Use of Cubic Splines to Calculate BOD First-Order Model Coefficients When There is a Lag Phase

[1] Mr. Rajendra Kumar Roul, [2]Mr.Abhijit Chhatar*
[1] Asst. Professor, Dept. OF Civil Engineering, NIT BBSR,*
Asst. Professor DEPT. of Civil Engineering, NIT, BBSR
[1]rajendraroul@thenalanda.com , abhijitchhatar@thenalanda.com*

Abstract: A new technique is presented for determining the associated coefficients (k and L) of the BOD first order model equation and for detecting the presence of a lag phase. The new approach relies on cubic spline interpolation, MATLAB, and a dimensionless solution to the first order problem with a lag phase. Theoretical first order model curves for the first five days of BOD divided by theoretical BOD5 curves with lag phases for various k values are drawn. By dividing the experimental BOD values for the first five days by the experimental BOD5, the dimensions of those values become dimensionless.

For various lag times, these numbers are connected seamlessly using the cubic spline approach. When both theoretical curves have the same lag phase, the one that is closest to the cubic spline curve in MATLAB is chosen and used to calculate the values for k, L, and the lag period. This method makes it easy to see how closely the experimental data resembles the first order model with a lag phase.

Keywords: dimensionless method; cubic spline; BOD kinetics; BOD with a lag phase.

1 Introduction

The biochemical oxygen demand (BOD) test is typically used to assess the organic content of wastewater. Mathematical models can be used to calculate the final BOD if the first order BOD model is assumed (Ramalho, 1977; Steel and McGhee, 1991; Cutrera et al., 1999; Bassa and Chetty, 2002; Metcalf and Eddy Inc., 2004; Singh, 2004; Siwiec et al., 2011) and the BOD values for the first five to six days are measured. The first order BOD model predicts:

$$BOD = L(1 - e^{-kt}) \quad (1)$$

where

BOD (mg/l) is the amount of oxygen that was consumed (or expended) at time t.

t the amount of time since the test began (day)

L BOD or BODu maximum (mg/l)

k (1/day) reaction constant

Based on BOD measurements for the first five to six days, a variety of approaches have been employed to forecast the values of L and k in the first order model equation. The least squares approach, the Fujimoto method, and the Thomas (1950) method are the three most often utilised techniques (Marquardt, 1963; Cutrera et al., 1999; Bassa and Chetty, 2002; Metcalf and Eddy Inc., 2004; Zainudin et al., 2010). A approach based on the geometric series and logarithm series expansion of the BOD first order model was recently introduced by Ammary and Al-Samraie (2014).

None of the above mentioned methods can be used when, or can predict the presence, of a lag period or lag phase in the first part of the BOD curve. A lag phase is the first phase in a typical bacterial growth curve which is observed when bacteria are placed in a medium with the necessary nutrients. During this phase, bacteria do not reproduce and do not increase in population. Instead, they are creating the necessary enzymes and other factors necessary for growth in their new environment and their new food (Rolfe et al., 2012). Microorganisms which use waste as food are becoming acclimatised and assuming dominance in the system (Pfafflin and Ziegler, 2006). The lack of adequate seeding is one reason for the presence of such lag period (Moore et al., 1950). The presence of toxic chemicals in wastewater is another reason. The first order BOD equation (1) in the presence of a lag period (t_0) can be written as (Moore et al., 1950):

$$BOD = L(1 - e^{-k(t - t_0)}) \quad (2)$$

Moore et al. (1950) have extended the moment method to reflect the presence of a lag phase. The slope method has also been extended to reflect the presence of a lag phase (Thomas, 1940). Braun and Berthouex (1970) have used Monod kinetics to develop a model to analyse BOD curves with a lag phase. Other modelling efforts have also been suggested to solve the BOD curve with a lag phase (Marsilt-Libelli, 1986; Swamee and Ojha, 1991). The complexity of all of these methods has made their use very limited.

The present paper introduces a new method that determines the coefficients k, L, and the lag period t_0, if present, in the BOD first order equation with a lag period

[equation (2)]. The method is based on a dimensionless approach to the BOD first order equation with a lag phase.

2 The dimensionless approach

The dimensionless approach in the absence of a lag phase is based on dividing the theoretical BOD values up to BOD_5 by the theoretical value of BOD_5 for different k values of the BOD first order model equation [equation (1)]. The curves for the different k values with no lag phase thus start from 0.0 at day 0.0 and ends at 1.0 at day 5.0.

Similarly, the BOD first order model equation with a lag phase [equation (2)] can be made dimensionless by dividing the theoretical value of BOD up to BOD_5 by the theoretical value of BOD_5 for different k values and for different lag phase periods (t_0).

For example, the value of BOD_1 over BOD_5 for the case when k = 0.2/day and for a lag phase of 12 hours (0.5 day) would be computed as follows:

$$BOD_1 = L\left(1 - e^{k(1-t_0)}\right) = L\left(1 - e^{-0.2(1-05)}\right) = 0.09516L \quad (3)$$

$$BOD_5 = L\left(1 - e^{-k(5-t_0)}\right) = L\left(1 - e^{-0.2(5-05)}\right) = 0.59343L \quad (4)$$

and thus the value of BOD_1/BOD_5 would be equal to 0.16036. The values of BOD_u/BOD_5 or L/BOD_5 can also be calculated using equation (4) for the same conditions to be equal to

$$\frac{L}{BOD_5} = \frac{1}{\left(1 - e^{-k(5-t_0)}\right)} = \frac{1}{\left(1 - e^{-0.2(5-0.5)}\right)} = 1.685 \quad (5)$$

In the present paper, the values of BOD/BOD_5 for continuous k values (from 0 up to 0.7) and for continuous lag phase periods (from 0 up to 24 hours) were calculated using MATLAB (Hahn and Valentine, 2010; McMahon, 2007). MATLAB was also used to draw the different theoretical curves for BOD/BOD_5 for different k values and different lag phase periods. Only a limited number of k values and lag phase period values are shown in this paper for reasons of clarity and for demonstration purposes.

3 Application of the dimensionless curves on experimental BOD data

As the experimental values of the BOD_1 through BOD_5 are measured, the dimensionless values of these experimental BOD data are calculated. This is done by dividing each experimental value by the experimental BOD_5 value. These dimensionless values are then drawn on the theoretical dimensionless curves drawn using MATLAB for different k values and different lag phase periods. The k value and the lag phase period value of the closest theoretical dimensionless curve to the experimental data are then used to calculate k, L, and the lag phase period of the experimental data.

The closest curve to the dimensionless experimental value can either be found manually if the experimental data are very close to a theoretical dimensionless curve, or by using any other appropriate method. In this paper, the use of cubic spline method (Shikin and Pils, 1995; Knott, 1999) and MATLAB were used for this purpose.

In the cubic spline method, a cubic polynomial function connects every two measured adjacent dimensionless BOD values. Every two adjacent points are connected by a different cubic polynomial function. The different cubic polynomial functions should pass through each measured dimensionless BOD value and be continuous in its first and second derivatives at the interior dimensionless BOD values (De Boor, 1978). In this method, a cubic polynomial function connects points BOD_1/BOD_5 and BOD_2/BOD_5. Another cubic polynomial function connects points BOD_2/BOD_5 and BOD_3/BOD_5 and so on. Further details about cubic spline method are available elsewhere (McKinley and Levine, 2013; Al-Samrraie et al., 2015). Equation (6) shows the form of a cubic polynomial function.

$$S(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i \quad \text{for } i = 1, 2, \ldots, n-1. \tag{6}$$

where a, b, c, and d are the coefficients of the third order polynomial functions, and x_i is the time at which the function starts. For example, when a function S_3 starts from day 2 and ends at day 3, then x_i would be 2 days for the function S_3. The value of x_i for the function S_4 would then be 3 days as the next function starts from day 3 and so on. To evaluate these coefficients, equations for the interior points or nodes and for the two boundary conditions should be written. For the boundary conditions, it was assumed here that the second derivative at the endpoints is equal to that at the points immediately adjacent to them. This method is called parabolic runout spline (Knott, 1999; Gerald and Wheatley, 2004). This type of boundary condition results in a parabolic curve at the endpoint. It is assumed that this type is more appropriate than the many other types of boundary conditions usually used in cubic spline interpolation.

A MATLAB code has been developed to solve the matrix that results for the interior nodes and the two boundary conditions. MATLAB is a very powerful tool for many engineering applications that include matrices, as is the case here.

The cubic spline method draws a smooth curve that passes through each of the dimensionless experimental data. For a BOD curve without a lag phase, the cubic spline curve starts from day zero on the time axis, and thus the start coordinates are (0.0, 0.0), and the end coordinates are (5.0, 1.0). For a BOD curve with a lag phase of t_0, the cubic spline starts from t_0 on the time axis, and thus the start coordinates of the cubic spline curve are (t_0, 0.0). This smooth cubic spline curve is actually a number of cubic polynomial curves that connect smoothly at the point of intersection.

The MATLAB code developed here performs the following tasks:

1 The code calculates the dimensionless experimental BOD values by dividing BOD_1 through BOD_6 values by BOD_5 value. The sixth day BOD (i.e., BOD_6/BOD_5) is used to ensure that when cubic spline curves are drawn, the value at day 5 does not go above the value 1.0. Theoretically, the cubic spline curves for high k values could go above 1.0, just before the fifth day if cubic splines are drawn for only the 5 days values of BOD. Therefore, the value of BOD_6 was used in drawing all the cubic spline curves between 0.0 and 5.0 days. It should be noted that only the area below these curves (between 0.0 and 5.0 days) was calculated and drawn (see below). Figures 1 to 3 show these values for the example shown in Table 1.

Table 1 Example for applying the dimensionless approach to BOD data

Day	*0*	*1*	*2*	*3*	*4*	*5*	*6*
BOD	0	34.1	72.2	104.5	129	150	167
BOD/BOD_5	0	0.227	0.481	0.697	0.860	1.00	1.11

Note: BOD values for days 0 to 6 are divided by BOD5 value.

In Figure 1, the dimensionless BOD at time zero day (BOD_0/BOD_5) is included as a measured value, whereas, in fact it is not. For the case where there is no lag phase, it is assumed that if BOD at time zero is measured, the result would be zero. Similarly, for a lag period of (x days), as in

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Figures 2 to 5, the dimensionless BOD at (x days) is assumed to be zero and included as a measured BOD value. For example, for
0.5 day lag period (as in Figure 2) it is assumed that if BOD is measured after
0.5 day from the time of incubation, the value of BOD would be zero. Therefore, the dimensionless BOD value at time 0.5 day would be zero ($BOD_{0.5}/BOD_5 = 0$) and included in the experimental BOD data. The same was done for Figures 3 to 5.

2 The code then determines the cubic polynomial functions that connect each of the dimensionless experimental data for different lag periods. The lag periods used in this MATLAB code were 25 different lag periods (0.0, 1.0, 2.0, …, 24 hours). They start from (0.0) hour (i.e., no lag period) and end at (24) hours with a 1.0 hour sequence. Different lag periods times can be used, but this was done here to reduce the calculation time. Figures 1 to 3 show the different cubic spline curves connecting the dimensionless data shown in Table 1 for 0, 12, and 18 hours (0, 0.5, and 0.75 days) lag periods, as examples.

Figure 1 Cubic spline curve connecting the dimensionless BOD data and the theoretical BOD curves for k values of 0.05, 0.2, 0.2, 0.3, 0.4, and 0.5 per day and no lag period (see online version for colours)

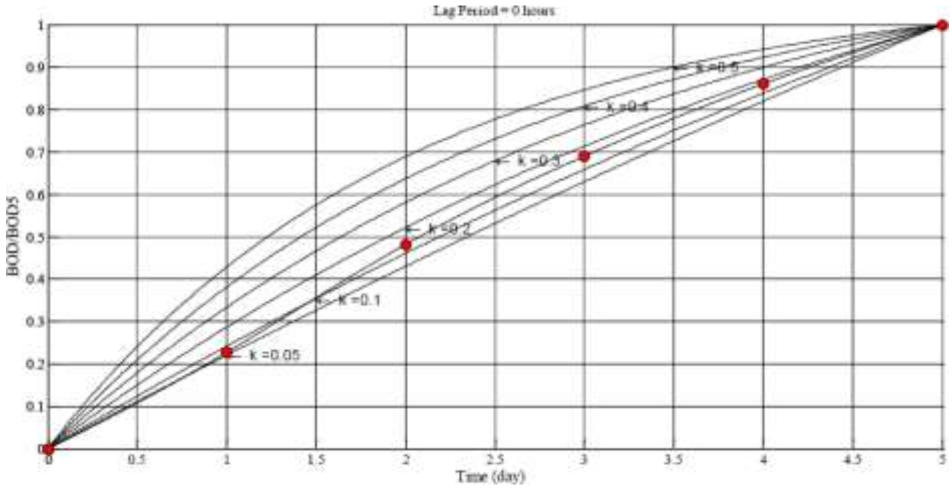


Figure 2 Cubic spline curve connecting the dimensionless BOD data and the theoretical BOD curves for k values of 0.05, 0.2, 0.2, 0.3, 0.4, and 0.5 per day and 0.5 day lag period (see online version for colours)

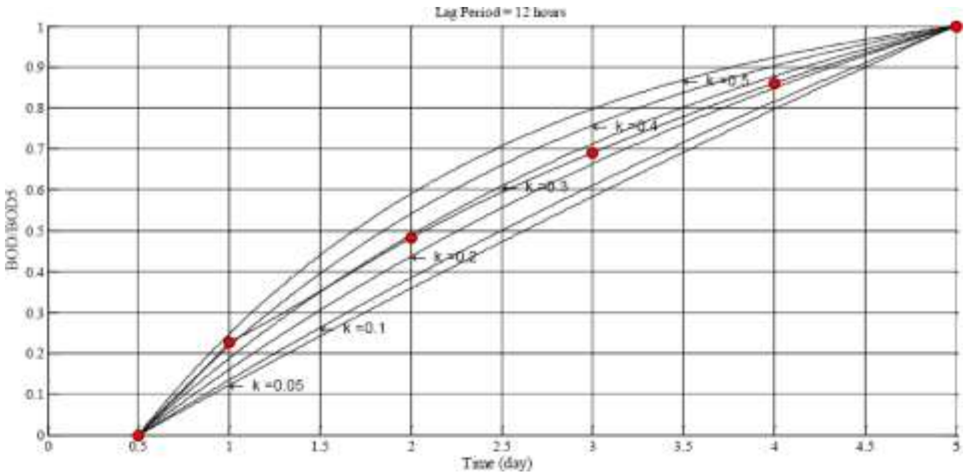
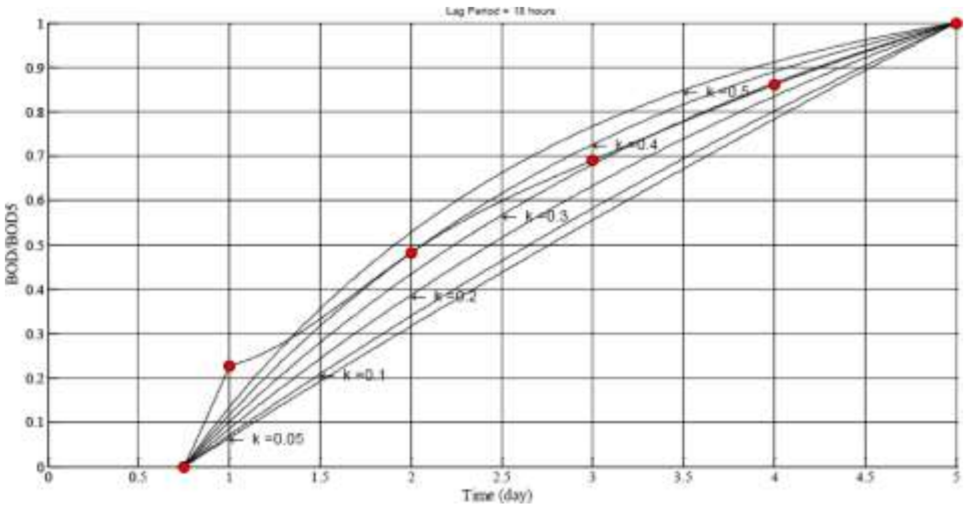


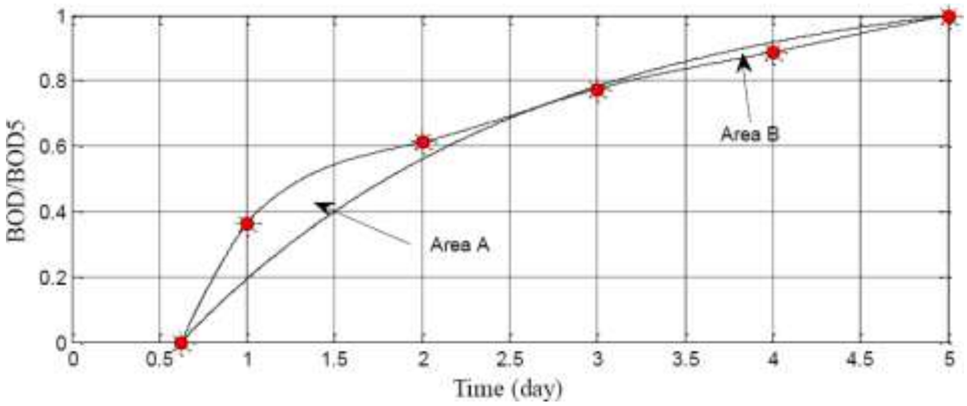
Figure 3 Cubic spline curve connecting the dimensionless BOD data and the theoretical BOD curves for k values of 0.05, 0.2, 0.2, 0.3, 0.4, and 0.5 per day and 0.75 day lag period (see online version for colours)



3 The code then determines the area below the cubic spline curves between day zero and day five for each different lag phase period t_0 (0.0, 1.0, 2.0, …, 24 hours).

4 Then for each lag phase period, a theoretical dimensionless curve with the same area below it as that with the cubic spline curves is determined. The code selects this curve by trying different values of k and calculating the area below each of these curves. The curve with the area closest to the area below the cubic spline curves is selected. As the areas below these two types of curves are equal, this implies that the area that lies below the cubic spline curves and above the theoretical dimensionless curve (area A in Figure 4) is equal to the area that lies above the cubic spline curve and below the theoretical dimensionless curve (area B in Figure 4).

Figure 4 The two areas (area A and area B) that should be equal in order for the areas below the cubic spline curve and the theoretical dimensionless curve to be equal (see online version for colours)



Note: Minimum area A (or area B) indicates that the two curves are the closest.

5 Now the code has 25 theoretical dimensionless curves each with a different value of k for the 25 different lag periods each with a different cubic spline curve. Each of these 25 theoretical curves has the same area below it as the corresponding cubic spline curve with the same lag period.

Table 2 Function coefficients for the cubic spline curves [see equation (6)], $S_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i$ in Figure 5(c) with a lag period of 6 hours (0.25 day).

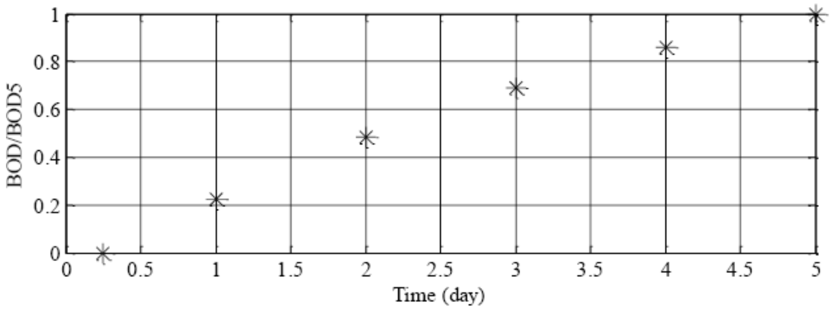
Function	*a*	*b*	*c*	*d*
S_1*	0	0.037161	0.274929	0
S_2**	–0.02579	0.037161	0.243028	0.2271
S_3[\$]	0.008624	–0.04021	0.239983	0.4815
S_4[\$]	–0.00071	–0.01433	0.185441	0.6899
S_5[\$]	0.001502	–0.01645	0.154652	0.8603

Notes: *Function S_1 describes the function that connects time (0.25 day) and time (1 day) on Figure 5(c) and is equal to: $S_1(x) = 0\,(x - 0.25)^3 + 0.037161\,(x - 0.25)^2 + 0.274929\,(x - 0.25) + 0$.
**Function S_2 describes the function that connects time (1 day) and time (2 day) on Figure 5(c) and is equal to: $S_2(x) = -0.02579\,(x - 1)^3 + 0.037161\,(x - 1)^2 + 0.243028\,(x - 1) + 0.2271$.
[\$]Functions S_3, S_4, and S_5 connect (day 2–day 3), (day 3–day 4), and (day 4–day 5) on Figure 5(c), respectively. The values of x_i in equation (6) above for S_3, S_4, and S_5 are 2, 3, and 4 days, respectively.

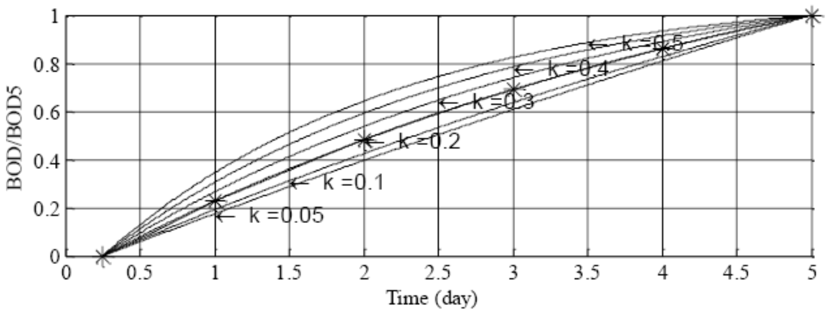
6 The code then selects the curve that has the minimum values of area A (or area B). The theoretical dimensionless curve that produces minimum area A means that the cubic spline curve and the theoretical dimensionless curve are the closest compared to any other theoretical dimensionless curve. Figure 5 shows the theoretical dimensionless curve that produces minimum area A and of course minimum area B

(see Figure 4 for the definition of area A and area B). The k value and the lag period value for this theoretical curve, in this case 0.25 day lag period and a k value of 0.195/day, is the k value and the lag period value of the first order BOD equation.
The values of the cubic spline coefficients for the curves shown in Figure 5 with the same lag period (0.25 day) are shown in Table 2.

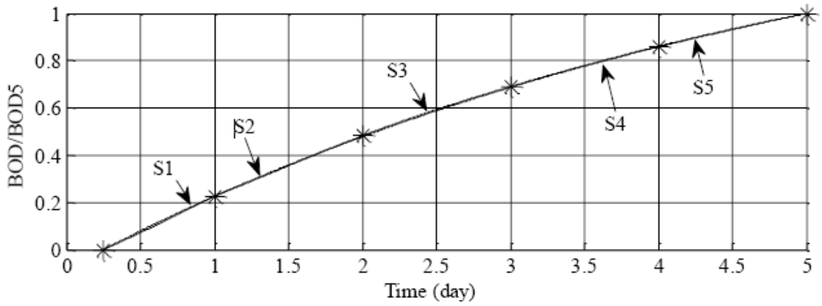
Figure 5 The closest theoretical dimensionless curve to the cubic spline curves (S_1–S_5) for data in Table 1



(a)



(b)



(c)

Notes: Lag period = 0.25 day, k = 0.195428, BOD factor = 1.60356, Difference in area below the cubic spline curve and below the theoretical first order curve = 9.57314e-005, area A = 0.0064 (spline curve above first order), area B = –0.0061 (spline curve under first order curve).

7 The ultimate BOD is then calculated using equation (5). In this equation, the value of BOD_u is calculated by multiplying BOD_5 for the experimental data by the value of BOD_u/BOD_5 (the BOD_5 factor) obtained from equation (5). The MATLAB code also calculates the BOD_5 factor for any k value for the theoretical dimensionless BOD curve. The theoretical BOD_5 factor calculated in Figure 5 is equal to (1.60356). Therefore, the ultimate BOD (BOD_u or L) in this case is calculated as:

$$BOD_u = (BOD_5 \text{ factor})(BOD_5 \text{ value}) = 1.60356\,(150 \text{ mg l}^{-1}) = 240 \text{ mg/l}$$

4 Conclusions

A new dimensionless method is introduced for the detection of the presence of a lag phase and the determination of the corresponding coefficients of the first order BOD equation with a lag phase. A MATLAB code determines the closeness of the cubic spline interpolation of the experimental dimensionless BOD data to the theoretical dimensionless BOD first order equation, each having the same lag phase period. The MATLAB code is capable of determining the k value that best describes the experimental data and calculates the ultimate BOD directly. The advantages of such method include better visualisation, understanding, and comparison of experimental data to the BOD first order model with lag phase.

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