

Parameters sensitivity analysis of DO in water quality model of QUAL2K

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Abstract. QUAL2K is a comprehensive longitudinal one-dimension steady-state water quality model, which considers the effect on dissolved oxygen (DO) through nitrogen circulation, algae growth and sediment oxidation process. And this model integrated hydrological model and temperature model, so it is widely adopted in the overseas. Because of its complexity and multiple parameters, the application of this model is restricted in China. Parameters optimization is inevitable in the usage of the water quality model. The modified Morris screening method is used and DO is selected as study index to proceed sensitivity analysis and further optimize related parameters. The high sensitive parameters, sensitive parameters and low sensitive parameters are determined.

1. Introduction

QUAL2K model is a comprehensive and diversified water quality one-dimensional model developed by the US Environmental Protection Agency. It is widely used not only for complex dendritic river systems, but also for multiple intakes, outlets, and inflows Applied to the total amount of pollutants in the basin control and water quality management .The basic equation of QUAL2K water quality model is one-dimensional advection-dispersion material delivery and reaction equation that considers advection-dispersion, dilution, self-reactions within water quality components and interactions between them ,as well as the impact of external source and sink on the concentration of components, therefore, it is widely adopted in the overseas [1-5]. QUAL2K model contains numerous parameters simultaneously. The determination of these parameters will have a directly impact on applicability of model, which is used to simulate the evolution of characteristics of water quality variables in water [6]. DO is a significant indicator reflecting biological growth status and water pollution level [7], what's more, it's a necessary condition in water. So the analysis on related parameters of DO in QUAL2K model has a great importance. In this paper, the Morris screening method and the Modified Morris screening method are used and DO is selected as study index to proceed sensitivity analysis to simplify the parameter determination.

2. Methods

2.1. DO parameter analysis

DO concentration increases with the photosynthesis of bottom algae and phytoplankton, which are



restrictively affected in combined temperature, nutrients and light. It is necessary to consider the nitrogen (N), phosphorus quota, light constant of bottom algae and phytoplankton, salt concentration and the effect of chlorophyll extinction coefficient on phytoplankton etc. [8]. At the same time, the effects of carbonized biochemical oxygen demand (CBOD) oxidation, ammonia nitrogen nitrification, microorganism and plant respiration on the decrease of DO concentration should be premeditated [9]. As well as river concrete conditions such as hydraulic works, river depth, velocity, other related parameters, point source pollution load and river water temperature influences DO concentration. There are hydraulic, hydrological, and water quality parameters relating to DO in table 1.

Table 1. Hydraulic hydrological and water quality parameters of DO and the value.

Category	NO.	Parameter	Unit	Parameter Description	Value ^a
Hydraulic parameters	1	n	—	Manning roughness	0.0700
	2	Q ₀	m ³ /s	River source discharge	0.713
	3	T _B	°C	B point source of the average water temperature	15.00
	4	Q _B	m ³ /s	B point source flow	0.5900
	5	adam	—	Water quality correction factor	1.2500
	6	bdam	—	Dam type correction factor	0.9000
Hydrological parameters	7	C _{B(DO)}	(mgO ₂ /L)	B point source emissions DO average concentration	4.00
	8	CV	%	Algae coverage at the bottom of the river	70
	9	a	—	River flow velocity section coefficient	0.2457
	10	b	—	River flow velocity section coefficient	0.451
	11	α	—	River water depth section coefficient	0.6271
	12	β	—	River water depth section coefficient	0.435
Water quality parameters	13	r _{oc}	(gO ₂ /gC)	Organic carbon oxidation coefficient	2.69
	14	r _{on}	(gO ₂ /gN)	Ammonia nitrification oxygen consumption coefficient	4.57
	15	k _{na}	(d ⁻¹)	Ammonia nitrification rate coefficient	1.649
	16	k _{gp}	(d ⁻¹)	Phytoplankton growth rate	2.50
	17	k _{rp}	(d ⁻¹)	Phytoplankton respiration rate	0.10
	18	k _{socf}	L/mgO ₂	CBOD Oxygen inhibition parameters	0.60
	19	k _{sona}	L/mgO ₂	Nitric oxide inhibition parameters	0.60
	20	k _{sodn}	L/mgO ₂	Denitrifying oxygen increases the parameters	0.60
	21	k _{sop}	L/mgO ₂	Plant respiratory oxygen inhibition parameters	0.60
	22	k _{sob}	L/mgO ₂	Algae respiratory oxygen increase parameters	0.60
	23	γ	(d ⁻¹)	River reoxygenation coefficient	0
	24	θ _{dcs}	—	CBOD _s oxidation temperature correction factor	1.047
	25	θ _{hc}	—	CBOD _s Hydrolysis temperature correction factor	1.047
	26	θ _{dc}	—	CBOD _f oxidation temperature correction number	1.047
	27	θ _{na}	—	Ammonia nitrogen nitration temperature correction factor	1.07
	28	θ _a	—	Reaeration temperature correction factor	1.024
		k _{db}	(d ⁻¹)	Bottom algae death rate	0.09

30	k_{dc}	(d ⁻¹)	CBOD _f oxidation rate	5.0
31	k_{dcs}	(d ⁻¹)	CBOD _s oxidation rate	5.0
32	k_{Lb}	langley/d	Bottom algae light constants	76.319
33	k_{eb}	(d ⁻¹)	Bottom algae excretion rate	0.5
34	k_{Lp}	langley/d	Phytoplankton light constant	57.6
35	k_{rb}	(d ⁻¹)	Bottom algae respiration rate	1
36	k_{dt}	(d ⁻¹)	Debris dissolution rate	7.179
37	k_{ep}	(d ⁻¹)	Phytoplankton excretion rate	0.5
38	k_{dp}	(d ⁻¹)	Phytoplankton death rate	0.09
39	C_{gb}	mgA/m ² /d	Bottom algae maximum growth rate	999.991
40	q_{ON}	mgN/mgA	Bottom algae nitrogen quota	5.024
41	q_{op}	mgP/mgA	Bottom algae phosphorus quota	0.002
42	k_{eb}	/m	Background extinction coefficient	0.2
43	α_p	1/m-(ugA/L)	Linear chlorophyll extinction coefficient	0.0088
44	α_{pn}	1/m-(ugA/L) ^{2/3}	Nonlinear chlorophyll extinction coefficient	0.054
45	α_s	1/m-(mgD/L)	ISS extinction coefficient	0.052
46	α_o	1/m-(mgD/L)	Particle organic matter extinction coefficient	0.174
47	u_w	m/s	Wind speed u_w (water surface 7m)	2.00
48	v_a	m/d	Phytoplankton sedimentation rate	0.15

^a water quality model of QUAL2K recommended value

2.2. Parameter sensitivity analysis method

Sensitivity analysis of model parameters includes local and global sensitivity analysis [10]. In this paper, local sensitivity analysis use the Modified Morse classification screening to test the influence of single parameters [11], the other use the Morse classification screening to test the overall effect of multiple parameters on the model results [12].

2.2.1. Modified Morse classification screening method. The modified Morse classification screening method use independent variables to fixe step-changes. The parameter sensitivity index takes the average of the Morse coefficients calculated over multiple disturbances.

$$S = \sum_{i=0}^{n-1} \frac{(Y_{i+1} - Y_i)/Y_0}{(P_{i+1} - P_i)/100} / (n-1) \quad (1)$$

In the above formula: S is Morse coefficient; Y_0 is the initial calculation result after the parameters determined; Y_i and Y_{i+1} respectively is model output value of the i and i+1 times operation; P_i , P_{i+1} respectively is the percent change of the i and i + 1 times model parameter relative to the initial value; n is the number of model runs.

2.2.2. Morse classification screening method. Morse classification screening method selects one of the variables, which named x_i in the model, and fixes the rest parameters. The value of x_i is changed randomly within the threshold range of the variable and the value of the objective function $y(x) = y(x_1, x_2, x_3, \dots, x_n)$ is obtained by running the model. The influence value e_i is used to judge the influence of the parameter variation on the output value.

$$e_i = (y - y_0) / \Delta i \quad (2)$$

In the above formula: e_i is Morse coefficient; y_0 and y respectively is model output value before and after the change of parameters; Δi is the variation range of the parameter i .

By calculating the influence of water quality concentration under a certain parameter rate of change and comparing its sensitivity. According to the sensitivity degree, this paper identifies the local sensitivity analysis hierarchy [11] as shown in table 2.

Table 2. Delineation of the sensitivity.

Sensitivity level	Sensitivity range	Sensitivity
I	$0 \leq s_i < 0.05$	Insensitive
II	$0.05 \leq s_i < 0.2$	Weak sensitive
III	$0.2 \leq s_i < 1$	Sensitive
IV	$ s_i > 1$	Highly sensitive

2.3. River overview

Research chooses Boulder Creek River, abbreviated BC River, which the average width is 12.50 m, total length is 13.53 km and the flow is 0.713 m³/s. The study divided the river into five sections and 25 units according to the sources and hydraulic characteristics, as shown in tables 3, 4, and 5 and the entire river can be summarized as shown in figure 1.

Table 3. Delineation of Boulder Creek river reach and computational element.

Serial number	The upper reaches of the river	The lower reaches of the river	Length of the river	Computational element
1	0.00	0.65	0.65	2
2	0.65	4.32	3.67	7
3	4.32	5.71	1.39	2
4	5.71	8.18	2.47	4
5	8.18	13.53	5.35	10

Table 4. Point source distribution.

Project	Name	A	B	C
Position (km)		0.12	4.46	7.12
Nitrate (μgN/L)		2337.04	1000.00	0.00
Organic phosphorus (μgP/L)		647.96	1000.00	0.00
Inorganic phosphorus (μgP/L)		3932.78	1000.00	0.00
Alkalinity (mgCaCO ₃ /L)		125.74	120.00	0.00
pH		6.84	7.00	0.00
Flow (m ³ /s)		1.0000	0.5900	1.9000
Average water temperature (°C)		20.06	15.00	0.00
DO (mg/L)		3.57	4.00	0.00
CBOD _s (mg/L)		0.00	2.00	0.00
CBOD _F (mg/L)		26.70	0.00	0.00
Organic nitrogen (μgN/L)		1044.81	1000.00	0.0000
Ammonia nitrogen (μgN/L)		1121.11	1000.00	0.00

Table 5. Non-point source distribution.

Name	Top (km)	Lower end (km)	Flow (m ³ /s)	Average water temperature (°C)	Conductivity (umhos)	Nitrate (μgN/L)	Alkalinity (mgCaCO ₃ /L)	pH
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D	0.06	6.79	0.2574	16.00	600.00	4000.00	150.00	6.50
E	6.79	13.53	0.2426	16.00	600.00	4000.00	150.00	6.50

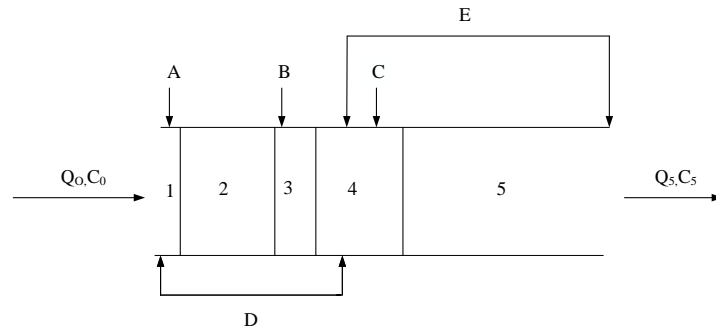


Figure 1. Delineation of the river.

A and B are point sources; C is farmland water intake; D and E are surface source of pollution; 1, 2, 3, 4, 5 are serial number of river reach; Q_0 is source of BC river flow, C_0 is the source of the BC river of DO concentration, Q_5 is the end of BC river flow, C_5 is the end of the BC river of DO concentration.

3. DO parameter sensitivity analysis

3.1. Local sensitivity analysis

Table 6. Result of local sensitivity analysis.

NO.	Parameter name	Sensitivity	NO.	Parameter name	Sensitivity
1	n	0.3429	25	θ_{hc}	0.0000
2	Q_0	0.1952	26	θ_{dc}	0.5190
3	T_B	0.1905	27	θ_{na}	0.6381
4	QB	0.1810	28	θ_a	-2.5143
5	adam	0.0000	29	k_{db}	0.0224
6	bdam	0.0000	30	k_{db}	-0.2429
7	$C_{B(DO)}$	0.1143	31	k_{dcs}	-0.0238
8	CV	0.1562	32	k_{Lb}	0.0689
9	a	-0.2021	33	k_{eb}	0.0412
10	b	0.0701	34	k_{Lp}	0.0000
11	α	0.2310	35	k_{rb}	-0.0834
12	β	0.0866	36	k_{dt}	-0.0524
13	r_{OC}	-0.5667	37	k_{ep}	0.0000
14	r_{on}	-0.2571	38	k_{dp}	0.0000
15	K_{na}	-0.2667	39	C_{gb}	0.1359
16	k_{gp}	0.0000	40	q_{ON}	0.0846
17	k_{rp}	0.0000	41	q_{OP}	0.0000
18	K_{socf}	-0.0557	42	k_{eb}	0.0000
19	K_{sona}	-0.0557	43	α_p	0.0000
20	k_{sodn}	0.0000	44	α_{pn}	0.0000
21	k_{sop}	0.0000	45	α_s	0.0000
22	k_{sob}	0.0000	46	α_o	0.0000
23	γ	0.8810	47	u_w	0.0000

24 CBOD_s 0.0286 48 v_a 0.0000

Compare the sensitivity of each parameter through studying the effect of concentration changes on DO from the value of parameters diversification in table 1. The modified Morse classification screening method was used to analyze the local sensitivity of all the parameters in table 1, where disturbing every parameter value with fixed step of 5%, respectively, the value was from -20% to 20%, DO output results shown in table 6:

Through the analysis of the local sensitivity of the parameters, it can be concluded that the θ_a is the only highly sensitive parameter of DO. The sensitive parameters include the γ , θ_{na} , r_{oc} , CBOD_f, θ_{dc} , n , K_{na} , r_{on} , k_{dc} , α and a ; The weak sensitive parameters include the Q_0 , T_B , Q_B , CV , C_B (DO), q_{0N} , k_{rb} , K_{Lb} , β , b , K_{socf} , K_{sona} and k_{dt} ; The others are insensitive parameters.

We can draw eight bottom algal parameters from table 6, which have less effect on DO, involving q_{0N} , K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db} and k_{dt} . During local sensitivity analysis processing, the mutual interaction of parameters was neglected, therefore, next, it researches the further global sensitivity analysis for these eight parameters.

3.2. Global sensitivity analysis

This analysis selects above eight parameters to get $X = [q_{0N}, K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt}]$, in order to get credible analysis results and simplify calculations, using the Morse method to assume the parameters increasing or decreasing by 10%. According to the principle of global sensitivity analysis and the method of Section 2.2, the matrix B of 9×8 dimensions is obtained. Then the parameters of each row of the matrix B are respectively brought into the QUAL2K model. Finally calculate the difference between outputs of the model. In line with the principle of sensitivity analysis, different combinations of parameters can be received. Through the data processing, the sensitivity of the interaction among parameters can be got too. The details are shown in table 7.

Table 7. Result of parameters global sensitivity analysis (a).

Parameter group	Parameter combination	Sensitivity	Parameter group	Parameter combination	Sensitivity
1	q_{0N}	0.0857	19	$K_{socf}, K_{sona}, k_{eb}$	-0.0821
2	K_{Lb}	0.0616	20	K_{sona}, k_{eb}, k_{db}	0.0043
3	k_{rb}	-0.0845	21	k_{eb}, k_{db}, k_{dt}	0.0041
4	K_{socf}	-0.0568	22	$q_{0N}, K_{Lb}, k_{rb}, K_{socf}$	0.0063
5	K_{sona}	-0.0565	23	$K_{Lb}, k_{rb}, K_{socf}, K_{sona}$	-0.1359
6	k_{eb}	0.0323	24	$k_{rb}, K_{socf}, K_{sona}, k_{eb}$	-0.1658
7	k_{db}	0.0284	25	$K_{socf}, K_{sona}, k_{eb}, k_{db}$	-0.0524
8	k_{dt}	-0.0567	26	$K_{sona}, k_{eb}, k_{db}, k_{dt}$	-0.0525
9	q_{0N}, K_{Lb}	0.1475	27	$q_{0N}, K_{Lb}, k_{rb}, K_{socf}, K_{sona}$	-0.0510
10	K_{Lb}, k_{rb}	-0.0231	28	$K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}$	-0.1041
11	k_{rb}, K_{socf}	-0.1420	29	$k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}$	-0.1375
12	K_{socf}, K_{sona}	-0.1130	30	$K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt}$	-0.1095
13	K_{sona}, k_{eb}	-0.0242	31	$q_{0N}, K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}$	-0.0180
14	k_{eb}, k_{db}	0.0610	32	$K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}$	-0.0760
15	k_{db}, k_{dt}	-0.0281	33	$k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt}$	-0.1934
16	q_{0N}, K_{Lb}, k_{rb}	0.0630	34	$q_{0N}, K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}$	0.0112
17	K_{Lb}, k_{rb}, K_{socf}	-0.0795	35	$K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt}$	-0.1330
18	$k_{rb}, K_{socf}, K_{sona}$	-0.1979	36	$q_{0N}, K_{Lb}, k_{rb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt}$	-0.0471

Table 7 shows the average value about sensitivity of the combination of parameters when all parameters increase or reduce 10% simultaneously. Through the sensitivity analysis of individual parameters in local and global sensitivity analysis, it can be seen that q_{0N} , K_{Lb} , k_{eb} , and k_{db} are positively correlated with DO and k_{rb} , K_{socf} , K_{sona} , k_{dt} are negatively correlated with DO. In order to more accurately reflect the sensitivity of the parameter combinations, parameters such as q_{0N} , K_{Lb} , k_{eb} and k_{db} positively correlated with DO were increased by 10%, and the parameters K_{socf} , K_{sona} , k_{rb} and k_{dt} negatively correlated with DO were decreased by 10%. The results of maximum sensitivity of parameters combination are shown in table 8.

Table 8. Result of different combination-patterns of parameters global sensitivity analysis (b).

Parameter group	Parameter combination	Sensitivity	Parameter group	Parameter combination	Sensitivity
1	q_{0N}	0.0857	19	K_{socf} , K_{sona} , k_{eb}	0.1397
2	K_{Lb}	0.0567	20	K_{sona} , k_{eb} , k_{db}	0.1111
3	k_{rb}	-0.0845	21	k_{eb} , k_{db} , k_{dt}	0.1105
4	K_{socf}	-0.0559	22	q_{0N} , K_{Lb} , k_{rb} , K_{socf}	0.2857
5	K_{sona}	-0.0556	23	K_{Lb} , k_{rb} , K_{socf} , K_{sona}	0.255
6	k_{eb}	0.0276	24	k_{rb} , K_{socf} , K_{sona} , k_{eb}	0.2254
7	k_{db}	0.0275	25	K_{socf} , K_{sona} , k_{eb} , k_{db}	0.1676
8	k_{dt}	-0.0549	26	K_{sona} , k_{eb} , k_{db} , k_{dt}	0.1667
9	q_{0N} , K_{Lb}	0.1428	27	q_{0N} , K_{Lb} , k_{rb} , K_{socf} , K_{sona}	0.3429
10	K_{Lb} , k_{rb}	0.1416	28	K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb}	0.2833
11	k_{rb} , K_{socf}	0.1408	29	k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db}	0.2535
12	K_{socf} , K_{sona}	0.1117	30	K_{socf} , K_{sona} , k_{eb} , k_{db} , k_{dt}	0.2235
13	K_{sona} , k_{eb}	0.0833	31	q_{0N} , K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb}	0.3714
14	k_{eb} , k_{db}	0.0552	32	K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db}	0.3116
15	k_{db} , k_{dt}	0.0826	33	k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db} , k_{dt}	0.3099
16	q_{0N} , K_{Lb} , k_{rb}	0.2286	34	q_{0N} , K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db}	0.4000
17	K_{Lb} , k_{rb} , K_{socf}	0.1983	35	K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db} , k_{dt}	0.3683
18	k_{rb} , K_{socf} , K_{sona}	0.1972	36	q_{0N} , K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db} , k_{dt}	0.4571

The sensitivity of the combination of weak sensitive parameters is higher than a single parameter in table 8, indicating that the collective effect of multiple parameters will have a greater impact on the concentration of DO. For example, the sensitivities of q_{0N} and K_{Lb} are 0.0857 and 0.0567, respectively, but the sensitivity of their combination is 0.1428. The sensitivity of the combination parameters obtained by the Morse classification screening method is not a simple numerical addition of a single parameter. The sensitivity of the eight parameter combinations reaches 0.4571, indicating that the QUAL2K model needs to consider the values of the eight weak sensitive parameters when simulating DO, which can not be neglected in the model definition and calibration. Thus, the method of determining DO related parameters in the QUAL2K water quality model was confirmed as shown in table 9.

Table 9. Recommended methods for choosing parameters.

Category	Name
Field measured or laboratory determination	θ_a , γ , θ_{na} , r_{oc} , θ_{dc} , n , K_{na} , r_{on} , k_{dc} , α , a , q_{0N} , K_{Lb} , k_{rb} , K_{socf} , K_{sona} , k_{eb} , k_{db} , k_{dt}
Adopt QUAL2K water quality model recommended value	Q_0 , T_B , Q_B , C_V , $C_{B(DO)}$, β , b , $adam$, $bdan$, k_{gp} , k_{rp} , k_{sodn} , k_{sop} , k_{sob} , $CBOD_S$, k_{dcs} , k_{Lp} , k_{dp} , q_{op} , k_{eb} , α_p , α_n , α_s , α_o , u_w , V_a , θ_{hc} , k_{ep} , C_{gb}

4. Conclusions

Through the local and global sensitivity analysis of DO-related parameters, it can be seen that the most important process affecting DO in the QUAL2K water quality model is the river reoxygenation, CBOD oxidation, ammonia nitrogen nitrification and oxygenation. Algae of bottom photosynthesis also have a certain impact on DO and algae respiration on the impact of DO is relatively small. On this basis, the method of determining the different parameters is confirmed.

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