

A review of development and application on River comprehensive water quality model QUAL2K

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Abstract: After more than 40 years research and development, the river comprehensive water quality model QUAL2K which is designed by the United States Environmental Protection Bureau has got lots of achievements in the field of water quality simulation. In recent years, QUAL2K model also has been widely used by more and more scholars and units in domestic. This article will introduce the development history, characteristics and application prospects of QUAL2K model so as to provide references for further promotion and application of QUAL2K in China.

1. Introduction

As the prevention and control of water pollution has been carried out in depth, the water quality model which reflects the change rule of pollutant and the relationship between water quality components in water environment, has played an increasingly important role in water environmental protection planning. Abroad, the QUAL2K model as a comprehensive water quality model has been widely used in water quality simulation^[1-3], but domestic institutions and scholars still have rarely touched on it in recent years. This paper will emphatically presents the development history of QUAL2K model, application characteristics of model software, advantages and disadvantages and future application prospects, aiming at providing reference for promoting the popularization and application of QUAL2K model in China.

2. History of the development of water quality model

Internationally, that development and research of water quality models has been divided into four stages of development since the first time Streeter-Phelps has established a water quality model in 1925^[4]. Stage one (1925-1965): scientists developed a relatively simple bilinear system model of biochemical oxygen demand and dissolved oxygen (bod-do). One-dimensional calculation method is used for river and estuary problems. Stage two (1965-1970): with the development and applications of computing technology, and the understanding of the process of biochemical oxygen consumption, in addition to continuing to study and develop the multi parameter estimation of the BOD DO model, the water quality model is developed from the bilinear model to six linear models, and the calculation method is developed from one dimension to two dimensions. Also, in addition to river and estuary problems, lake and gulf problems are being calculated. Stage three (1970-1975): a nonlinear system model is developed which is based on a nutrient nitrogen and phosphorus cyclic reaction system and phytoplankton and animal biological chain system. The system also study the relationship between



biomass growth rate and nutrient, sunlight and temperature. In terms of calculation method, since the interaction is non-linear, it can only be solved by numerical method, and in space, it can be calculated by one-dimension and two-dimensional method. Stage four (after 1975) : on the basis of continuing studies on the food chain in Phase three, a variety of interaction systems have been developed, such as those involving interactions with toxic substances. Space scales have also evolved into three dimensions. However, as the water quality model simulation targets become more diversified and simulated, and on account of water environment capacity calculation, water function division, water resource allocation and other decisions are also more dependent on the water quality model. All these laid a technical requirement for the construction of comprehensive water quality model QUAL2K^[5-6].

3. The development history of the QUAL2K model

The state variables of pollutant components in the previous models were mostly BOD and DO, but when the pollutant enters the water, it will not only cause the changes of BOD and DO in the water, but also cause other changes in water quality, such as water temperature, algae and ammonia nitrogen. Therefore, a new comprehensive water quality model is needed to describe water quality comprehensively. Commissioned by the US environmental protection agency (USEPA), American water resources engineering company collaborated with the Texas Water Development Department have successfully developed a river integrated water quality model in 1970. So the QUAL model emerges as the times require which helped the U.S. government solve the river pollution problem in Ohio. Subsequently, WRE worked with EPA and SEMCOG to develop improved versions of the model in 1972 and 1976 respectively. This version of the model can simulate 13 kinds of water quality components and give a range of values to the parameters in its partial differential equation. And the model has 23 parameters, wherein 12 of which vary with the river, and the rest does not. The parameters that do not change with the river section generally do not need to be measured, and can be evaluated according to the reference literature. But the parameters that change with the river section should be measured in the actual river section. Then Brown and Barnwell developed the one-dimensional stable model QUAL2E based on the original version in 1987. In the QUAL2E model, a one-dimensional equation of mass transport and reaction was used to simulate the interaction of various water quality components in branched river system. And the classical implicit backward difference method is used to solve the steady state and steady state problems. Finally, after decades of development and improvement, the EPA released a new version of the QUAL2K model in January 2009, the model's functionality and performance have become more mature and reliable.

4. Characteristics, mathematical models and simulation factors of QUAL2K model

Qual2K model as a comprehensive water quality model, its basic equation is one-dimensional advection-dispersion material transport and reaction equations, which is considering the responses of water quality components such as water advection dispersion, dilution and external source import or change. It has the following settings: (1) One-dimensional, the water in the channel is completely mixed vertically and horizontally. (2) The water flow of the river is stable. (3) External factors, such as heat budget, temperature, humidity, wind power and humidity, are all measured in days, and the internal meteorological equations are simulated on the daily time axis. (4) Daily input and output of point source and non-point source are all to be simulated.

And the new functions of the QUAL2K model are as follows: (1) Carbonaceous BOD speciation. Q2K uses two forms of carbonaceous BOD to represent organic carbon. These forms are a slowly oxidizing form (slow CBOD) and a rapidly oxidizing form (fast CBOD). (2) The relationship between algae, nutrients and light was corrected, and added to the simulation of new factors, like algae BOD, anti-nitrification and various pathogens. (3) pH. Both alkalinity and total inorganic carbon are simulated. The river's pH is then computed based on these two quantities. (4) Weirs and waterfalls. The hydraulics of weirs as well as the effect of weirs and waterfalls on gas transfer is explicitly included.

The reaction equation of the water quality component is as follows:

$$\frac{\partial \rho}{\partial t} + U \frac{\partial \rho}{\partial x} = E_x \frac{\partial^2 \rho}{\partial x^2} + \frac{d\rho}{dt} + \frac{S}{V} \quad (1)$$

In the formula, ρ is the mass concentration of the component, mg/L; X is the step length of the calculation unit, m; t is the time, s; U is the flow velocity, m/s; S is the mass concentration of the external input and output of the component, mg/L; V is the volume of the calculation unit, L; E_x is the longitudinal dispersion coefficient of the river, m²/s.

Because of $d\rho/dt$ is the mass concentration function of the water quality index ρ , may as well set up $d\rho/dt = k\rho$, and using the finite difference method for its numerical solution, the finite difference equation is decomposed as follows:

set $x_i = i\Delta x, t_j = j\Delta t, k_i = k\Delta t, \rho(x_i, t_j) = \rho_i^j$, $i = (0, 1, 2, \dots, n)$, n is the number of calculation units after generalization of river section, $j = (1, 2, \dots, m)$, m is the pumping time, d.

$$\text{There are} \quad \frac{\partial \rho_i}{\partial t} = \frac{\rho_i^{j+1} - \rho_i^j}{\Delta t} \quad (2)$$

$$\frac{\partial \rho_i}{\partial x} = \frac{\rho_i^j - \rho_{i-1}^j}{\Delta x} \quad (3)$$

$$\frac{\partial^2 \rho_i}{\partial x^2} = \frac{\rho_i^j - 2\rho_{i-1}^j + \rho_{i-2}^j}{\Delta x^2} \quad (4)$$

Substituting equations (2), (3) and (4) into equations (1), we can get:

$$\frac{\rho_i^{j+1} - \rho_i^j}{\Delta t} = E_{xi} \frac{\rho_i^j - 2\rho_{i-1}^j + \rho_{i-2}^j}{\Delta x^2} - U_i \frac{\rho_i^j - \rho_{i-1}^j}{\Delta x} - k_i \rho_{i-1}^j + \frac{S}{V} \quad (5)$$

$$\rho_i^{j+1} = \rho_{i-2}^j \Delta t \frac{E_x}{\Delta x^2} + \rho_{i-1}^j \left(\frac{U\Delta t}{\Delta x} - 2 \frac{E_x \Delta t}{\Delta x^2} - k\Delta t \right) + \rho_i^j \left(1 - \frac{U\Delta t}{\Delta x} + \frac{E_x \Delta t}{\Delta x^2} \right) + \Delta t \frac{S}{V} \quad (6)$$

When $i = 1$, set $\rho_{-1}^j = \rho_0^j, \rho_0^0 = 0, \rho_0^j$ is the initial boundary condition, At this point, E_x, U, k, S, A and V in equation (6) are all known initial conditions and boundary conditions.

Analogue factor aspect, QUAL2K has expanded the calculation function, and users can simulate 15 kinds of water quality components according to the desired combination, including :BOD, DO, temperature, alga -- chlorophyll a, organic nitrogen, ammonia nitrogen, nitrite nitrogen, nitrite nitrogen, organic phosphorus, dissolved phosphorus, Escherichia coli, an optional attenuated radioactive component and three refractory inert components. Figure 1 shows Model kinetics and mass transfer processes.

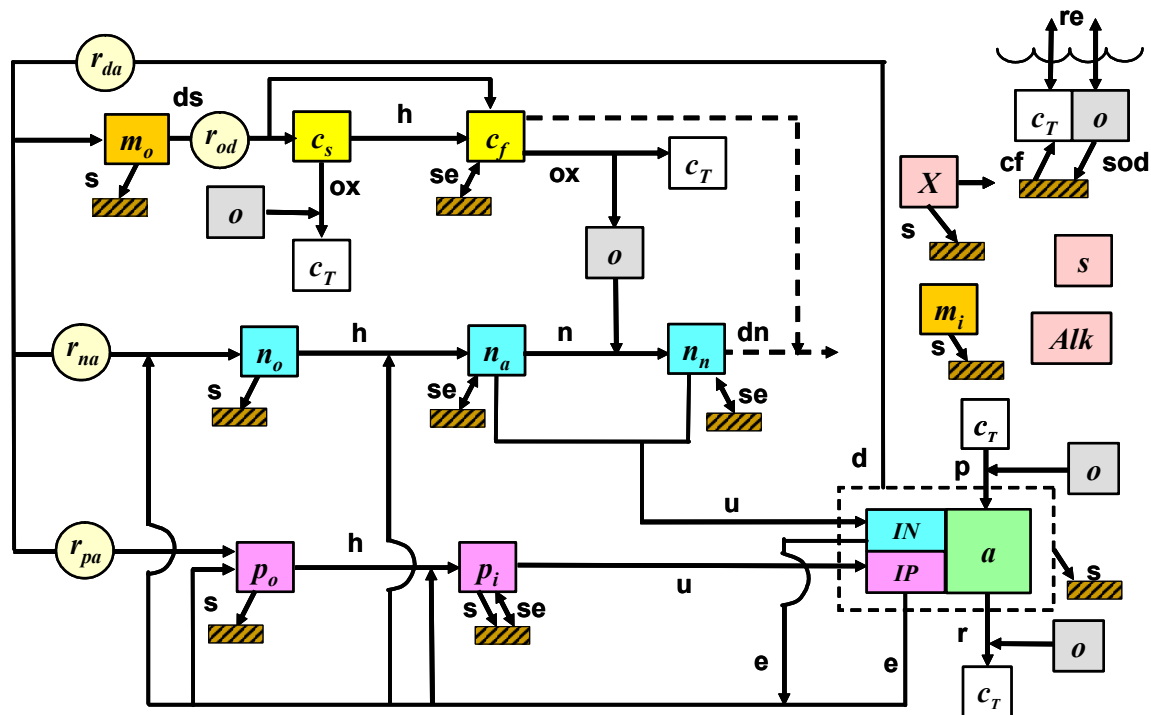


Figure 1. Model kinetics and mass transfer processes

5. QUAL2K model application guide

QUAL2K first divides the simulated channel into a series of constant non-uniform flow segments, and then divides each segment into several equal length calculation units. The unit is the smallest unit of calculation in QUAL2K, and each unit is an ideal hybrid reactor. To describe the spatial distribution characteristics of rivers, QUAL2K defines the unit as the following eight types. The model unit classification is shown in the following table.

Table 1. Model unit classification

| No. | Unit type | definition | Maximum allowable amount |
|-----|-------------------------------|--|---|
| 1 | Source unit (H) | The source of the main stream and its tributaries | 10 |
| 2 | Junction unit (J) | A tributary import unit | 9 |
| 3 | Upstream unit of junction (U) | The last unit of a junction unit in the mainstream | 20 |
| 4 | System final unit (L) | The last cell in the simulation system | 1 |
| 5 | Intake unit (P) | A unit containing water intake | 50 |
| 6 | Discharge outlet unit (W) | The units containing the emissions | 50 |
| 7 | Hydraulic building unit (D) | A unit containing a hydraulic structure | 50 |
| 8 | Standard unit (S) | All units except the above 7 are defined as standard units | Each river should not exceed 20, and the whole process should not exceed 500. |

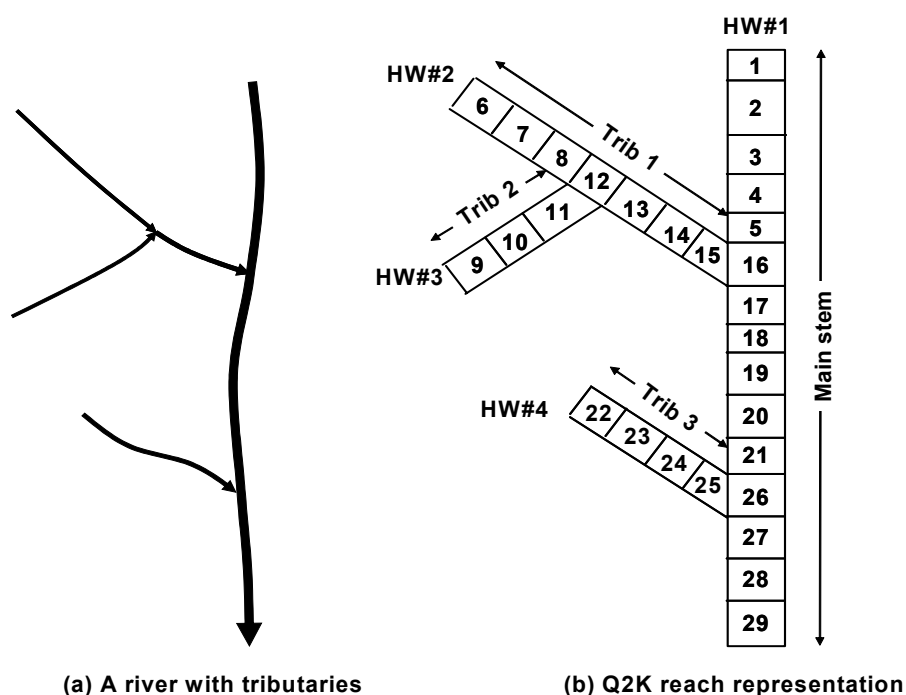


Figure 2. QUAL2K segmentation scheme for (a) a river with tributaries

The model requires the following several aspects of the data. The first is the hydrological data and spatial information of the basin such as the data of river basin hydrology and drainage system, the trend of river basin and the flow of tributaries, flow velocity, flow rate, velocity of flow, section shape of river channel, siltation and so on. The second is the boundary condition and the point source data, for example: Boundary conditions are the boundary of the administrative region, the tributaries are remittance, etc. Point source statistics need to investigate industrial pollution sources (factory outlets), large-scale urban life sources (rain and sewage pumping stations, sewage treatment plants). And the non-point source statistics include agricultural non-point source, poultry, livestock farms, rural living sources, etc. It is also necessary to collect the monitoring data for calibration and validation the parameters in model.

6. Successful application of the QUAL2K models in China

In references [7], Zhejiang University has used QUAL2K model and one-dimensional water quality model to simulate the water quality of Qian Tang River Basin in 2009. The paper estimates the capacity of COD, ammonia nitrogen and BOD in the water body of the whole river basin, and uses the TMDL management model to carry out the research on the reduction and distribution of COD, ammonia nitrogen and BOD load in the typical river sections, providing a theoretical basis for the total amount control of the river basin.

In references [8], Nanchang University has applied the QUAL2K model and the one-dimensional heavy metal migration and transformation water quality model to carry out the comprehensive improvement of lean river environment in Jiangxi province in 2013. The model simulates the COD_{cr} , $\text{NH}_3\text{-H}$, C_u , P_b and other elements of the river in the river. And the quantitative calculation is carried out by using analytical method and functional area first control method, which provides a technical basis for local government to carry out water pollution prevention and control.

In references [9], according to the characteristics of water quality in the Qinhuai River, Hohai University selects DO, $\text{NH}_3\text{-N}$ and COD as the simulation factors and uses QUAL2K model to construct the optimal management model of water quality in the Qinhuai River in 2013.

7. The prospect of QUAL2K model

QUAL- II series model has been used in many practical applications of water quality simulation in a number of rivers and rivers abroad since 1970. In addition to some river sections, the error is generally within 20%. The simulation results match the actual monitoring values relatively well. Although the QUAL- II series model has broad application prospects, according to the actual situation in China, the application and improvement of the model should focus on the following three aspects:

(1) The model application and reasonable model evaluation index system need to be further deepened. Based on the simulation of water quality by the QUAL2K model, the optimization of water environment should first combine with the development of economy and society, select evaluation indicators from social economy, resource environment, technology management and other fields, and build an indicator structure with a clear hierarchical system. Then it is necessary to determine the weight of each index and establish a comprehensive evaluation model of water environmental capacity of the river basin. Then the weight of each index is determined and a comprehensive evaluation model of water environment carrying capacity is set up to provide ideas for the reduction and distribution of pollution load, the implementation of the optimal reduction measures and the optimization of the discharge outlet for the next stage.

(2) The selection and determination of water quality and hydraulics parameters need further study. The water quality and hydraulics parameters of different water bodies in China are different. As for some empirical parameters, if the model is used to provide value, it may be quite different from the actual situation of China's specific rivers, resulting in low accuracy of simulation. In view of the excessive demand of the model for data volume, the influence coefficient method and genetic algorithm (POMIG) adopted by QUAL2Kw in reference^[10] are also a new improvement method.

(3) Coupling with other water quality models and software needs further development. Reference^[11] takes the Dunda basin and west lake basin in Oklahoma as examples. The QUAL2E model is integrated into the SWAT model to modify the hourly time step dynamic framework of the model, then the SCE algorithm is adopted to the water quality target goal alignment and integration. Finally, statistical methods were used to make the aggregation target function as individual variables to avoid the weight problem, thus enhancing the water quality simulation function of SWAT model. This kind of related research has just begun in China, and will be one of the trends in the future.

Acknowledgments

This research was supported in part by the National Nature Science Foundation of China (51709237), The Science and Technology Plan Project of Department of Water Resources of Zhejiang Province (RA1603), Projects Supported by Zhejiang Provincial Scientific Research Institutes (2017F30009) and National Key R&D Program of China (2016YFC0401603).

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