FORECASTING DISSOLVED OXYGEN AND BIOCHEMICAL OXYGEN DEMAND IN A RIVER WITH NUMERICAL SOLUTION OF ONE-DIMENSIONAL BOD-DO MODEL

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Abstract. As a main measure of water quality, the concentration of DO always gets much attention. The chemical reactions in water bodies are mainly related to DO, so the concentration of DO has much relationship with the water quality. Biochemical oxygen demand and dissolved oxygen (BOD-DO) model is used to show the relationship of the concentration of BOD or DO with the physical characteristic of the river. For this model, it is difficult to determine the analytical solution, so numerical solution of the model is obtained with Chebyshev orthogonal polynomial. With this method, the model is rewritten with differential form, and then the four order differential of the oxygen deficit was expressed with the Chebyshev orthogonal polynomial, which had coefficients. Lastly, a simulation test was conducted to verify the rationality of the model. The actual BOD and oxygen deficit values are calculated using the original model. With the actual values and formulas, the coefficients could be solved and the predicted values calculated. The forecasting values of concentration of BOD and DO are compared with the actual values. Five statistical measures were used to evaluate the predicted results.
Keywords: *water quality; analytical solution; Chebyshev orthogonal polynomial; statistic index; oxygen deficit*

Introduction

Many water bodies have become polluted due to rapid economic and social development (Qu and Fan, 2010; Zhang et al., 2011; Liu et al., 2012; Ma et al., 2009). River water quality has been substantially affected by industrial, agricultural and municipal waste water. So it is necessary to assess and predict water quality (Sun et al., 2005). The main pollution indicators are biochemical oxygen demand (BOD), five day biochemical oxygen demand (BOD_5) and the permanganate index (COD_{Mn}). From China official report, among 60 lakes and reservoirs in China, 25.0% are eutrophic, 18.3% are mildly eutrophic and 6.7% are moderately eutrophic. The main indicators are total phosphorus (TP), five-day biochemical oxygen demand (BOD_5) and the permanganate index. In the same time, the concentration of dissolved oxygen (DO) is always low which makes the pollution more serious (Ministry of Environmental Protection of the People’s Republic of China, 2012). Water quality assessment evaluates the pollution levels of rivers or water areas with quality or quantity indicators (Yu et al., 2006; Chen et al., 2005).

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Water quality mathematical models can help establish the relationship between the emission of pollutants and changes in water quality. Such models change a complicated river system into suitable mathematical equations and simulations (He et al., 2013; Lin et al., 2015). As comprehensive indicators that reflect the organic pollution of water body, biochemical oxygen demand (BOD) and dissolved oxygen (DO) are two important parameters for judging the degree of water cleanliness. The well-established BOD-DO water quality model describes the change the law of BOD and DO in a river and is a mature water quality model. It forms the basis of many amended and complex BOD-DO models (Yuan et al., 2003; Zeng et al., 2000). The analytical solution of the model is difficult to obtain and it is necessary to determine the numerical solution (Zhu et al., 2001). Revelli and Ridolfi established a one-dimensional water quality model and obtained the probability density function of BOD (Revelli and Ridolfi, 2004). The finite element and Monte Carlo methods were also used to solve the water quality model separately (Xu et al., 2004a; Guo et al., 2004), and the two methods were combined to solve the problem (Xu et al., 2004b). STREAM II modeling package simulates the DO and BOD parameters in a two-dimensional model (Sharma and Singh, 2009).

Materials and methods

BOD-DO model equations

The research and development of water quality model has gone through a number of stages (Fan and Lv, 2008; Fu, 1987). The first stage was from 1925 to 1980, during which the research object of water quality models was the water body, including the components of water quality. In 1925, Streeter and Phelps proposed the first water quality model. Based on their research, other scholars used and improved the model for water quality forecasting (Guo et al., 2002). The second stage was from 1980 to 1995, involved the use of water quality models in more complicated systems and in combination with the watershed models, thus allowing non-point pollution sources to be treated as initial inputs (Liao and Tim, 1997). The third stage was from 1995 to the present during which the water quality models were developed into a comprehensive model from reaction models. The most common research interests have concentrated on eutrophication of reservoirs and lakes (Quan and Yan, 2001).

The one-dimensional reach is the minimum unit of a river. In this situation, there is only one sewage outlet or tributary at beginning of the reach. The BOD-DO model describes the changes in pollutant concentration, and is expressed by oxygen deficit as:

$$\begin{cases} u\dfrac{\partial L}{\partial x} = D_x \dfrac{\partial^2 L}{\partial x^2} - k_1 L \\ -u\dfrac{\partial D}{\partial x} = -D_x \dfrac{\partial^2 D}{\partial x^2} - k_1 L + k_2 D \end{cases} \tag{Eq.1}$$

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where L is the concentrations (g/m^3) of BOD, u is the flow velocity (km/day or km/d) of water, D is the oxygen deficit, (g/m^3), D_x is the dispersion coefficient (m^2/d), k_1 is the attenuation coefficient of BOD (d^{-1}), and k_2 is the coefficient of reoxygenation of river (d^{-1}). Under steady state, the concentration of indicators does not change, that is $\frac{\partial L}{\partial t}=0, \frac{\partial C}{\partial t}=0$. When considering the effect of dispersion, the analytical solution of the equations can be expressed as follows:

$$\begin{cases} L=L_0 e^{\beta_1 x} \\ D = D_0 e^{-k_2 x/u} - \dfrac{k_1 L_0}{k_1 - k_2}(e^{-k_1 x/u} - e^{-k_2 x/u}) \end{cases} \tag{Eq.2}$$

The expressions of β_1 and β_2 are both complex formulas and there is no regular patterns to obtain their approximate value. So the two equations can be transformed as follows:

$$\begin{cases} \beta_1 = \dfrac{u(1-\sqrt{1+\frac{4D_x k_1}{u^2}})}{2D_x} \dfrac{1+\sqrt{1+\frac{4D_x k_1}{u^2}}}{1+\sqrt{1+\frac{4D_x k_1}{u^2}}} = -\dfrac{2k_1}{u} \dfrac{1}{1+\sqrt{1+\frac{4D_x k_1}{u^2}}} \\ \beta_2 = \dfrac{u(1-\sqrt{1+\frac{4D_x k_2}{u^2}})}{2D_x} \dfrac{1+\sqrt{1+\frac{4D_x k_2}{u^2}}}{1+\sqrt{1+\frac{4D_x k_2}{u^2}}} = -\dfrac{2k_2}{u} \dfrac{1}{1+\sqrt{1+\frac{4D_x k_2}{u^2}}} \end{cases} \tag{Eq.3}$$

From the transformation above, we can conclude that when the parameters obey the relationship $\frac{D_x k_1}{u^2} << 1$ and $\frac{D_x k_2}{u^2} << 1$, the model has an analytical solution. For other situations, however, it is difficult to obtain the analytical solution for the model.

BOD-DO model solution

As referred to above, the BOD-DO model determines the relationship between the concentration of BOD and DO and the river location. In Eq. (1), some parameters need to be estimated. First, the numerical solution is obtained with the parameters, and then certain methods are applied to obtain the parameter values. The next step shows the processes to solve the BOD-DO model. From the first part of Eq. (1), we can obtain the expression of L with other parameters and symbols. The expression of L, the derivative of L, and the second derivative of L are summed up as follows:

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$$\begin{cases} L = \dfrac{1}{k_1}(-D_x \dfrac{d^2D}{dx^2} + u\dfrac{dD}{dx} + k_2 D) \\ \dfrac{dL}{dx} = \dfrac{1}{k_1}(-D_x \dfrac{d^3D}{dx^3} + u\dfrac{d^2D}{dx^2} + k_2\dfrac{dD}{dx}) \\ \dfrac{d^2L}{dx^2} = \dfrac{1}{k_1}(-D_x \dfrac{d^4D}{dx^4} + u\dfrac{d^3D}{dx^3} + k_2\dfrac{d^2D}{dx^2}) \end{cases} \quad \text{(Eq.4)}$$

After the calculation, the three equations above can be substituted into the second formula of Eq. (1). Eq. (4) shows the relationship of the differential and the parameters of the model. We can conclude that the solution of the model refers to a high order-nonlinear problem. The Chebyshev orthogonal polynomial is an effective way to solve this high order differential equation.

$$\frac{D_x^2}{k_1}\frac{d^4D}{dx^4} - \frac{2u}{k_1}D_x\frac{d^3D}{dx^3} + (\frac{u^2}{k_1} - \frac{k_2}{k_1}D_x - D_x)\frac{d^2D}{dx^2} + u(\frac{k_2}{k_1}+1)\frac{dD}{dx} + k_2 D = 0 \quad \text{(Eq.5)}$$

Chebyshev orthogonal polynomial

When the interval is [-1, 1], and the weight function is $\rho(x) = \frac{1}{\sqrt{1-x^2}}$, the orthogonal polynomial combined with the orthogonalization series {1, x, …, x^n, …} is called the Chebyshev orthogonal polynomial. The expression of the nth item is $T_n(x) = \cos(n \arccos x),\ |x| \le 1$. Let $x = \cos\theta$, when x varies in the interval $[-1,1]$ and θ varies in the interval $[0,\pi]$. The expression can be rewritten as $T_n(x) = \cos(n\theta), 0 \le \theta \le \pi$ instead. The general term formula is $T_n(x) = \frac{n}{2}\sum_{m=1}^{[\frac{n}{2}]}(-1)^m \frac{(n-m-1)!}{m!(n-2m)!}(2x)^{n-2m}$, with Tn(x) being the polynomial of degree n with the coefficient of the first item being 2^{n-1}. The recursion formula of the differential coefficient form of the Chebyshev orthogonal polynomial is $2T_n(x) = \frac{1}{n+1}\frac{d}{dx}T_{n+1}(x) - \frac{1}{n-1}\frac{d}{dx}T_{n-1}(x)$. The value of x is between -1 and 1, which is not appropriate for river position. Notation z can be used to replace x, such that $z = a(1-x)$, with the interval of z being from 0 to $2a$. The relationship of x and z is given as follows: $x = 1 - \frac{z}{a}, \frac{dx}{dz} = -\frac{1}{a}, \frac{dz}{dx} = -a$.

According to the relationship of x and z, the connection of θ and z can be deduced. The Chebyshev orthogonal polynomial can be expressed with z.

$$T_n(z) = \frac{n}{2}\sum_{m=1}^{[\frac{n}{2}]}(-1)^m \frac{(n-m-1)!}{m!(n-2m)!}[2(1-\frac{z}{a})]^{n-2m} \quad \text{(Eq.6)}$$

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When $z = a(1-x)$, the recursion formula of the differential coefficient form of the Chebyshev orthogonal polynomial is changed into:

$$2T_n(z) = \frac{1}{n+1}\frac{dT_{n+1}(z)}{dz}\frac{dz}{dx} - \frac{1}{n-1}\frac{dT_{n-1}(z)}{dz}\frac{dz}{dx} \qquad \text{(Eq.7)}$$

Solving the BOD-DO model with the Chebyshev orthogonal polynomial

To solve the problem mentioned in Eq. (5), the four order derivate of the concentration of the dissolved oxygen deficit, $\frac{d^4D}{dz^4}$, should be expanded by the Chebyshev orthogonal polynomial.

$$\begin{aligned}\frac{d^4D}{dz^4} &\approx \sum_{i=1}^{n} d_i f_i(z) = [d_1\ d_2 \cdots d_n][f_1(z)\ f_2(z) \cdots f_n(z)]^T \\ &= d^T f,\ f = [T_0(z)\ T_1(z)\ T_2(z) \cdots T_N(z)]^T, d^T = [d_1\ d_2 \cdots d_n]^T\end{aligned} \qquad \text{(Eq.8)}$$

The next step is to integrate $\frac{d^4D}{dz^4}$. When performing integration, the value of $d^T Hf|_{z=z_0}$ is lost and it should be added when calculating $\frac{d^3D}{dz^3}$. When $z = z_0$, the value of $d^T Hf|_{z=z_0}$ is a constant, denoted as A_3. Because f consists of the polynomial of z, $d^T \int_{z_0}^{z} fdz$ is still composed of the polynomial of z. We can then obtain the expression of $\frac{d^3D}{dz^3}$ in Eq. (9). The calculation of $\frac{d^2D}{dz^2}, \frac{dD}{dz}$ and D are much the same as the calculation of $\frac{d^3D}{dz^3}$. Eq. (9) shows the expressions of these derivatives. Like A_3, the values of A_2, A_1 and A_0 are all constants.

$$\frac{d^3D}{dz^3} = d^T Hf + A_3,\ \frac{d^2D}{dz^2} = d^T H^2 f + A_2,\ \frac{dD}{dz} = d^T H^2 f + A_1,\ D = d^T H^4 f + A_0 \qquad \text{(Eq.9)}$$

The five equations from Eq. (8) to Eq. (9) are substituted into the first part of Eq. (1) and the expression of L can be expressed with the Chebyshev orthogonal polynomial. Lastly, the derivatives of D to x are substituted into Eq. (5). The problem of obtaining the solution of the BOD-DO model is now turned into solving Eq. (10).

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$$\begin{aligned}&\frac{D_x^2}{k_1}d^T f-\frac{2u}{K_1}D_x(d^T Hf+A_3)+(\frac{u^2}{k_1}-\frac{k_2}{k_1}D_x-D_x)(d^T H^2 f+A_2)\\&+u(\frac{k_2}{k_1}+1)(d^T H^3 f+A_1)+k_2(d^T H^4 f+A_0)=0\end{aligned} \quad \text{(Eq.10)}$$

Because other parameters can be obtained or calculated with chemical or physical indicators, the main step during the process of solving Eq. (10) is to solve matrix H.

Matrix

From Eq. (9), $\frac{d^3D}{dz^3}\approx d^T\int_{z_0}^{z} fdz+d^T Hf\,|_{z=z_0}=d^T Hf+A_3$, the expression of H can be deduced as $\int_{z_0}^{z} fdz=Hf$. To obtain the expression of matrix H, the first step is from the derivate form: $T_n(z)=\frac{a}{2(n+1)}\frac{d}{dz}T_{n+1}(z)-\frac{a}{2(n-1)}\frac{d}{dz}T_{n-1}(z)$, in the interval $[z_0,z]$. If $t=0$, then $z(0)=0$, that is to say $z_0=0$. When $n\neq 0$ and $n\neq 1$, performing integration for the equation: $T_n(z)=\frac{a}{2(n+1)}\frac{d}{dz}T_{n+1}(z)-\frac{a}{2(n-1)}\frac{d}{dz}T_{n-1}(z)$. In water quality analysis, $z_0=0$ means the position is the start of the river. In this situation, $\int_{z_0}^{z}T_n(z)dz=-\int_{z_0}^{z}\frac{a}{2(n+1)}\frac{d}{dz}T_{n+1}(z)dz+\int_{z_0}^{z}\frac{a}{2(n-1)}\frac{d}{dz}T_{n-1}(z)dz$ can replace this formula and the formula can be simplified (Eq. (11)). The value of the two expressions can then be determined, they are $\frac{a}{2(n+1)}T_{n+1}(z)\big|_{z=0}$ and $\frac{a}{2(n-1)}T_{n-1}(z)\big|_{z=0}$. The analysis is shown below:

$$\begin{aligned}&\int_0^z T_n(z)dz=-\int_0^z\frac{a}{2(n+1)}\frac{d}{dz}T_{n+1}(z)dz+\int_0^z\frac{a}{2(n-1)}\frac{d}{dz}T_{n-1}(z)dz\\&=-\frac{a}{2(n+1)}T_{n+1}(z)+\frac{a}{2(n-1)}T_{n-1}(z)+\frac{a}{2(n+1)}T_{n+1}(a)\big|_{z=0}-\frac{1}{2(n-1)}T_{n-1}(z)\big|_{z=0}\end{aligned} \quad \text{(Eq.11)}$$

When n=0, $\int_0^z T_0(z)dz=aT_0-aT_1=[a-a\,0\,0\cdots0][T_0\;T_1\;T_2\;T_3\cdots T_n]^T$. Thus, the first row of matrix H has just two elements that are not zero, $H_1=[a-a\,0\,0\cdots0]$. When n=1, $\int_0^z T_1(z)dz=-\frac{a}{2}(1-\frac{z}{a})^2+\frac{a}{2}=[\frac{a}{4}\,0-\frac{a}{4}\,0\cdots0][T_0\;T_1\;T_2\;T_3\cdots T_n]^T$. From this we can obtain the second row of matrix H, which also has two elements that are not zero, $H_2=[\frac{a}{4}\,0-\frac{a}{4}\,0\cdots0]$. These two rows can only be observed according to the form $\int_0^z T_0(z)dz$

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and $\int_0^z T_1(z)dz$. When $n \geq 2$, however, we can obtain the recursion formula. According to Eq. (11), the next problem is to calculate the value of the last two items of this equation.

$$\begin{aligned}
&\frac{a}{2(n+1)}T_{n+1}(z)\Big|_{z=0} - \frac{a}{2(n-1)}T_{n-1}(z)\Big|_{z=0} \\
&= \frac{a}{4}\sum_{m=1}^{[\frac{n+1}{2}]}(-1)^m \frac{(n-m)!}{m!(n+1-2m)!}\times 2^{n-2m} - \frac{a}{4}\sum_{m=1}^{[\frac{n-1}{2}]}(-1)^m \frac{(n-3-m)!}{m!(n-1-2m)!}\times 2^{n-2m-2}
\end{aligned} \qquad \text{(Eq.12)}$$

When $n \geq 2$, the value of the corresponding row of the matrix are $H_{n+1}(1) = -\frac{1}{(n-1)(n+1)}a$, $H_{n+1}(n) = \frac{1}{2(n-1)}a$, and $H_{n+1}(n+2) = -\frac{1}{2(n+1)}a$. According to the analysis above, the structure of matrix H can be obtained as $H_1 = [a - a\,0\,0 \cdots 0]$, $H_2 = [\frac{a}{4}\,0 - \frac{a}{4}\,0 \cdots 0]$, $\cdots\cdots$, $H_{n+1}(1) = -\frac{1}{(n-1)(n+1)}a$, $H_{n+1}(n) = \frac{1}{2(n-1)}a$, and $H_{n+1}(n+2) = -\frac{1}{2(n+1)}a$.

Results and discussion

To illustrate the effectiveness of this method in solving the BOD-DO model, we conducted a simulation experiment to determine if the method could be used to predict water quality. According to the empirical data and actual situation, we assumed that the river was in a steady state and that there were no tributaries or other sewage outlets in the study reach. The parameters of the model mentioned above were also given proper values, $D_0 = 2.48\, g/m^3$, $u = 16\, km/d$, $L_0 = 64.2\, ml/L^3$, $k_1 = 0.114\, d^{-1}$, $k_2 = 2.183\, d^{-1}$, and $D_x = 38.5\, m^2/d$. The distance between two sample sites was 1 km and there were 500 sites in total.

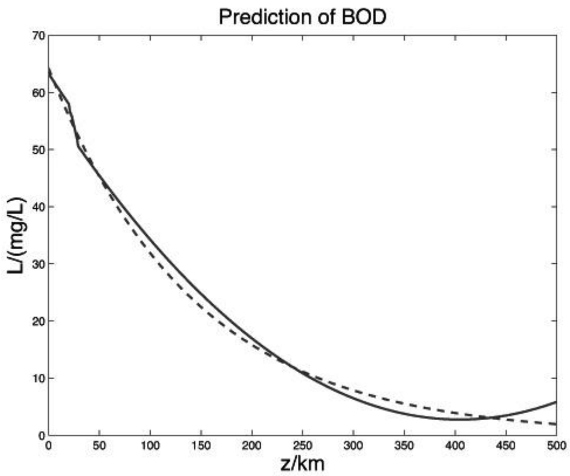

Figure 1. *Actual and predicted data of BOD*

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According to the initial equation (Eq. 1), the actual values of L and D in each site were calculated. Then the coefficient values of the Chebyshev orthogonal polynomial expansion were obtained by Eq (12). Lastly, the predicted values of L and D were acquired. The actual values and predicted values of BOD and DO were compared and the results are shown in *Fig. 1* and *Fig.* 2. The curve of the predicted data was very close to that of the actual data. Although in some sites, the predicted data were not very accurate, the forecasted results as a whole followed the same trend as the actual situation. Thus, the solution method solved the BOD-DO model.

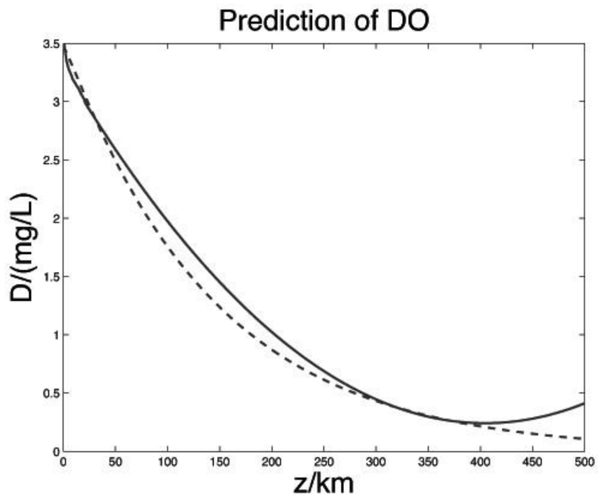

Figure 2. *Actual and predicted data of oxygen deficit*

Comparing the forecast value with the actual value on the surface, five statistical assessment indices, specifically R Squared, the mean absolute error (MAE), the mean absolute percentage error (MAPE), the mean squared error (MSE) and the root-mean-square error (RMSE), were also used to evaluate whether the predicted results were good or bad (*Table 1*).

Table 1. *Statistical assessment measures for model prediction*

	L (concentration of BOD)	D (oxygen deficit)
R Squared	0.9906	0.9775
MAE	1.3901	0.1089
MAPE	0.0240	0.0538
MSE	2.5596	0.0189
RMSE	1.5999	0.1373

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The coefficient of determination, denoted as R^2 (R squared), indicates how well data points fit a statistical model. The R squared of L and D were 0.9906 and 0.9775 respectively. These values were very close to 1, demonstrating that the forecast values of L and D could explain the concentration trends of DO and BOD. The mean absolute error (MAE) is used to measure how close predictions are to eventual values. From *Table 1*, the MAE value for BOD was 1.3901, which was a little higher, and was 0.1089 for oxygen deficit. However, this measure was an absolute value not a percentage value. Further, the interval of the centration of BOD was from 0 to 64.2 (g/m^3) and the interval of oxygen deficit was from 0 to 2.48 (g/m^3). This might explain why the MAE value for BOD was a little larger. The mean absolute percentage error (MAPE) measures the accuracy of a method for constructing fitted time series values, specifically in trend estimation. It usually expresses accuracy as a percentage. This produces a percentage value and appropriate for BOD and oxygen deficit. The mean squared error (MSE) of an estimator is way to quantify the differences between forecast and actual values of the quantity being estimated. An MSE of zero, meaning that the forecast value predicts observations of the parameter with perfect accuracy, is the ideal, however, it is practically impossible to achieve. MSE is calculated by $MSE = \sum_{t=1}^{n}(F_t - A_t)^2/n$. The MSE of the oxygen deficit was less than 0.02, which was an ideal value for the model. Similar to MAE, however, this value is a mean squared error and it also magnifies the error. The MSE value of BOD was 2.5596 which was a little large, but still within the scope of acceptability. The root-mean-square deviation (RMSD) or root-mean-square error (RMSE) is a frequently used measure of the differences between values predicted by a model or an estimator and the values actually observed. RMSD is a good measure of accuracy and is calculated as $RMSD = \sqrt{\sum_{t=1}^{n}(F_t - A_t)^2/n}$. This measure is the square root of MSE, so it has a similar trend to MSE. Because MSE is a sum of square value, RMSD is more objective and reasonable. They were used to evaluate the rationality of the present model, with the results (*Table 1*) illustrating that solving the numerical solution with the proposed method was very suitable.

Conclusion

In this study, a new method was proposed to obtain the numerical solution of the differential equation. It was used to solve the standard BOD-DO water quality model. The derivative of BOD of the model was calculated first. The four orders, three orders, and one order of oxygen deficit were also calculated. The four order differential of oxygen deficit was expressed by the Chebyshev orthogonal polynomial and corresponding coefficients. With the integral of the four orders differential, other differential equations were also expressed. Thus, the BOD-DO model could be denoted with the Chebyshev orthogonal polynomial. After that, we solved the coefficients with

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simulation data. With the solution method and coefficients, the simulated values of BOD and oxygen deficit were calculated. Two figures were used to compare the actual and predicted data. Also there are some irregular points that deviated from the curve, the results as a whole is receivable. Five statistical measures were also used to evaluate the results of the model. These results showed that the predicted values were very similar to the actual values. The simulation test showed that the present method using the Chebyshev orthogonal polynomial to obtain the numerical solution was acceptable and reasonable.

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