoellhamer (1987) developed the model which has been widely used by U.S. Geological Survey and elsewhere (California Water Resources Control Board 1996; Drewes and Conrads 1995; Graf 1995; Weiss et al. 1994; Bulak et al. 1993; Wiley 1993).

3.2.2 Model system

The main stream reach is divided into sub-reaches. It employs finite difference solution of the mass transport and reaction equations and most determinants are simulated as 1st-order decays. The modelling system has five levels- EQULTMP, SOLAR to process time-series of meteorological data; INTRP, MRG programs to process time-series data; BBLTM, BQUAL2E to build input files for transport model; BLTM, QUAL2E to define reaction kinetics and CTPLT, CXPLT as a post processor plotting programs. The model uses Lagrangian reference frame in which the computational nodes move with the flow to solve 1D advective dispersion equation. The USEPAs stream-water-quality model QUAL2 (EPA-QUAL2) version QUAL2E (Brown and Barnwell 1987) was supplied as a subroutine to the BLTM called QBLTM for simulating the reaction kinetics. The software is available for electronic retrieval by means of either the internet at http://water.usgs.gov/software/ and via anonymous File Transfer Protocol (FTP) from water.usgs.gov (path:/pub/software). The format for data input is described in Jobson and Schoellhamer (1987, p. 8–10

and Appendix A). The input data required includes stream/river parameters, global variable forcing functions. QUAL2E is extensively used for waste load allocation, discharge permit determinations, and other conventional pollutant evaluations and has limitations like it assumes uniform hydraulics, steady-state flow, must be assumed and uniformly spaced computational elements. When combined with BLTM, these limitations are reduced (Fig. 2) and make it a dynamic model wherein both flow and water-quality conditions can be estimated. Further details on the reaction kinetics and rate constants are available by Bowie et al. (1985). The presence of decay-coefficient subroutine in the model can provide the reaction kinetics for up to 10 constituents.

3.2.3 Governing equations

Basic equation

$$\frac{\partial C_L}{\partial t} = \frac{\partial}{\partial \xi}\left(D\frac{\partial C_L}{\partial \xi}\right) + S_L + \Phi_L + \sum_{n=1}^{m} K_{L,n}(C - CR_{L,n})$$

DO

$$\frac{d_{DO}}{dt} = (C_8 - C)K_2 - (\alpha_3\mu - \alpha_4\rho)A - K_1L - \frac{K_4}{D} - \alpha_5\beta_1[NH_4] - \alpha_6\beta_2[NO_2]$$

CBODu

$$\frac{d_{CBODu}}{dt} = K_1L - K_3L$$

Nitrogen

$$\frac{dN_o}{dt} = \alpha_1\rho A - \beta_3N_0 - \sigma_4N_0, \frac{d[NH_4N]}{dt} = \beta_3N_0 - \beta_1[NH_4N] + \frac{\sigma_3}{D} - F_1\alpha_1\mu A$$

$$\frac{d[NO_2N]}{dt} = \beta_1[NH_4N] - \beta_2[NO_2N], \frac{d[NO_3N]}{dt} = \beta_2[NO_2N] - (1-F)\alpha_1\mu A$$

Phosphorus

$$\frac{dP_o}{dt} = \alpha_2\rho A - \beta_4P_0 - \sigma_5P_0, \frac{dP_d}{dt} = \beta_4P_0 + \frac{\sigma_2}{D} - \alpha_2\mu A$$

Notations C_L = concentration; S_L = rate of production of concentration independent of zero-order rate; Φ_L = rate of change in concentration due to tributary inflow; D = longitudinal dispersion coefficient; $K_{L,n}$ = rate coefficient for the production of constituent L due to presence of constituent; $CR_{L,n}$ = constituent (n) concentration at which production of constituent L due to n cases; K_1 = rate of oxidation of the CBOD; K_3 = rate of CBOD loss due to settling; K_4 = rate of SOD; β_1 = rate coefficient parameter for the biological oxidation of ammonium (i.e., nitrification); NH_4N = ammonium-N; NO = organic-N; NO_2N = nitrite N; NO_3N = nitrate–N; P_d = concentration of inorganic or dissolved P; D = depth; Po = concentration of organic P; t = time; U = mean velocity; x = distance along the element; α_1 = fraction of algal biomass that is N; α_2 = source rate of P from the sediments; α_3 = P content of algae; α_4 = rate of respiratory oxygen uptake per unit of algal respiration; α_5 = rate of oxygen utilization per unit of ammonium oxidized during nitrification; α_6 = rate of oxygen uptake per unit of nitrite oxidized; β_2 = rate coefficient for the oxidation of NO_2N; β_3 = rate coefficient parameter for hydrolysis of organic N to ammonium; β_4 = organic P decay rate; ΔS = net concentration influence of external sources and sinks; μ = algal growth rate; ρ = algal respiration rate; σ_1 = settling rate; σ_4 = rate coefficient parameter for settling of organic N; σ_5 = organic P settling rate.

3.2.4 Strengths

The lagrangian reference frame minimizes the numerical dispersion. The dispersion coefficients vary with sub-reach in the model.

3.2.5 Assumptions and limitations

Solutes are assumed to be completely mixed across the cross section and dispersive transport is expected to be proportional to concentration gradient. The model is unable to convert algal death to CBOD and is inappropriate where macrophytes are simulated. The model includes only limited number of reaches, computational elements, and junctions.

3.2.6 Applicability

Model has been applied to various study area like San Joaquin River in California where a rainfall-runoff

model, a runoff-quality model, a 1D river-flow model, and BLTM have been used to simulate water quality of urban runoff (Guay 1991). Conrads and Roehl (1999) compared and evaluated the results obtained by BLTM with other selected models like physical model, BRANCH model and neural network technique for Cooper and Wando rivers in South Carolina. They found neural network models have more accuracy for parameters like salinity, temperature and DO. The model has also been applied to Texas River (Lizarraga 1996), Wateree River, South Carolina (Feaster and Conrads 1999), Mississippi River Basin (Broshears et al. 2001) and Catawba River, South Carolina (Feaster et al. 2003).

3.3 EPD-RIV1

3.3.1 Development

The basic model for EPD-RIV1 was originally developed at Ohio State University as requested by USEPA. Thereafter, the WES contracted Ohio State University to modify the model code to handle control structures. Subsequent, update and modifications were made, resulting in Version 1.0 of CE-QUAL-RIV1, released in 1991. WES further modified and supported CE-QUAL-RIV1, releasing Version 2.0 of the model in 1995 (Environmental Laboratory 1985). At the onset of the Chattahoochee River Modeling Project (CRMP), the Environmental Protection Division (EPD) of the Georgia Department of Natural Resources selected CE-QUAL-RIV1. Due to certain limitations in CE-QUAL-RIV1, an extensive development was undertaken, resulting in the software described in this series of documents and the modified version of CE-QUAL-RIV1, referred to as the EPD-RIV1.

3.3.2 Model system

The model simulates multiple branches, and in-stream hydraulic control structures. It employs explicit two-point, 4th-order accurate, Holly-Preissman scheme to solve the mathematical formulations. It has hydrodynamic mode (RIV1H) and water quality mode (RIV1Q) designed to simulate the dynamic conditions in rivers and streams for the purpose of analyzing existing conditions and performing waste load allocations, including allocations of total maximum daily loads (TMDLS). The input data required is geometric data, initial conditions, model forcing data, hydraulic and control parameters and calibration data. The model has the capability to resolve the longitudinal variations in hydraulic and quality characteristics and is applicable where lateral and vertical variations are small. The software has Computer System Shell; pre-processor; deliberator; post-processor, and pre-run. The water quality module can simulate the interactions of 16 state variables, including water temperature, nitrogen species, phosphorus species, DO, CBOD (two types), algae, iron, manganese, coliform bacteria and two arbitrary constituents. The model has the capability to resolve the longitudinal variations in hydraulic and quality characteristics and is applicable where lateral and vertical variations are small. It can also simulate the impacts of macrophytes on DO and nutrient cycle, time-varying point and non-point sources on the hydrodynamics and water quality of a stream. Moreover, the model can represent recycling of nutrients and combined fate; and effects of toxic chemicals. The model can solve differential equations to represent changing values of state variables, normally with a reporting time step of 1 day (Martin et al. 2002).

3.3.3 Governing equations

Basic equation

$$\frac{\partial \alpha}{\partial t} + \overline{u}\frac{\partial \alpha}{\partial x} = D\frac{\partial^2 \alpha}{\partial x^2} + \frac{q}{A}(\gamma - \alpha) - K_5\alpha + SINKS$$

DO

$$\begin{aligned}\frac{d_{DO}}{dt} = {} & K_2 * (DO_{SAT} - DO) - K_1 * CBOD \\ & - ONITRI * KN * NH_4N + OPDECY \\ & + \left[ONEQUI * \left(\frac{NO_3^- N}{NO_3^- N + NH_4^+ N}\right)\right] \\ & * (ALGRO + MGRATE)\cdot \\ & OPDECY * (1.FCBOD) \\ & * (ALGADK + MDEATH) - OFEDC \\ & * KFEDK * FE - OMNDEC * KMNDK \\ & * MN - K_{SOD}\end{aligned}$$

CBODu

$$\frac{d_{CBODu}}{dt} = \left(K_1 + KDN + \frac{CBOD_{SR}}{H}\right) * CBOD + OPDECY * \frac{(KOCB_1 + DO_X * FCBOD)}{(DO_X + KOCB_1)} * (ALGADK + MDEATH)$$

Nitrogen

$$\frac{dON}{dt} = -\left(KIN + KDN + \frac{XONS}{H}\right) * ORGAN + (ANCONT * ALGADK + MNCONT * MDEATH)$$

$$\frac{dNH_4}{dt} = (KIN + KDN) * ORGAN - ANCONT * 1 - \frac{NH_4}{NH_4 - N + NO_3^- - N} * (ALGRO - ALGADK) - MNCONT * 1 - \frac{NH_4}{NH_4 - N + NO_3^{-N}} * (MGRATE - MDEATH) + KBNNH_3 - KN * NH_4^+ - N$$

$$\frac{dNO_3 - N}{dt} = ONEQUI * KDN * CBOD + KN * NH_4N - (ANCONT * ALGRO + MNCONT * MGRATE) * \left(\frac{NO_3^- - N}{NH_4^+ - N + NO_3^- - N}\right) - (KDNO_2 * NO_3^- - N)$$

Phosphorus

$$\frac{d_P}{dt} = -ORG - P * \left(KPDK + \frac{KPSET}{H}\right) + (MPCONT * MDEATH + APCONT * ALGADK) + ORG - P * KPDK + KBENPO_4 - (APCONT * ALGRO + MPCONT * MGRATE) - APO_4 * TH\_SORP^{(TEMP.-20)} * OPO_4$$

Algal model

$$ALGRO = C(12.1) * KALGRO\left(\frac{1}{KEXT * H}\right) * In\left(\frac{KLITE + SWALG}{KLITE + SWALG * EXP(KEXT * H)}\right) * FN * FP$$

$$ALGRO = C(12.1) * KALGDK * \left(\frac{DO}{DO + KOALDK}\right)$$

Notations KIN = temperature and DO corrected rate coefficient for organic-N, day^{-1} as computed from K1 N = ACK * TH_K1 N(T-20.)*(1. + KOCB1)/ DO; KDN = temperature corrected rate coefficient for nitrate reduction and anaerobic CBOD oxidation, day^{-1}; KNSET = rate coefficient for removal of organic-N by settling, m/day, H = stream depth, m, ORGAN = concentration of organic-N, C(3,I), g-N/m^3, ACK = rate coefficient for organic-N hydrolysis to NH^{+4}, day^{-1}, AKN = specific rate coefficient for organic-N decay, day^{-1}, ANCONT = nitrogen-to-biomass ratio in algae, g/g, MNCONT = nitrogen-to-biomass ratio in macrophytes, g/g, ALGADK = rate of algal decay, g/m^3/day, MDEATH = rate of macrophyte decay, g/m^3/da, KN = nitrification rate coefficient, day-1, NH^{4+}–N = ammonia-N concentration, g-N/m, AKN = uncorrected rate coefficient for nitrification, day^{-1}, TH_KNH_3 = temperature coefficient for ammonium oxidation (suggested value is 1.1), KON = Monod half-velocity constant for oxygen limitation of nitrification, g O_2/m, ANCONT = nitrogen-to-biomass ratio in algae, MNCONT = nitrogen-to-biomass ratio in macrophytes, NH^{4+}–N = concentration of ammonium nitrogen, g-N/m^3, C(4,I), NO_3–N = concentration of nitrate nitrogen, g-N/m^3, C(5,I), ALGRO = growth rate of algae, g/m^3/day, MGRATE = growth rate of macrophytes, g/m^3/da, BENNH3 = benthic release rate, g-N/(m^2 day), TH_BENN = temperature coefficient for ammonia release, H = depth, m, T = temperature, °C; A CK = rate coefficient for organic-N hydrolysis to

NH^{+4}, day^{-1}; AKN = specific rate coefficient for organic-N decay, day^{-1}; ALGADK = algal death rate g/(m^3 day); ALGRO = growth rate of algae, g/m^3/day; ANCONT = nitrogen-to-biomass ratio in algae, g/g; APCONT = phosphorus-to-biomass ratio in algae; APO4 = phosphate loss rate (1/day); BEN-NH_3 = benthic release rate, g-N/(m^2 day); BEN-PO_4 = benthic release rate, g-P/(m^2 day); C(12,I) = algae concentration at node i, g/m^3; CBOD = concentration of CBOD, g O_2/m^3, from previous time-step, C(2,I) or C(13,I); CBODSR = rate coefficient for CBOD type 1 removal by settling (RBODSR for type 2), m/day; D = dispersion coefficient; DAMK = reaeration coefficient, m; DO = average dissolved oxygen (g/m^3); DOSAT = local solubility of oxygen, g O_2/m^3; DOSAT = saturation DO concentration, g/m^3;ELEV0 = reference elevation of the waterbody, ft; FCBOD = fraction of algal and macrophyte mortality contributing to CBOD (FCRBOD for type 2); FE = concentration of reduced iron, g/m^3; FL = light growth adjustment factor; ALGADK = algal decay rate, g/(m^3 day); FN = nitrogen growth adjustment factor; FP = phosphorus growth adjustment factor; H = depth, m; K_1 = temperature corrected rate coefficient for aerobic oxidation of CBOD, day^{-1}; K_2 = reaeration rate coefficient, day^{-1}; K_2(T) = reaeration rate coefficient at ambient temperature, 1/day; KALGDK = maximum specific algal decay rate, day^{-1}; KALGRO = maximum specific algal growth rate, day^{-1}. Input as KALGRO, renamed ALG_1 in subroutine SEG; KDN = temperature corrected rate coefficient for nitrate reduction and anaerobic CBOD oxidation, day^{-1}; KEXT = light extinction coefficient, m^{-1}, corrected for algal self-shading; H = hydraulic depth, A/B, m; KFEDK = oxidation rate for iron, day^{-1}; KIN = temperature and DO corrected rate coefficient for organic-N, day^{-1} as computed from K_1N = ACK * TH_K1 N(T^{-20}.)*(1. + KOCB1)/DO; KDN = temperature corrected rate coefficient for nitrate reduction and anaerobic CBOD oxidation, day^{-1}; KNSET = rate coefficient for removal of organic-N by settling, m/day; KLITE = half-velocity constant for light intensity, watt/m^2; KMNDK = oxidation rate for manganese, day^{-1}; KN = nitrification rate coefficient, day^{-1}; NH^{4+-}N = ammonia-N concentration, g-N/m^3; KOALDK = DO half-velocity constant for algal decay, g/m^3; KOCB1 = Monod half velocity constant for oxygen-limited aerobic systems, g O_2/m^3; KPSET = organic-P settling rate, m/day; H = depth, m;ALGRO = growth rate of algae, g/m^3/day; Ks = biochemical uptake or decay rates (+) and growth rates (−); KS is $KDNO_2$, where KDSED sediment denitrification rate. The coefficient ONEQUI (suggested value 0.35) is a conversion factor for oxygen to nitrogen equivalents; MDEATH = macrophyte death rate, g/(m^3 day); MGRATE = growth rate of macrophytes, g/m^3/day; Mn = concentration of reduced manganese, g/m^3; MNCONT = nitrogen-to-biomass ratio in macrophytes, g/g; MPCONT = phosphorus-to-biomass ratio in macrophytes; NH^{4+}–N = concentration of ammonium nitrogen, g-N/m^3, C(4,I); NO^3–N = concentration of nitrate nitrogen, g-N/m^3, C(5,I); OFEDEC = oxygen-to-iron ratio for iron oxidation; OMNDEC = oxygen-to-manganese ratio for manganese oxidation; OPDECY = oxygen-to-biomass ratio for oxygen production by algae and macrophytes when ammonia is nitrogen source; OPO_4 = phosphate concentration (mg/l) ORGAN = concentration of organic-N, C(3,I), g-N/m^3; ORG-P = organic-P concentration, C(6,I), g/m^3; KPDK = organic-P hydrolysis rate, day^{-1}; q = lateral inflow rate; SINKS = biochemical sources (+) and sinks (−); SWALG = short-wave radiation intensity at the water surface, watt/m^2; T, TEMP = temperature, oC; TH_BENN = temperature coefficient for ammonia release; TH_$BENPO_4$ = temperature coefficient for phosphate release; TH_K_2 = temperature coefficient, unitless; TH-SORP = temperature coefficient for phosphate sorption or loss; u = velocity; x = longitudinal distance; α = constituent (i.e. DO, temperature, etc.); γ = concentration of the runoff input to the channel by distributed flow q; ΔH = elevation change, m.

3.3.4 *Strengths*

The geometry specification and time series input of the model are flexible. It can account for time-varying flow, elevation, and water quality constituent changes from unsteady flow. The model includes direct explicit interaction of flow and elevation on the constituent distributions and can be applied to a river channel of arbitrary cross section and specified bottom slope. The lateral inputs of water and pollutant concentrations are accounted and multiple branches and in-stream hydraulic control structures can also be simulated (Martin et al. 2002).

3.3.5 Assumptions and limitations

The river body is assumed to be homogenous across the section. Lateral and vertical gradients are assumed to be small and can be neglected. The model is limited to 1D simulation and does not include sediment transport processes.

3.3.6 Applicability

The model has found limited applications worldwide. Few recent studies includes the evaluation of total maximum daily load for the Coosa River to maintain DO is rarely applied to simulate the river quality http://www.gaepd.org/Documents/coosa_modeling.html and another wherein the model has been applied to Chattahoochee River near Atlanta http://www.gaepd.org/Documents/capps_ferry_do_monitoring.html.

3.4 QUAL2 kw

3.4.1 Development

In 2002, QUAL2 k was developed after identifying limitations of QUAL2E, QUAL2EU. The major enhancement included the strengthening of computational structure and addition of new constituent interactions, such as algal BOD, denitrification, and DO change caused by plants (Chapra and Pelletier 2003). The latest version, QUAL2 Kw was developed by Pelletier and Chapra (2005) by modifying QUAL2 K.

3.4.2 Model system

The QUAL2Kw is 1D, steady state (flow is assumed to be in steady-state but water quality is simulated in a dynamic mode with diel water quality kinetics and heat budget) stream water quality model which is implemented in the Microsoft Windows environment (http://www.ecy.wa.gov/).

The river can be simulated as collection of reaches (equal or unequal lengths) and tributaries are represented as point sources. The input data required is flow and concentrations for headwater, discharges and withdrawals; reach segment lengths, elevations, hydraulic geometry and weather data parameters. It can also simulate a generic pathogen as a function of temperature, light, and settling velocity (Pelletier and Chapra 2005). The model can simulate temperature, pH, conductivity, inorganic suspended solids, DO, slowly reacting CBOD, fast-reacting CBOD, organic nitrogen, ammonia nitrogen, nitrate nitrogen, organic phosphorus, inorganic phosphorus, phytoplankton, detritus, pathogen, alkalinity, total inorganic carbon, bottom algae (periphyton) biomass, bottom algae (periphyton) nitrogen, bottom algae (periphyton) phosphorus. Most of the determinants are simulated as 1st-order decays but DO, nitrate, and phosphate are represented in more detail.

3.4.3 Governing equations

Basic equation

$$\frac{dc_i}{dx} = \frac{Q_{i-1}}{V_i}c_{i-1} - \frac{Q_i}{V_i}c_i - \frac{Q_{ab,i}}{V_i}c_i + \frac{E'_{i-1}}{V_i}(c_{i-1} - c_i) + \frac{E'_i}{V_i}(c_{i+1} - c_i) + \frac{W_i}{V_i} + S + \frac{E'_{hyp,i}}{V_i}(c_{2,i} - c_i)_i;$$

$$\frac{dc_{2,i}}{dx} = S_{2,i} + \frac{E'_{hyp,i}}{V_{2,i}}(c_i - c_{2,i}); \frac{da_{b,i}}{dx} = S_{b,i}; \frac{dIN_b}{dt} = S_{bN,i}; \frac{dIP_b}{dt} = S_{bp,i}; \frac{da_{h,i}}{dt} = S_{ah,i}$$

DO

$$\begin{aligned} S_o &= r_{oa}(PhytoPhoto - PhytoResp) \\ &\quad + r_{od}(BotAlgPhoto - BotAlgResp)\frac{A_{st,i}}{V_i} \\ &\quad - r_{oc}FASTCOxid - r_{oc}SlowCOxid - r_{on}NH_4Nitr \\ &\quad + Reaeration - COD_{oxid} - SOD\frac{A_{st,i}}{V_i} \\ &= r_{oa}\cdot(k_{gp}\phi_{Np}\phi_{Lp}a_p - F_{oxp}\cdot k_{rp}\cdot a_p) \\ &\quad + r_{od}[BotAlgPhoto \\ &\quad -F_{oxb}(k_{rb1}\cdot a_b - k_{rb2}BotAlgPhoto)] \\ &\quad \times\frac{A_{st,i}}{V_i} - r_{oc}\cdot(F_{oxcf}\cdot k_{dc}\cdot C_f) \\ &\quad - r_{oc}(F_{oxcf}\cdot k_{dcs}\cdot C_s) \\ &\quad - r_{on}(F_{oxnd}k_n n_a) + Reaeration - k_{COD}[COD] \\ &\quad - SOD\frac{A_{st,i}}{V_i} \end{aligned}$$

$$Reaeration = k_a[(e^{(lnO_s)}(1 - 00001148elev) - O)]$$

$$InOs = -139.3411 + \frac{1.575701 \times 10^5}{T_a} - \frac{6.642308 \times 10^7}{T_a^2} + \frac{1.2438 \times 10^{10}}{T_a^3} - \frac{8.621949 \times 10^{11}}{T_a^4}$$

CBODu

$$S_{cs} = r_{od}DetrDiss - SlowChydr - SlowCOxidSlowCHydr = k_{hc}(T)C_S$$

$$S_{cf} = SlowCHydr - FastCOxid - r_{ondn}Denitr + J_{CH4,d}\frac{A_{st,i}}{Vi}$$

$$SLowCOxid = F_{oxcf}k_{dcs}(T)C_S; FastCOxid = F_{oxcf}k_{dc}(T)f$$

Nitrogen

$$S_{DO} = r_{na} \cdot \left(k_{dp} \cdot a_p\right) + qN\left(\frac{k_{db}a_b}{H}\right) - k_{hn} \cdot n_o - \frac{v_{on}}{H} \cdot n_o S_{na} = k_{hn} \cdot n_o - F_{oxna} \cdot k_{na} + r_{na}\left(F_{oxp}k_{rp}\right)a_p - r_{na}P_{ap}\left(k_{gp}\emptyset_{Np}\emptyset_{Lp}\right)a_p + [J_{NH_4} - P_{ab}BotAlgUptakeN(NUpWCfrac)]\frac{A_{st,i}}{V_i}$$

$$P_{ap} = \frac{n_a n_n}{\left(k_{hnxp} + n_a\right)\left(k_{hnxp} + n_n\right)} + \frac{n_a k_{hnxp}}{(n_a + n_b)\left(k_{hnxp} + n_n\right)}$$

$$P_{ab} = \frac{n_a n_n}{(k_{hnxb} + n_a)(k_{hnxb} + n_n)} + \frac{n_a b}{(n_a + n_b)(k_{hnxb} + n_n)}$$

$$S_{nn} = F_{oxna} \cdot k_{mn} \cdot n_a - (1 - F_{oxdn})k_{dn}n_n - r_{na}\left(1 - P_{ap}\right) \cdot \left(k_{gp}\emptyset_{Np}\emptyset_{Lp}\right)a_p \cdot + [J_{NO_3} - (1 - P_{ab})BotAlgUptakeN(NUpWCfrac)]$$

Phosphorus

$$S_{po} = r_{pa} \cdot \left(k_{dp} \cdot a_p\right) + q_p\left(\frac{K_{db}a_b}{H}\right) - k_{hp} \cdot p_o - \frac{v_{op}}{H} \cdot p_o$$

$$S_{po} = k_{hp} \cdot p_o + r_{pa}\left(F_{oxp} \cdot k_{rp} \cdot a_p\right) - r_{pa}\left(k_{gp}\emptyset_{Np}\emptyset_{Lp}\right)a_p - \frac{v_{ip}}{H}P_i + [J_{PO_4} - BotAlgUptakeP \times (PUpWCfrac)]\frac{A_{st,i}}{V_i}S_{mi} = -\frac{v_i}{H}m_i$$

Notations Ah = biofilm of attached heterotrophic bacteria in the hyporheic sediment zone; ap = phytoplankton concentration (mgA/m^3), ab bottom algae concentration (gD/m^2); Ast,i = surface area of the reach (m^2); BotAlgPhoto = bottom algae photosynthesis (gO$_2$/m^2/day); BotAlgUptakeN = uptake rate for nitrogen in bottom algae (mgN/m^2/day); BotAlgUptakeP = uptake rate for phosphorous in bottom algae (mgP/m^2/day); BotAlResp = bottom algae respiration (gO$_2$/m^2/day); c^2,i = concentration in hyporheic sediment zone (mg/L); ci = concentration in the surface water in reach i (mg/L); ci − 1 = concentration in the upstream reach i − 1 (mg/L); CODoxid = oxidation of non-carbonaceous non-nitrogenous chemical oxygen demand (gO$_2$/m^2/day); Denitr = rate of denitrification [mgN/L/day]; E'i − 1, Ei′ = bulk dispersion coefficients between reaches i − 1 and i and i and i + 1 (m^3/day), respectively; E'hyp,j bulk dispersion coefficients between hyporheic zone and reach i (m^3/day); FastCOxid = fast CBOD oxidation (gO$_2$/m^2/day); Foxcf = attenuation due to low oxygen [dimensionless]; Foxna = attenuation due to low oxygen on ammonia nitrification (dimensionless); Foxp = attenuation due to low oxygen of phytoplankton respiration; H$_2$,i = the thickness of the hyporheic zone (cm); INb intracellular nitrogen concentration in bottom algae (mgN/m^2); IPb intracellular phosphorus concentration in bottom algae (mgP/m^2); JCH$_4$,d is the sediment flux of dissolved methane in oxygen equivalents (gO$_2$/m^2/day); JNH$_4$ = sediment flux of ammonia (mgN/m^2/day); JNO$_3$ = sediment flux of nitrate (mgN/m^2/day); JPO4 = the sediment flux of inorganic P (mgP/m^2/day); ka = reaeration rate (1/day); kdc(T); kdcs(T) = temperature-dependent fast CBOD oxidation rate [/day]; kdp = phytoplankton death rate (/day); kgp = maximum photosynthesis rate at temperature (/day); khc(T) = temperature-dependent slow CBOD hydrolysis

rate [/day]; khn = organic nitrogen hydrolysis rate (1/day); khnxb = preferences coefficient of bottom algae for ammonium (mgN/m^3); khnxp = preferences coefficient of phytoplankton for ammonium (mgN/m^3); khp = organic phosphorus hydrolysis rate (/day); kna = nitrification rate for ammonia nitrogen (1/day); knn = temperature-dependent nitrification rate for ammonia nitrogen (1/day); krp = phytoplankton respiration rate (1/day); NH4nitr = ammonium nitrification ($gO_2/m^2/day$); NUpWCfrac = fraction of N uptake from the water column by bottom plants; Os = saturation concentration of dissolved oxygen (mgO_2/L); Pab = preferences for ammonium as nitrogen source for bottom algae; Pap = preferences for ammonium as nitrogen source for phytoplankton; Phytophoto = phytoplankton photosynthesis ($gO_2/m^2/day$); PhytoResp = Phytoplankton respiration ($gO_2/m^2/day$); PUpWCfrac = fraction of P uptake from the water column by bottom plants; Qab,i = total flow abstractions from the reach I; Qi = outflow from reach i = Qi–1 inflow from the upstream reach i–1; qN = actual cell quotas of nitrogen (mgN/gD); qP = actual cell quotas of phosphorous (mgP/gD); Reaeration = ($gO_2/m^2/day$); rna = ratio of nitrogen to chlorophyll a (mgN/mgA); rod = ratio of oxygen consumed to detritus (mgO_2/mgD) during bottom algae respiration; ron = ratio of oxygen consumed nitrogen during nitrification (mgO_2/mgN); roa = ratio of oxygen generated to phytoplankton growth (mgO_2/mgA); roc = ratio of oxygen consumed during CBOD oxidation (mgO_2/mgO_2); rpa = ratio of phosphorus to chlorophyll a (mgP/mgA); S_2,i = sources and sinks of the constituent in the hyporheic sediment zone due to reactions; Sah,i = sources and sinks of heterotrophic bacteria in the hyporheic sediment zone due to reactions ($gD/m^2/days$; Sb,i = sources and sinks of bottom algae biomass due to reactions ($gD/m^2/day$); SbN,i = sources and sinks of bottom algae nitrogen due to reactions ($mgN/m^2/day$); SbP,i = sources and sinks of bottom algae phosphorus due to reactions ($mgP/m^2/day$); Si = sources and sinks of constituent i due to reactions and mass transfers (mg/L/day); SlowCOxid = slow CBOD oxidation ($gO_2/m^2/day$); Ta = absolute temperature (°K), elev = elevation of the area (m); V_2,i (= Φs, iAst, iH_2, i/100) volume of pore water in the hyporheic sediment zone (m^3); Vi = volumes of reach i (m^3), t is time (day); vi = inorganic suspended solids settling velocity (m/day); vip = inorganic phosphorus settling velocity (m/day); von = organic nitrogen settling velocity (m/day); vop = organic phosphorus settling velocity (m/day); Wi = external loading of the constituent to reach i (mg/day); ΦLp = phytoplankton light attenuation factor (dimensionless); ΦNp = phytoplankton nutrient attenuation factor (dimensionless); Φs,i = porosity of the hyporheic sediment zone.

3.4.4 Strengths

The model includes multiple loading and abstractions and can simulate both point and non-point pollution for 20 water quality parameters. It can also simulate water exchange between surface water column and hyporheic zone and sediment pore-water quality. It uses two forms of CBOD (slow and fast) and is capable of converting algal death to CBOD, macrophytes and detritus. The model can accommodate anoxia by reducing oxidation reactions to zero at low oxygen levels. Besides, denitrification is modeled as a 1st-order reaction that becomes pronounced at low oxygen concentrations. Sediment–water fluxes of dissolved oxygen and nutrients are simulated internally rather than being prescribed. The model explicitly simulates attached bottom algae. Light extinction is calculated as a function of algae, detritus and inorganic solids. Alkalinity, total inorganic carbon and river pH are simulated. It has inbuilt automatic calibration system using genetic algorithm (Pelletier and Chapra 2005).

3.4.5 Assumptions and limitations

The flow is assumed to be in steady state. The model simulates only the main stem of a river and does not simulate branches of the river system. It does not presently include an uncertainty component.

3.4.6 Applicability

QUAL series have been applied to numerous rivers. Here, a few applications of QUAL2kw model have been given which includes the water quality simulation of Wenatchee River, Washington State (Cristea and Pelletier 2005); Umpqua River, Oregon, USA (Turner et al. 2006) and Bagmati River, Nepal (Kannel et al. 2007a, b).

3.5 WASP 7

3.5.1 Development

The development of WASP model started in 1970s (Wool et al. 2001; Ambrose et al. 2006; Nikolaidis et al. 2006) with its latest enhanced version 7 (Ambrose and Wool 2009). WASP7, is freely available at USEPA's website. It is a dynamic compartment-modeling program to simulate the fate and transport of contaminants in surface waters.

3.5.2 Model system

The model is based on the concept of flexible compartmentalization and simulates conservation of mass both spatially and temporally which is accounted using FD equation for each segment. The processes of transport, loading, and transformation are simulated using advection dispersion and kinetic transformation. It can be applied in 1D, 2D and 3D (Wool et al. 2001). Ambrose et al. (2006) included the benthic algae and multiple phytoplankton classes in WASP7. Besides EUTRO for water quality and TOXI for toxicants, WASP7 has additional sub-models like advanced EUTRO (named Periphyton), MERCURY and HEAT. The model simulates the variations in detrital and periphyton concentrations based upon the QUAL2 K algorithm (Chapra and Pelletier 2003).

The basic program includes time-varying processes of advection, dispersion, point and diffuse mass loading and boundary exchange. The model has a user-friendly windows-based interface with a pre-processor; sub-model processors and a graphical postprocessor. The transport options for simulating hydrodynamics include internal stream transport algorithms and external linkage to Environmental Fluid Dynamics Code (EFDC) and the Hydrodynamic Program (DYNHYD) (Ambrose and Wool 2009). The input data requires the details regarding output control, model segmentations, boundary concentrations, point and diffuse source waste loads, kinetic parameters, constants, time series flow and initial concentrations. It can simulate the transport and transformation reactions for 14 state variables (Ambrose et al. 1993). WASP7 includes DO, N (organic, ammonia, nitrite, nitrate), P (organic, inorganic), phytoplankton and periphyton (bottom algae C, N. P), particulate detritus (N, P, C), CBOD (fast, intermediate, slow), temperature, salinity, coliform bacteria, silica, cohesive sediments, non-cohesive sedi-ment, sediment diagenesis, conservative tracer, pesticides, organic chemicals, mercury, heavy metals, and inorganic solids (Ambrose et al. 2006).

3.5.3 Governing equations

Basic equation

$$\frac{\partial(AC)}{\partial t} = \frac{\partial}{\partial x}\left(-U_x AC + E_x A\frac{\partial C}{\partial x}\right) + A(S_L + S_B) + AS_k$$

DO

$$\frac{\partial C_6}{\partial x} = k_a(C_{sat} - C_6) - k_d\left(\frac{c_6}{k_{BOD} + c_6}\right)C_5 - \frac{64}{14}k_{12}\left(\frac{c_6}{k_{NIT} + c_6}\right)c_1 - \frac{SOD}{D,} + G_{pl}\left(\frac{32}{12} + \frac{48}{14} + \frac{14}{12}(1 - P_{NH_3})\right)C_4 - \frac{32}{12}k_{1R}C_4$$

CBODu

$$\frac{\partial c_5}{\partial t} = a_{oc}k_{1d}c_4 - k_d\left(\frac{c_6}{k_{BOD} + c_6}\right)C_5 - \frac{5}{4}\frac{32}{14}k_{2d}\left(\frac{K_{NO_3}}{K_{NO_3} + c_6}\right)c_2;$$

$$BottleBOD_5 = c_5\left(1 - e^{-5knbot}\right) + a_{oc}c_4\left(1 - e^{-5k_{1R}}\right)$$

Nitrogen

$$\frac{\partial(c_4 a_{nc})}{\partial x} = \left(G_{pl} - D_{pl} - \frac{V_{s4}}{D}\right)\cdot c_4 a_{nc};$$

$$\frac{\partial c_7}{\partial t} = D_{pl}(a_{nc}\cdot f_{cn})c_4 - k_{71}\left(\frac{c_4}{k_m P_c + c_4}\right)\cdot c_7 - \frac{V_{s7}(1 - f_{d7})}{D}c_7$$

$$\frac{\partial c_1}{\partial t} = D_{pl}a_{nc}(1 - f_{on})c_4 + k_{71}\left(\frac{c_4}{k_{mPc} + c_4}\right)c_7 - k_{12}\left(\frac{c_6}{k_{NIT} + c_6}\right)\cdot c_1 - G_{pl}\cdot a_{nc}\cdot P_{NH_3}c_4$$

$$\frac{\partial c_2}{\partial t} = k_{12}\left(\frac{c_6}{k_{NIT} + c_6}\right)c_1 - G_{pl}\cdot a_{nc}\cdot(1 - P_{NH_3})c_4 - k_{2D}\left(\frac{k_{NO_3}}{k_{NO_3} + c_6}\right)\cdot c_2$$

$$P_{NH_3} = \left(\frac{c_2}{(k_{mN} + c_1)(k_{mN} + c_2)}\right)c_1 + \left(\frac{k_{mN}}{(c_1 + c_2)(k_{mN} + c_2)}\right)$$

Phosphorus

$$\frac{\partial(c_4 a_{pc})}{\partial x} = \left(G_{pl} - D_{pl} - \frac{V_{s4}}{D}\right) \cdot a_{pc} c_4$$

$$\frac{\partial c_8}{\partial t} = (D_{pl} \cdot a_{pc} \cdot f_{op}) \cdot c_4 - k_{83}\left(\frac{c_4}{k_{mPc} + c_4}\right) c_8 - \frac{V_{s3}(1 - f_{d8})}{D} c_8$$

$$\frac{\partial c_3}{\partial t} = D_{p1} a_{pc}(1 - f_{op}) c_4 + k_{83}\left(\frac{c_4}{k_{mPc} + c_4}\right) c_8 - G_{p1} \cdot a_{pc} \cdot c_4$$

Notations A cross-sectional area (m^2); anc = nitrogen to carbon ratio = 0.25 mgN/mgC; aoc = oxygen to carbon ratio = 32/12 (mgO_2/mgC); apc = phosphorus to carbon ratio (mgP/mgC),; C : concentration of water quality (g/m^3); c1 = ammonia–nitrogen (mgN/L); c_2 = nitrate nitrogen (mg/L); c_3 = phosphate phosphorus (mg/L); c_4 = the phytoplankton biomass in carbon units (mg/L); c_5 = CBOD (mg/L); c_6 = DO (mg/L); c_7 = organic nitrogen (mg/L); c_8 = organic phosphorus (mg/L); c_{sat} = saturated concentration of DO (mg/L); D = depth of water (m); Dp_1 = phytoplankton death rate (1/day); Ex = longitudinal diffusion coefficient (m^2/day); f_{d5} = dissolved fraction of CBOD; f_{d7} = fraction of dissolved organic nitrogen; f_{d8} = fraction dissolved organic phosphorus; fon = fraction of dead and respired phytoplankton recycled to the organic nitrogen pool; fop = fraction of dead and respired phytoplankton recycled to the organic phosphorus pool; Gp_1 = phytoplankton growth rate (1/day); k_{12} = nitrification rate (1/day); k_1d = phytoplankton death rate (1/day); k_1R = phytoplankton respiration rate at 20 °C (1/day); k_2d = denitrification rate (1/day); k_{71} = organic nitrogen mineralization rate (1/day); k_{83} = dissolved organic phosphorus mineralization (1/day; ka = re-aeration rate (1/day); k_{BOD} = half saturation constant for oxygen limitation for CBOD (mg/O_2/L); kd = CBOD deoxygenation rate (1/day); $k_d$bot = the laboratory "bottle" deoxygenation rate constant (1/day); kmN = Michaelis value for ammonia preference (μgN/L); kmPc = half saturation constant for phytoplankton limitation of phosphorous recycle (mgC/L); knbot = the laboratory "bottle" nitrification rate constant (1/day); kNIT = half saturation constant for oxygen limitation for nitrification (mgN/L); kNO_3 = half saturation constant for oxygen limitation of de-nitrification (mgO_2/L); PNH_3 = preference for ammonia term; SB = boundary loading rate including upstream, downstream, benthic, atmospheric (g/m^3 day); Sk = transformation term (total kinetic transformation rate; positive source, negative sink, g/m^3 day for variable i in a segment); SL = diffusion loading rate (g/m^3 day); SOD = sediment oxygen demand (mg/m^2/day); T = time (day); Ux = longitudinal velocity (m/day); Vs_3 = organic matter settling velocity (m/day); Vs_4 = phytoplankton settling velocity (m/day).

3.5.4 Strengths

WASP has a very flexible modeling framework and can simulate water quality in 1D/2D/3D. The volume control structure enables to follow the principle of mass-conservation. The model provides the transport computational framework and can be combined with EUTRO and TOXI to simulate eutrophication, nutrient, metals, toxics, and sediment transport.

3.5.5 Assumptions and limitations

The model assumes completely mixing control volume in the river. It requires an external hydrodynamic model to provide flow file for solving advection. The model has over-simplified sediment flux calculation and is unable to simulate periphyton or macroalgae. In addition, the sediment transport processes are not related to shear stress and the user-specified dispersion coefficient and temperature are used. Besides, the models uses 1st-order UPWIND difference in space which may cause significant numerical diffusion.

3.5.6 Applicability

A few applications of WASP series models can be found in Gualtieri and Rotondo (1996a, b), Pickett (1997), Tufford and McKellar (1999), Wool et al. (2003), Caruso (2004) and Ambrose et al. (2005). It has been used extensively to simulate nutrients, PCBs, organic compounds and heavy metals in many lake and coastal systems such as the Great Lakes; the estuaries of Potomac, James, Delaware, Gulf of Greece and deep rivers (Wool et al. 2001; Rygwelski et al. 1999; Stansbury and Admiraal 2004; Nikolaidis et al. 2006).

3.6 WQRRS

3.6.1 Development

It was originally developed by Chen and Orlob (1975) of Water Resources Engineers, with subsequent modification and continued maintenance and distribution by the Corps of Engineers Hydrologic Engineering Center (HEC). The model has been used to evaluate water quality conditions in river and reservoir systems.

3.6.2 Model system

The model is based on conservation of heat energy and mass both spatially and temporally. It is discretized into series of layers and elements. It includes settling, 1st-order decay, reaeration, chemical transformation, biological uptake and release, growth, respiration and mortality including predation. It includes 3 models, namely reservoir module (WQRRSR), Stream Hydraulics Package (SHP) to simulate the flow and Stream Water Quality (WQRRSQ) to simulate the water quality of stream networks. The input data required is geometric, meteorological, initial conditions, boundary conditions, hydraulic and kinetic parameters.

Model can simulate up to 18 state variables including: temperature, fish (three functional groups), aquatic insects, benthic animals, zooplankton, phytoplankton (two functional groups), benthic algae (two functional groups), detritus, organic sediment, inorganic suspended solids (up to five types), inorganic sediment, dissolved orthophosphorus, dissolved ammonia, dissolved nitrate, dissolved BOD (i.e., DOC), coliform bacteria, total inorganic carbon, alkalinity, TDS, and pH (not all of the possible state variables are included). Temperature simulations were performed based on the head budget method, which evaluates the five major components of the heat budget of a waterbody. In this model, the discharges, velocities, and depths can be computed as a function of time and location in a stream. The input stage-discharge relationships, hydrologic routing, kinematic routing, steady flow equations, or the full unsteady flow St. Venant equation can be used to perform hydraulic computations. (USACE-HEC 1978 [revised on 1986]).

3.6.3 Governing equations

Basic equation

$$\overline{v}\frac{\partial C}{\partial t} = \Delta z^{*} Q_z \frac{\partial C}{\partial t} + \Delta z \cdot A_z \cdot D_c \frac{\partial C^2}{\partial Z^2} + Q_i C_i - Q_o C \pm \Delta S$$

DO

$$\begin{aligned}\frac{\partial O_2}{\partial t} &= K_O\left(O_2^{*} - O_2\right) - KL \cdot L - KNH_3 \cdot NH_3 \cdot O_2NH_3 \\ &\quad - KNO_2 \cdot NO_2 \cdot O_2NO_2 \\ &\quad - KDET \cdot (DET + S) \cdot O_2DET \\ &\quad - \sum BIO \cdot O_2R\left[BTOR + BIOG\left(\frac{1}{BIEFF} - 1\right)\right. \\ &\quad \left.\times(1 - EXF)\right] + \sum A(O_2P \cdot AG - O_2R \cdot AR)\end{aligned}$$

CBODu

$$\frac{\partial L}{\partial t} = -L \cdot KL$$

Nitrogen

$$\begin{aligned}\frac{\partial NH_3}{\partial x} &= -KNH_3 \cdot NH_3 + KDET(DET + S)DN \\ &\quad + \sum BIO \cdot BION\left[BIOR + BIOG\left(\frac{1}{BIEFF} - 1\right)\right. \\ &\quad \left.\times(1 - EXF)\right] - \sum A \cdot AP(AG \cdot FNN - AR)\end{aligned}$$

$$\begin{aligned}\frac{\partial NO_2}{\partial t} &= KNH_3 \cdot NH_3 - KNO_2 \cdot NO_2; \frac{\partial NO_3}{\partial t} \\ &= KNO_2 \cdot NO_2 - \sum A \cdot AN \cdot AG(1 - FNN)\end{aligned}$$

Phosphorus

$$\begin{aligned}\frac{\partial PO_4}{\partial t} &= KDET(DET + S)DP \\ &\quad + \sum BIO \cdot BIOP\left[BIOR + BIOG\left(\frac{1}{BIEFF} - 1\right)\right. \\ &\quad \left.\times(1 - EXF)\right] \\ &\quad - \sum A \cdot AP(AG - AR)\end{aligned}$$

Notations Δz = element thickness; A = algae concentration (i.e., phytoplankton and benthic algae); AG = algal growth rate; AN = nitrogen fraction of

algae; AP = phosphorus fraction of algae; AR = algal respiration rate; Az = cross sectional area at the fluid element boundary; BIEFF = biota digestive efficiency; BIO = biota concentration excluding algae; BIO = biota concentration including algae; BIOEFF = biota digestive efficiency; BIOG = biota growth rate; BION = nitrogen fraction of biota; BIOG = biota growth rate; BIOP = phosphorus fraction of biota; BIOR = biota respiration rate; C = the constituent concentration; DET = detritus concentration; DN = nitrogen fraction of detritus; DP = phosphorus fraction of detritus; Dz = effective diffusion coefficient; EXF = particulate fraction of total excrement; FNN = ammonia fraction of available nitrogen; KDET = detritus decay rate; KL = rate of BOD removal by oxygen uptake; KNH_3 = ammonia decay rate; KNH_3 = ammonia decay rate; KNH_3 = ammonia decay rate; KNO_2 = nitrite decay rate; Ko = surface exchange coefficient for dissolved oxygen; L = concentration of ultimate BOD; NH_3 = ammonia concentration as nitrogen; NO_2 = concentration of nitrite nitrogen; NO_3 = nitrate concentration as nitrogen; O_2 = nitrite concentration as nitrogen; O_2^* = concentration of dissolved oxygen at saturation; O_2 = concentration of dissolved oxygen; O_2DET = stoichiometric equivalence between oxygen and nitrite; O_2NH_3 = stoichiometric equivalence between oxygen and ammonia; O_2NO_2 = stoichiometric equivalence between oxygen and nitrite; O_2P = oxygenation factor for algal photosynthesis; O_2R = stoichiometric equivalences between oxygen and biomass respiration; PO_4 = phosphate concentration as phosphorus; S = concentration equivalent of organic sediment; S = source and sinks; t = computation time increment; Q = flow; $\bar{v}$ = the volume of the fluid element.

3.6.4 Strengths

The model assesses eutrophication related processes and effects in a simplified manner. The model can evaluate the vertical stratification of physical, chemical, and biological parameters in a reservoir.

3.6.5 Assumptions and limitations

The dispersion is assumed to be instantaneous for all inflow quantities and constituents throughout the horizontal layers. The river is assumed to have 1D homogeneous element and longitudinal and lateral variations are neglected. It does not consider competition between individual species.

3.6.6 Applicability

The application of the model can be found in Lopes et al. (2003); Li et al. (2003) and Kerachian et al. (2005). Karamouz et al. (2008), provided a methodology for conflict resolution over water allocation for Karkheh river-reservoir system (Iran). They linked WQRRS with the optimization model to determine the quality of outlet release, as well as the temporal and spatial variations of the concentration of water quality variables in the reservoir.

4 Errors in WQMs

The models have been developed for specific topographical region and are based on certain default values for rate coefficients which limit their applicability to other geographical areas. However, they can be applied to other study regions by incorporating various statistical tools for calibration, validation, sensitivity and uncertainty analysis. The extent of uncertainty depends upon the quality of data and nature of the model. The errors in the simulation arise due to structural uncertainty, input data uncertainty and uncertainty of the model parameters (Harremoës 1988; Refsgaard et al. 2007; Freni et al. 2009; Mannina and Viviani 2009). Therefore, eliminating the errors and uncertainties is a major task for any river quality modeling study. Consequently, it is important to adjust the rate coefficients according to the river profile in accordance with the chosen WQM. Nevertheless, these values can be adjusted only in the range of default values via calibrating the model. Thomann and Muller (1982) have described the verification of WQMs. Seng Lung and Larson (1995) demonstrated the usefulness of calibration in evaluating water pollution control strategies in upper Mississippi River and Lake Peppin. All the WQMs reviewed have wide range of default values and require hourly frequency of the dataset, which can be changed depending upon the data availability.

It is also inevitable to nullify or minimize the errors related to monitoring of input parameters. In this context, the Global Environment Monitoring System

(GEMS) was formulated to standardize a global network for freshwater quality monitoring. Initially, under the flagship of GEMS the important water quality parameters to be monitored were DO, BOD, faecal coliforms, nitrates and chemical constituents such as major, minor and trace contaminants, heavy metals and toxic organic compounds. However, the research has demonstrated that sampling the above mentioned parameters is insufficient in formulating the river restoration plans. Therefore, analysis of suspended matter, bottom sediment, biological tissue and ecological parameters is inevitable to plan the improvement in river water quality (Helmer 1994). It is noteworthy that worldwide, most of the input parameters are not being monitored regularly like total carbon (organic/inorganic); light extinction; heat budget; nutrients; nitrogen and its compounds; phosphorus and its compounds; sand/silt/clay; sediments and various forms including SOD; toxicants (organic/inorganic); solid (organic/inorganic and suspended/dissolved), aquatic plants and animals; benthic plants and animals; microbes; algae and various forms, pathogens, various forms of BOD like NBOD, CBOD (slow and fast); brines; salinity; silica, conservative tracer, pesticides, synthetic organics; hyporheic metabolism; iron; manganese etc.

Furthermore, apart from GEMS, there exists many global agencies aiming to promote good governance in water management like Water Environment Partnership in Asia (WEPA), Land and Water Development Division of Food and Agriculture Organization of the United Nations (LWDD, FAO); Global International Waters Assessment (GIWA); Water Portal; United Nations Development Programme (WP:UNDP) and many more. Also, in addition to GEMs stations, most of the countries have their own monitoring agencies like USA have United States Environment Protection Agency (USEPA), India has Central water commission (CWC), Central Pollution Control Board (CPCB) etc. Existence of various regulatory bodies, leads to mismatch between the data required by a WQM and actual data monitored for the study area. Such, diversification negatively impacts the frequency and the robustness of the input data ultimately leading to the adoption of various assumptions for the river quality modeling studies and intervention analysis. Ambrose et al. (2009) concluded that no comprehensive model exists that has all functionalities and each model has its own set of assumptions and limitations.

All these gaps and existence of default values lead to underutilization of the models. Such differences between the data available and the model requirements lead to the development of weak pollution abatement strategies. Therefore, it is important to perform the systematic analysis and implementation of the data monitored (Helmer 1994). This fact was further strengthened in a study done by Zhulidov et al. (2000) on the derailed water quality programme in Russia which was affected by chronic underfunding; poor functioning of the network design including choice of parameters, sample collection, analytical conditions; data quality including its handling and accessibility; and by large the 'question of institutionalized flexibility required to meet local data needs'. Similarly, Bhardwaj (2005) highlighted few constraints of water quality monitoring in India like limited resources (finances and manpower), infrastructure sustainability, improper reporting of units, variation in analysis methods and quality control of chemicals, no usage of sophisticated statistical packages for data validation etc. Likewise, Strobl et al. (2006) gave the methodology to select the critical sampling points within a watershed via water quality monitoring network design.

Therefore, it is very crucial to comprehend the strengths, assumptions and limitations of the WQM along with the comprehensive understanding of the errors associated.

5 Discussion

The models described in the study are either steady-state or dynamic in nature. They can estimate the real-field mathematical approximation of the various physical, chemical and biological changes. The models have been compared on the basis of their capabilities, assumptions, basic equations, dimensions, limitations and strengths to simulate different parameters. On the basis of the review and literature collected, it can be stated that all the reviewed models are freely available online and have windows based graphical interface except for BLTM.

BLTM was found to be a simple model with comprehensive nutrient, algal and DO dynamics and is highly stable due to useage of special steady-state implemented for an implicit backward difference numerical scheme (Jobson and Schoellhamer 1987).

It was observed that all the reviewed WQMs models represent different levels of complexity in terms of underlying formulations. Comparatively, the water quality algorithms of EPD-Riv1 are most comprehensive. Whereas, AQUATOX is the most comprehensive model available for risk assessment. In terms of data requirements AQUATOX, QUAL2 Kw and WASP series are most data extensive models. However, QUAL series has certain advantages which makes it favorite among modellers like easy accessibility, frequent upgrades and more comprehensive formulations like simulating maximum numbers of parameters; chemical reactions in hyporheic zone etc. WQRRS can be used for both planning and design purposes. However, its requirement of intensive input data and complexity makes it difficult to be used by environmental planers. EPD-RIV1 model does not include processes like sediment transport such as scour and deposition. These are important factors that influence DO in a river (Park et al. (2008); Jobson and Schoellhamer (1987); Environmental Laboratory (1985); Pelletier and Chapra (2005); Ambrose and Wool (2009); USACE-HEC 1978 [revised on 1986]).

Table 1, describes the capabilities of the WQMs in terms of water quality parameter being simulated. Three models namely QUAL2kw, WASP and AQUATOX are capable of simulating maximum number of parameters. AQUATOX, QUAL2 Kw and WASP include the sediment diagenesis model for remineralization. QUAL2kw can also simulate SOD and hyporheic metabolism which are vital for predicting river water quality and planning the management options. As observed, WASP model has an advantage of simulating toxicants as well.

When analyzed for dimension, hydraulic, state, process description, nature of data, pollution transport and solution method characteristics (Table 2), it was observed that BLTM, and EPD Riv1 models can simulate unsteady flow and QUAL series and AQUATOX simulates steady flow. Whereas, WASP and WQRRS can simulate both steady and unsteady flow. Except for BLTM which is empirical all the models are mechanistic according to the process description. Further, all models are deterministic except for AQUATOX which is both deterministic and stochastic depending upon the data type. All models solve the equation using numerical solution method. In addition, QUAL2kw, AQUATOX and WASP provide uncertainty analysis tools as well.

6 Conclusions

The river quality models have come a long way and a wide variety of models are available today for planning river quality restoration projects. These models have incorporated the developments in basic research to offer application in various conditions and for various types of pollutants. The selection of a model for a particular policy objective is a critical task, as it requires assessment of theoretical validity, data availability, understanding the advantages and limitations of a model. The river quality modelling requires the strengths of input data in terms of information on hydrodynamics, geochemical, atmospheric and anthropogenic influences. Different models require varied sets of input data on the basis of frequency, pollutant type, water body type and solution method type. WQMs can handle large data sets required for comprehensive planning. However, a river system is very complex and therefore, no model is comprehensive enough to capture the entire gamut of real phenomenon. Each river quality model suffers from limitations mainly due to mathematical approximation of the physical, chemical and biological changes occurring in the river system. Hence, based on the review certain guidelines have been suggested to minimize the uncertainty and selecting the best-fit model for the application on the study area which is as follows:

6.1 Coherence in water quality assessment

Every country requires a mandate wherein the water quality monitoring agencies must follow the GEMS protocols of monitoring DO, BOD, faecal coliforms, nitrates and chemical constituents such as major, minor and trace contaminants, heavy metals, toxic organic compounds, analysis of suspended matter, bottom sediment, biological tissue and ecological parameters and other model specific parameters. Optimization of data collection (identifying critical sampling locations, collecting optimum numbers of replicates); identification of critical measurements and sampling locations (first order error analysis or sensitivity analysis) is crucial for minimizing the errors.

6.2 Uncertainty assessment of WQM

A model must be adopted for a particular river only after calibration of kinetic coefficients and matching

of simulated values with measured data. The range of validity of the calibrated model is further examined by validation of the model. The errors in the WQMs must be overcome by performing sensitivity and uncertainty analysis. The sensitivity analysis evaluates the contribution of the various sources of uncertainty to the model output and system performance. Uncertainty is a measure of the 'goodness of fit' of a result which forms the basis for decision making. Beck (1987), highlighted that parameter uncertainties must be evaluated to estimate their impact on model performance and calibration. Dubus et al. (2003) stated that before studying the effect of simulation it is important to identify the origin of uncertainty.

In the absence of these, river restoration projects may fail to provide the desired results due to overestimation or underestimation of predicted values out of an intervention.

6.3 Complexity of reviewed models

Most of the models studied are incapable of simulating heavy metals except EPD-Riv1 which can simulate Iron and Manganese. WASP is the only model which can predict Silica, conservative tracer, pesticides, synthetic organics. On the basis of comparison of process description, mathematical formulations, water quality parameters simulated and input data requirements, it was observed that BLTM and WQRRS are simple models with lower levels of complexity; QUAl2kw and WASP are easy to access and user-friendly and have intermediate level of complexity. However, AQUATOX and EPD-Riv1 are very comprehensive but they have higher levels of complexity. Based on the above discussion, it is concluded that QUAL2kw and WASP can be considered as the most effective tool for modelling the river water quality. Therefore, the above compared models can be classified according to the level of complexity which is as follows:

- Lower levels of complexity: BLTM and WQRRS
- Intermediate levels of complexity: QUAL2kw and WASP
- Higher levels of complexity: AQUATOX and EPD-Riv1

When compared, it was observed that out of all six models studied, QUAL2kw and WASP have following advantages:

- Public domain; graphical user interface; simple to use
- QUAL2kw: 1D and WASP:1D, 2D and 3D
- Simulates maximum number of water quality parameters
- QUAL2kw has inbuilt Auto calibration option
- Uncertainty analysis tool can be plugged-in both QUAL2kw and WASP

However, it is completely user's discretion to decide the 'best model' depending upon factors like the geographic region, study area, watershed type, size of the river, data availability and most importantly the type of pollutants to be monitored. It is therefore essential that a WQM be recognized by regulatory agencies for various rivers correlating with the physical conditions of the river. Next step is to design the water quality surveillance to provide not only the information on existing quality but also to meet the input requirements of the model and real in situ values (to avoid use of default values). This will save time and cost overruns in long term and avoidance of the use of non-suitable WQM, often selected on the basis of convenience. The comprehensive review on basic research and models as provided here can guide the planners and the researchers for the convergence of the objectives of water quality surveillance program, water quality modelling, and planning of river restoration projects.

Modellers have only compared these models qualitatively on the basis of their capabilities and applications. These models have not been applied to same river system leading to a major gap in understanding the model performance. Hence, there is an urgent need to apply different models on same river system using same input data and evaluating the model performance on the basis of quantitative comparisons. Such comparisons will not only evaluate the 'best uses' for each model but would also enhance the model strengths and capabilities by identifying their limitations in terms of process and applications. Comparative application of these models propels environment managers towards formulation of BMPs for river restoration plan.

Acknowledgments The authors would like to thank Ms Priyanka Banerjee for the editing and proof-reading the article.

References

Adrian DD, Sanders TG (1998) Oxygen sag equation for second-order BOD decay. Water Res 32(3):840–848

Adrian DD, Yu FX, Barbe D (1994) Water quality modeling for a sinusoidally varying waste discharge concentrations. Water Res 28(5):1167–1174

Ambrose RB, Wool TA (2009) WASP7 Stream transport-model theory and user's guide, supplement to water quality analysis simulation program (WASP) user documentation, EPA/600/R-09/100. USEPA, Washington, DC

Ambrose RB, Wool TA, Martin JL (1993) The water quality simulation program (WASP), version 5, Part A, Model documentation. Athens: Environmental Research Lab, UEPA

Ambrose RB, Barnwell TO, McCutcheon SC, Williams JR (1996) Computer models for water quality analysis. In: Mays LW (ed) Water Resources Handbook, Chap. 14, McGraw-Hill, New York

Ambrose RB, Tsiros IX, Wool TA (2005) Modeling mercury fluxes and concentrations in a Georgia watershed receiving atmospheric deposition load from direct and indirect sources. J Air Waste Manag Assoc 55(5):547–558

Ambrose RB, Martin JL, Wool TA (2006) WASP7 Benthic algae: model theory and user's guide, EPA/600/R-06/106. USEPA, Washington, DC

Ambrose RB, Wool TA, Barnwell TO Jr (2009) Development of water quality modeling in the United States, review. Environ Eng Res 14(4):200–210

Beck MB (1987) Water quality modelling: a review of the analysis of uncertainty. Water Resour Res 23(8):1393–1442

Bhardwaj RM (2005). Water quality monitoring in india-achievements and constraints. IWG-Env. International work session on water statistics, Vienna, June 20–22

Bhargava DS (1983) Most rapid BOD assimilation in Ganga and Yamuna rivers. J Environ Eng 109(1):174–178

Bowen RL, Young RA (1985) Financial and economic irrigation net benefit functions for Egypt's northern delta. Water Resour Res 21(9):1329–1335

Bowie GL, Mills WB, Porcella DB, Cambell CL, Pagenkopf JR, Rupp GL, Johnson KM, Chan PWH, Gherini SA (1985) Rates, constants, and kinetics formulations in surface water quality modeling (2nd edn). Athens, GA, US Environmental Protection Agency, Environmental Research Laboratory, EPA/600/3-85/040, p 455

Broshears RE, Clark GM, Jobson HE (2001) Simulation of stream discharge and transport of nitrate and selected herbicides in the Mississippi River. Hydrologic Process 15(7):1157–1167

Brown LC, Barnwell TO (1987) The enhanced stream water quality models QUAL2E and QUAL2E-UNCAS. Documentation and user manual, report EPA/600/3-87/007, U.S. EPA, Athens, GA

Bulak JS, Hurley NM Jr, Crane JS (1993) Production, mortality, and transport of striped bass eggs in congaree and wateree rivers: South Carolina. Am Fish Soc Symp 14:29–37

California Water Resources Control Board, 1996, Methodology for flow and salinity estimates in the Sacramento-San Joaquin delta and Suisun Marsh: seventeenth annual progress report to the state water resources control board in accordance with water right decision 1485, Order 9, June, 37 p

Camp (1963) First expanded BOD-DO model. In: Jolankai DG (ed) Basic river water quality models, IHP-V Project 8.1, 1997, 27–29

Caruso BS (2004) Modeling metals transport and sediment/water interactions in a mining impacted mountain stream. J Am Water Works Assoc 40(6):1603–1615

Chapra SC (1997) Surface water quality modelling. Mc Graw-Hill series in water resources and environmental engineering. McGraw-Hill, New York, p 844

Chapra SC, Pelletier GJ (2003) QUAL2 K: a modeling framework for simulating river and stream water quality (beta version): documentation and users manual. Civil and Environmental Engineering Department. Medford: Tufts University

Chen CW, Orlob GT (1975) Ecological simulation for aquatic environments. In: Patton BC (ed) Systems analysis and simulation in ecology, vol III. Academic Press, New York, pp 475–588

Clough JS (2004) AQUATOX (Release 2): Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems, vol. 3, User's Manual for the BASINS (Version 3.1) Extension to AQUATOX Release 2. EPA-823-R-04-003, U.S. Environmental Protection Agency, Office of Water

Clough JS, Park RA (2005). AQUATOX: modeling environmental fate and ecological effects in aquatic ecosystems, release 2.1, addendum to release 2 technical documentation, US Environmental Protection Agency, Office of Water, Washington, DC

Conrads PA, Roehl EA (1999) Comparing physics-based and neural network models for simulating salinity, temperature, and dissolved-oxygen in a complex, tidally affected river basin. In: Proceedings of the south Carolina environmental conference, March 15–16, 1999, Myrtle Beach, SC

Cox BA (2003a) A review of dissolved oxygen modelling techniques for lowland rivers. Sci Total Environ 314–316:303–334

Cox BA (2003b) A review of currently available in-stream water-quality models and their applicability for simulating dissolved oxygen in lowland rivers. Sci Total Environ 314–316:335–377

Cristea N, Pelletier G (2005) Wenatchee river temperature total maximum daily load study. Publication number 05-03-011, Washington State Department of Ecology, Olympia, WA, http://www.ecy.wa.gov/biblio/0503011.html, Accessed on 28th may 2012

Dobbins WE (1964) BOD and oxygen relationships in streams. J Sanit Eng Div Am Soc Civ Eng 90(3):53–78

Drewes PA, Conrads PA (1995). Assimilative capacity of the Waccamaw River and the Atlantic Intracoastal Waterway near Myrtle Beach, South Carolina, 1989–92: U.S. geological survey water-resources investigations report, 95–4111, p 58

Dubus IG, Brown CD, Beulke S (2003) Sources of uncertainty in pesticide fate modelling. Sci Total Environ 317(1–3):53–72

Dudley NJ (1988) A single decision-maker approach to irrigation reservoir and farm management decision making. Water Resour Res 24(5):633–640

Environmental Laboratory (1985) CE-QUAL-RIV1: a dynamic, one-dimensional (longitudinal) water quality model for streams, user's manual, instruction report EL-95-2, US Army engineer waterways experiment station, Vicksburg, MS

Fair GM (1939) The dissolved oxygen sag-an analysis. Sew Works J Water Environ Fed 11(3):445
Feaster TD, Conrads PA (1999) Characterization of water quality and simulation of temperature, nutrients, biochemical oxygen demand, and dissolved oxygen in the Wateree River, South Carolina, 1996-1998: U.S. Geological Survey Water-Resources Investigations Report 99-4234, p 90
Feaster TD, Conrads PA, Guimaraes WB, Sanders CL Jr, Bales JD (2003) Simulation of temperature, nutrients, biochemical oxygen demand, and dissolved oxygen in the Catawba River, South Carolina, 1996–97: U.S. geological survey water-resources investigations report 03-4092, Columbia, South Carolina, p 123
Freni G, Mannina G, Viviani G (2009) Identifiability analysis for receiving water body quality modelling. Environ Model Softw 24(1):54–62
Graf JB (1995) Measured and predicted velocity and longitudinal dispersion at steady and unsteady flow, Colorado River, Glen Canyon Dam to Lake Mead. Water Resour Bull Am Water Resour Assoc 31(2):265–281
Gualtieri C, Rotondo G (1996a) Water quality modelling of Speed River. Part one: model calibration (in Italian). Ingegneria Sanitaria 2
Gualtieri C, Rotondo G (1996b) Water quality modelling of Speed River. Part two: model validation and application (in Italian), Ingegneria Sanitaria 5/6
Guay JR (1991) Simulation of urban runoff and river water quality in the San Joaquin River near Fresno, California: American water resources association symposium on urban hydrology, Denver, Colorado, November 4–8, 1990, Proceedings, p 177–181
Gundelach JM, Castillo JE (1976) Natural stream purification under anaerobic conditions. J (Water Pollut Contr Fed) Water Environ Fed 48(7):1753–1758
Harremoës P (1988) Stocastic models for estimation of extreme pollution from urban runoff. Water Resour 22(8):1017–1026
Helmer R (1994) Water quality monitoring: national and international approaches, hydrological, chemical and biological processes of transformation and transport of contaminants in aquatic environments, rostov-on-don symposium (May 1993) Proceedings, IAHSPubl. 219
James A (1993) An Introduction to water quality modelling. Technology & Engineering. Wiley, Chichester, p 311
Ji Z-G (2008) Hydrodynamics and water quality: modelling rivers, lakes, and estuaries. Wiley-Interscience, pp 704
Jobson HE, Schoellhamer H (1987) Users manual for a branched Lagrangian transport model: U.S. Geological Survey Water Resources Investigations Report 87-4163, pp 73
Jolankai G (1997) Basic river water quality models, IHP-V. Technical documents in hydrology No. 13, UNESCO, Paris
Kannel PR, Lee S, Kanel SR, Lee Y-S, Ahn K-H (2007a) Application of QUAL2Kw for water quality modelling and dissolved oxygen control in the river Bagmati. Environ Monit Assess 125(1–3):201–217
Kannel PR, Lee S, Lee Y-S, Kanel SR, Pelletier GJ (2007b) Application of automated QUAL2Kw for water quality modelling and management in the Bagmati River, Nepal. Ecol Model 202(3–4):503–517
Kannel PR, Kanel SR, Lee S, Lee Y-S, Gan TY (2010) A review of public domain water quality models for simulating dissolved oxygen in rivers and streams. Environ Model Assess. doi:10.1007/s10666-010-9235-1
Karamouz M, Moridi A, Fayyazi HM (2008) Dealing with conflict over water quality and quantity allocation: a case study. Scientia Iranica 15(1):34–49
Kerachian R, Karamouz M, Naseri AV (2005) River water quality management: application of stochastic genetic algorithm. Impacts of global climate change. In: Proceedings of world water and environmental resources congress
Kirchner JW, Dillon PJ, Lazerte BD (1993) Separating hydrological and geochemical influences on runoff acidification in spatially heterogeneous catchments. Water Resour Res 29(12):3903–3916
Koussis AD, Kokitkar P, Mehta A (1990) Modeling DO conditions in streams with dispersion. J Environ Eng, ASCE 116(3):601–614
Krysanova V, Bronstert A, Mûller-Wohlfeil DI (1999) Modelling river discharge for large drainage basins: from lumped to distributed approach. Hydrol Sci-Joumal-des Sciences Hydrologiques 44:2
Lee DJ, Howitt RE (1996) Modelling regional agricultural production and salinity control alternatives for water quality policy analysis. Am J Agric Econ 78(1):41–53
Lei BL, Huang SB, Jin XW, Wang ZJ (2010) Deriving the aquatic predicted no-effect concentrations (PNECs) of three chlorophenols for the Taihu Lake, China. J Environ Sci Health A 45(14):1823–1831
Li WH (1962) Unsteady dissolved-oxygen sag in a stream. J Sanit Eng Div Am Soc Civ Eng 88(3):75–85
Li WH (1972) Effects of dispersion on DO-Sag in uniform flow. J Sanit Eng Div Am Soc Civ Eng 98(1):169–182
Li CH, Hao FH, Cui L (2003) Forecast of water quality changes in the Baohe reservoir after its storage. Resour Environ Yangtze Basin 12(1):61–66
Lizarraga JNA (1996) Using QUALTX and DAFLOW/BLTM to simulate water quality in Texas Rivers. http://smig.usgs.gov/SMIG/features_0396/qualtx.html (Accessed 7th Jan 2011)
Lopes LFG, do Carmo JSA, Cortes RMV (2003) Influence of dam-reservoirs exploitation on the water quality. In: Brebbia CA (ed) River basin management II. Wessex Institute of Technology, UK, pp 512
Mannina G, Viviani G (2009) Parameter uncertainty analysis of water quality model for small river. 118th World IMACS/MODSIM Congress, Cairns, Australia 13-17 July 2009 http://mssanz.org.au/modsim09
Martin JL, McCutcheon SC (with contributions by Robert W.Schottman) (1999) Hydrodynamics and transport for water quality modelling. Lewis Publishers. pp 745
Martin JL, Wool T, Olson R (2002) A dynamic one-dimensional model of hydrodynamics and water quality EPD-RIV1 Version 1.0. User's manual by Roy Burke III, Georgia Environmental Protection Division, Atlanta, Georgia
McBride GB, Rutherford JC (1984) Accurate modelling of river pollutant transport. J Environ Eng Div Am Soc Civ Eng 110(4):809–827
Nikolaidis NP, Karageorgis AP, Kapsimalis V, Marconis G, Drakopoulou P, Kontoyiannis H et al (2006) Circulation and nutrient modeling of Thermaikos Gulf, Greece. J Mar Syst 60(1–2):51–62

Park RA (1990) AQUATOX, a modular toxic effects model for aquatic ecosystems. U.S. environmental protection agency, Corvallis, Oregon

Park RA, Clough JS (2004a) AQUATOX (Release 2): modeling environmental fate and ecological effects in aquatic ecosystems. volume 2: technical documentation. EPA-823-R-04-002, U.S. environmental protection agency, Office of Water, Washington, DC

Park RA, Clough JS (2004b) AQUATOX (Release 2): Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems. Vol. 1: User's Manual. EPA-823-R-04-001. U.S. Environmental Protection Agency, Office of Water, Washington, DC

Park RA, O'Neill RV, Bloomfield JA, Shugart HH Jr, Booth RS, Koonce JF, Adams MS, Clesceri LS, Colon EM, Dettman EH, Goldstein RA, Hoopes JA, Huff DD, Katz S, Kitchell JF, Kohberger RC, LaRow EJ, McNaught DC, Peterson JL, Scavia D, Titus JE, Weiler PR, Wilkinson JW, Zahorcak CS (1974) A generalized model for simulating lake ecosystems. Simulation 23(2):30–50

Park RA, Connolly CI, Albanese JR, Clesceri LS, Heitzman GW, Herbrandson HH, Indyke BH, Loehe JR, Ross S, Sharma DD, Shuster WW (1982) Modelling the fate of toxic organic materials in aquatic environments. Rept. EPA-600/S3-82-028. USEPA, Athens, GA

Park RA, Anderson JJ, Swartzman GL, Morison R, Emlen JM (1988). Assessment of risks of toxic pollutants to aquatic organisms and ecosystems using a sequential modelling approach. In: Fate and effects of pollutants on aquatic organisms and ecosystems, 153–165. EPA/600/9-88/001. USEPA, Athens, GA

Park K, Kuo AY, Shen J, Hamrick JM (1995) A three-dimensional hydrodynamic-eutrophication model (HEM-3D): description of water quality and sediment process submodels. Virginia Institute of Marine Science, College of William and Mary, Gloucester Point, VA

Park RA, Clough JS, Wellman MC (2008) Review: AQUATOX: modelling environmental fate and ecological effects in aquatic ecosystems. Ecol Model 213:1–15

Pelletier GJ, Chapra SC (2005) QUAL2Kw theory and documentation (version 5.1), a modeling framework for simulating river and stream water quality. Washington: Department of ecology

Pickett PJ (1997) Pollutant loading capacity for the Black River, Chehalis River system, Washington. J Am Water Resour Assoc 33(2):465–480

Raunch W, Henze M, Koncsos L, Reichert P, Shanahan P, Somlyódy L, Vanrolleghem P (1998) River water quality modelling: I. State of the art, presented at the IAWQ Biennial international conference, Vancouver, British Columbia, Canada, 21–26 June

Refsgaard JC, Van der Sluijs JP, Højberg AL, Vanrolleghem PA (2007) Uncertainty in the environmental modelling process: a framework and guidance. Environ Model Softw 22:1543–1556

Rygwelski KR, Richardson WL, Endicott DD (1999) A screening-level model evaluation of atrazine in the Lake Michigan basin. J Great Lakes Res 25(1):94–106

Seng Lung WU, Larson CE (1995).Water quality modelling of Upper Mississippi river and lake Peppin. J Environ Eng 121(EE10):691–699

Shanahan P, Henze M, Koncsos L, Rauch W, Reichert P, Somlyódy L, Vanrolleghem P (1998) River water quality modelling: II. Problems of the art, presented at the IAWQ biennial international conference, Vancouver, British Columbia, Canada, 21–26 June

Somlyódy L, Henze M, Koncsos L, Rauch W, Reichert P, Shanahan P, Vanrolleghem P (1998) River water quality modelling: III. Future of the art, presented at the IAWQ biennial international conference, Vancouver, British Columbia, Canada, 21–26 June

Stansbury J, Admiraal DM (2004) Modeling to evaluate macrophyte induced impacts to dissolved oxygen in a tail water reservoir. J Am Water Resour Assoc 40(6): 1483–1497

Streeter WH, Phelps EB (1925) A study of the pollution and natural purification of the Ohio River, 111. Factors concerned in the phenomena of oxidation and reaeration. Public Health Bulletin No. 146, US Public Health Service, Government Printing Office, Washington

Strobl RO, Robillard PD, Day RL, Shannon RD, McDonnell AJ (2006) A water quality monitoring network design methodology for the selection of critical sampling points: part II. Environ Monit Assess 122(1–3):319–334

The Georgia Department of Natural Resources (n.a.) Total maximum daily load evaluation for the Coosa River in the Coosa River basin for dissolved oxygen. http://www.gaepd.org/Documents/coosa_modeling.html, Accessed on 28th may 2012

The Georgia Department of Natural Resources (n.a.) Chattahoochee River at Capps Ferry monitoring. Environmental protection division, Georgia department of natural resources. http://www.gaepd.org/Documents/capps_ferry_do_monitoring.html (Accessed 7th Jan 2011)

Theriault EJ (1927) The dissolved oxygen demand of polluted waters. Public Health Bulletin No. 173, US Public Health Service, Washington, DC

Thomann RV (1963) Mathematical model for dissolved oxygen. J Sanit Eng Div Am Soc Civ Eng 89(SA5):1–30

Thomann RV, Mueller JA (1987) Principles of surface water quality modelling and control. Harper and Row, New York

Thomann RV, Muller JA (1982) Verification of water quality models. J Environ Eng 108(EE 5): 923–940

Thomas HA (1948) The pollution load capacity of streams. Water Sew Works 95(11):409

Tufford DL, McKellar HN (1999) Spatial and temporal hydrodynamic and water quality modelling analysis of a large reservoir on the South Carolina (USA) coastal plain. Ecol Model 114(2–3):137–173

Turner D, Kasper B, Heberling P, Lindberg B, Wiltsey M, Arnold G, Michie R (2006) Umpqua basin total maximum daily load (TMDL) and water quality management plan. Oregon Department of Environmental Quality, Portland, OR, http://www.deq.state.or.us/wq/tmdls/umpqua.html, Accessed on 28th may 2012

U.S. Army corps of Engineers Hydrology Engineering Center (1978) [revised on 1986] WQRRS: water quality for river-reservoir systems, user's manual

USEPA (2000a) AQUATOX for windows: a modular fate and effects model for aquatic ecosystems, vol. 1, User's Manual. EPA-823-R-00-006, Washington, DC

USEPA (2000b) AQUATOX for Windows: a modular fate and effects model for aquatic ecosystems, vol. 3, model validation reports. EPA-823-R-00-008, Washington, DC

USEPA (2000c) AQUATOX for Windows: a modular fate and effects model for aquatic ecosystems, vol. 2, Technical Documentation. EPA-823-R-00-007, Washington, DC

USEPA (2001a) AQUATOX for Windows: a modular fate and effects model for aquatic ecosystems: release 1.1, vol. 2, technical documentation (Addendum). EPA-823-R-01-007, Washington, DC

USEPA (2001b) AQUATOX for windows: a modular fate and effects model for aquatic ecosystems-release 1.1, vol. 3, model validation reports addendum: formulation, calibration, and validation of a periphyton submodel for AQUATOX release 1.1. EPA-823-R-01-008, Washington, DC

USEPA (2009) AQUATOX (RELEASE 3): modelling environmental fate and ecological effects in aquatic ecosystem. EPA-823-F-09-006

Van Genuchten MT, Alves WJ (1982) Analytical solutions of the one-dimensional convective-dispersive solute transport equation. Tech. Bull. No. 1661, U.S. Department of Agriculture, Agricultural Research Service, Washington, DC

Weiss LA, Schaffranek RW, deVries MP (1994) Flow and chloride transport in the tidal Hudson River, New York, in Hydraulic Engineering '94: Proceedings of the American Society of Civil Engineers, vol 2, pp 1300–1305

Whitehead PG (2006) Water quality. Encyclopedia of environmetrics. Copyright© 2002. Wiley & Sons, Ltd

Wiley JB (1993) Simulated flow and solute transport, and migration of a hypothetical soluble-contaminant spill for the new river in the New River Gorge National River, West Virginia U.S. Geological Survey Water-Resources Investigations report 93-4105, p 39

Wool TA, Ambrose RB, Martin JL, Comer EA (2001) Water quality analysis simulation program, WASP6. Part A: model documentation, U.S. Environmental Protection Agency, Center for exposure assessment modelling, Athens, GA

Wool TA, Davie SR, Rodriguez HN (2003) Development of three-dimensional hydrodynamic and water quality models to support total maximum daily load decision process for the Neuse River Estuary, North Carolina. J Water Resour Plan Manage 129(4):295–306

Wurbs RA (1994) Computer models for water resources planning and management, Texas A&M University, Department of Civil Engineering Environmental, Ocean and Water Resources Division College Station, Texas US Army Corps of Engineers, Institute for Water Resources, Water Resources Support Center, Alexandria, Virginia

Yu FX, Adrian DD, Singh P (1991) Modelling river quality by the superposition method. J Environ Syst 20(4):1–16

Zhulidov AV, Khlobystov VV, Robarts RD, Pavlov DF (2000) Critical analysis of water quality monitoring in the Russian Federation and former Soviet union. Can J Fish Aquat Sci 57(9):1932–1939

Zoppou C (2001) Review of urban storm water models. Environ Model Softw 16(3):195–231