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 |
|-------------------|-----|-----------|---------|----------------------------------------------------|-------|
| **Hydraulic**     | 1   | n         |         | Manning roughness                                  | 0.0700 |
|                   | 2   | Q₀        | m³/s    | River source discharge                             | 0.713 |
|                   | 3   | T₈        | °C      | B point source of the average water temperature    | 15.00 |
|                   | 4   | Q₈        | m³/s    | B point source flow                                | 0.5900|
|                   | 5   | adam      |         | Water quality correction factor                    | 1.2500|
|                   | 6   | bdam      |         | Dam type correction factor                         | 0.9000|
| **Hydrological**  | 7   | C₋₈(DO)   | mgO₂/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** | 13  | rₒc       | (gO₂/gC)| Organic carbon oxidation coefficient              | 2.69  |
|                   | 14  | rₒn       | (gO₂/gN)| Ammonia nitrification oxygen consumption coefficient | 4.57 |
|                   | 15  | kₐₐ       | (d⁻¹)   | Ammonia nitrification rate coefficient            | 1.649 |
|                   | 16  | kₚₕ       | (d⁻¹)   | Phytoplankton growth rate                         | 2.50  |
|                   | 17  | kₚₜ       | (d⁻¹)   | Phytoplankton respiration rate                    | 0.10  |
|                   | 18  | kₒₑₒᶠ     | L/mgO₂  | CBOD Oxygen inhibition parameters                 | 0.60  |
|                   | 19  | kₒₒₒₐₜ₃  | L/mgO₂  | Nitric oxide inhibition parameters                | 0.60  |
|                   | 20  | kₒₒₒₜ₃   | L/mgO₂  | Denitrifying oxygen increases the parameters      | 0.60  |
|                   | 21  | kₒₚᵦₕ₃   | L/mgO₂  | Plant respiratory oxygen inhibition parameters    | 0.60  |
|                   | 22  | kₒₒₑₒₜ₃  | L/mgO₂  | Algae respiratory oxygen increase parameters      | 0.60  |
|                   | 23  | γ         | (d⁻¹)   | River reoxygenation coefficient                   | 0     |
|                   | 24  | θₒₒ₋₃   |         | CBOD₃ oxidation temperature correction factor     | 1.047 |
|                   | 25  | θₒₜ₃     |         | CBOD₅ Hydrolysis temperature correction factor     | 1.047 |
|                   | 26  | θₒₜ₄     |         | CBOD₇ oxidation temperature correction number     | 1.047 |
|                   | 27  | θₒₜ₅     |         | Ammonia nitrogen nitration temperature correction factor | 1.07 |
|                   | 28  | θₒₜ₆     |         | Reaeration temperature correction factor          | 1.024 |
|                   |     | kₒₒ₃     | (d⁻¹)   | Bottom algae death rate                           | 0.09  |
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.

$$S = \frac{1}{n-1} \sum_{i=0}^{n-1} \left( \frac{Y_{i+1} - Y_i}{P_{i+1} - P_i} \right) / 100 \left( n - 1 \right)$$  \hspace{1cm} (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 \( y(x) = y(x_1, x_2, x_3, \cdots, x_n) \) 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.

$$e_i = \left( y - y_0 \right) / \Delta i$$  \hspace{1cm} (2)

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a water quality model of QUAL2K recommended value
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; $\Delta i$ 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 m$^3$/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 (℃) | | 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 Flow Average water Conductivity Nitrate Alkalinity pH |
|------|---------|-------------|--------------|--------------|--------------|---------------|
|      | (km)    | Lower (km)  | (m$^3$/s)  | temperature (℃) | (umhos) | (µgN/L) (mgCaCO$_3$/L) |
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 |
|-----|----------------|-------------|
| 1   | n              | 0.3429      |
| 2   | $Q_0$          | 0.1952      |
| 3   | $T_B$          | 0.1905      |
| 4   | $QB$           | 0.1810      |
| 5   | adam           | 0.0000      |
| 6   | bdam           | 0.0000      |
| 7   | $C_{B(DO)}$    | 0.1143      |
| 8   | CV             | 0.1562      |
| 9   | a              | -0.2021     |
| 10  | b              | 0.0701      |
| 11  | $\alpha$       | 0.2310      |
| 12  | $\beta$        | 0.0866      |
| 13  | $r_{OC}$       | -0.5667     |
| 14  | $r_{on}$       | -0.2571     |
| 15  | $K_{na}$       | -0.2667     |
| 16  | $k_{DP}$       | 0.0000      |
| 17  | $k_{Pp}$       | 0.0000      |
| 18  | $K_{socf}$     | -0.0557     |
| 19  | $K_{sona}$     | -0.0557     |
| 20  | $k_{soda}$     | 0.0000      |
| 21  | $k_{sodp}$     | 0.0000      |
| 22  | $k_{sodp}$     | 0.0000      |
| 23  | $\gamma$       | 0.8810      |
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 $\theta_6$ is the only highly sensitive parameter of DO. The sensitive parameters include the $\gamma$, $\theta_{5a}$, $\theta_{5c}$, $\text{CBOD}_5$, $\theta_{d}$, $n$, $K_{mn}$, $r_{on}$, $k_{dc}$, $\alpha$ and $a$; The weak sensitive parameters include the $Q_{0b}$, $T_{b}$, $Q_{a}$, $CV$, $C_B$ (DO), $q_{0a}$, $k_{eb}$, $K_{Lb}$, $\beta$, $b$, $K_{socf}$, $K_{sona}$ and $K_{db}$; The others are insensitive parameters.

We can draw eight bottom algal parameters from Table 6, which have less effect on DO, involving $q_{0a}$, $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$, $K_{db}$ 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 $X = [q_{0a}, K_{Lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb}, K_{db}, k_{dt}]$, 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 $9 \times 8$ dimensions is obtained. Then the parameters of each row of the matrix B are respectively brought into the QUAL2 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               | $q_{0a}$              | 0.0857      | 19              | $K_{socf}$, $K_{sona}$, $k_{eb}$ | -0.0821     |
| 2               | $K_{Lb}$              | 0.0616      | 20              | $K_{socf}$, $K_{sona}$, $k_{db}$ | 0.0043      |
| 3               | $k_{eb}$              | -0.0845     | 21              | $k_{eb}$, $k_{db}$, $k_{dt}$ | 0.0041      |
| 4               | $K_{socf}$            | -0.0568     | 22              | $q_{0a}$, $K_{Lb}$, $k_{eb}$, $K_{socf}$ | 0.0063      |
| 5               | $K_{sona}$            | -0.0565     | 23              | $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$ | -0.1359     |
| 6               | $k_{eb}$              | 0.0323      | 24              | $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$ | -0.1658     |
| 7               | $k_{db}$              | 0.0284      | 25              | $K_{socf}$, $K_{sona}$, $k_{eb}$, $k_{db}$ | -0.0524     |
| 8               | $k_{dt}$              | -0.0567     | 26              | $K_{sona}$, $K_{sona}$, $k_{db}$, $k_{dt}$ | -0.0525     |
| 9               | $q_{0a}$, $K_{Lb}$    | 0.1475      | 27              | $q_{0a}$, $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$ | -0.0510     |
| 10              | $K_{Lb}$, $k_{eb}$    | -0.0231     | 28              | $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$ | -0.1041     |
| 11              | $k_{eb}$, $K_{socf}$  | -0.1420     | 29              | $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{db}$ | -0.1375     |
| 12              | $K_{socf}$, $K_{sona}$| -0.1130     | 30              | $K_{socf}$, $K_{sona}$, $k_{eb}$, $k_{dt}$ | -0.1095     |
| 13              | $K_{sona}$, $k_{eb}$  | -0.0242     | 31              | $q_{0a}$, $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$ | -0.0180     |
| 14              | $k_{eb}$, $k_{db}$    | 0.0610      | 32              | $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{db}$ | -0.0760     |
| 15              | $k_{db}$, $k_{dt}$    | -0.0281     | 33              | $k_{db}$, $K_{socf}$, $K_{sona}$, $k_{db}$, $k_{dt}$ | -0.1934     |
| 16              | $q_{0a}$, $K_{Lb}$, $k_{eb}$ | 0.0630 | 34              | $q_{0a}$, $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$ | 0.0112 |
| 17              | $K_{Lb}$, $k_{eb}$, $K_{socf}$ | -0.0795 | 35              | $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$, $k_{dt}$ | -0.1330 |
| 18              | $k_{eb}$, $K_{socf}$, $K_{sona}$ | -0.1979 | 36              | $q_{0a}$, $K_{Lb}$, $k_{eb}$, $K_{socf}$, $K_{sona}$, $k_{eb}$, $k_{dt}$ | -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 \( q_0 \), \( K_{lb} \), \( k_{eb} \), and \( k_{db} \) are positively correlated with DO and \( k_{eb}, K_{socf}, K_{sona}, k_{dt} \) are negatively correlated with DO. In order to more accurately reflect the sensitivity of the parameter combinations, parameters such as \( q_0 \), \( K_{lb} \), \( k_{eb} \) and \( k_{db} \) positively correlated with DO were increased by 10%, and the parameters \( K_{socf}, K_{sona}, k_{eb} \) and \( k_{dt} \) negatively correlated with DO were decreased by 10%. The results of maximum sensitivity of parameters combination are shown in Table 8.

| Parameter group | Parameter combination | Sensitivity | Parameter group | Parameter combination | Sensitivity |
|-----------------|-----------------------|-------------|-----------------|-----------------------|-------------|
| 1               | \( q_0 \)             | 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               | \( k_{eb} \)          | -0.0845     | 21              | \( k_{db}, k_{dt} \) | 0.1105      |
| 4               | \( K_{socf} \)        | -0.0559     | 22              | \( q_0, K_{lb}, k_{eb}, k_{socf} \) | 0.2857      |
| 5               | \( K_{sona} \)        | -0.0556     | 23              | \( K_{lb}, k_{eb}, K_{socf}, K_{sona} \) | 0.255      |
| 6               | \( k_{eb} \)          | 0.0276      | 24              | \( k_{db}, K_{socf}, K_{sona}, k_{eb} \) | 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               | \( q_0, K_{lb} \)     | 0.1428      | 27              | \( q_0, K_{lb}, k_{eb}, K_{socf}, K_{sona} \) | 0.3429      |
| 10              | \( K_{lb}, k_{eb} \)  | 0.1416      | 28              | \( K_{lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb} \) | 0.2833      |
| 11              | \( k_{eb}, K_{socf} \) | 0.1408     | 29              | \( k_{eb}, K_{socf}, K_{sona}, k_{eb}, k_{db} \) | 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              | \( q_0, K_{lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb} \) | 0.3714      |
| 14              | \( k_{eb}, k_{db} \)  | 0.0552      | 32              | \( K_{lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb}, k_{db} \) | 0.3116      |
| 15              | \( k_{eb}, k_{dt} \)  | 0.0826      | 33              | \( k_{eb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt} \) | 0.3099      |
| 16              | \( q_0, K_{lb}, k_{eb} \) | 0.2286   | 34              | \( q_0, K_{lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb}, k_{db} \) | 0.4000      |
| 17              | \( K_{lb}, k_{eb}, K_{socf} \) | 0.1983 | 35              | \( K_{lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt} \) | 0.3683      |
| 18              | \( k_{eb}, K_{socf}, K_{sona} \) | 0.1972 | 36              | \( q_0, K_{lb}, k_{eb}, K_{socf}, K_{sona}, k_{eb}, k_{db}, k_{dt} \) | 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 \( q_0 \) 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 cannot 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 8. Result of different combination-patterns of parameters global sensitivity analysis (b).

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 \( q_0 \) 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 cannot 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.
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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