

CHAPTER -5

**APPLICATION OF LAPLACE
TRANSFORMATION TO A NONTRADITIONAL
DISSOLVED OXYGEN MODEL**

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5.1 Introduction

The first order BOD decay equation has been widely applied since 1925 in modeling the dissolved oxygen (DO) in a river stream (Streeter and Phelps, 1925). Literature reviews on BOD reaction orders which are three-halves order, second order, and multiorder are available (Adrian *et al.*, 1999; Adrian and Sanders, 1998; Adrian et al, 2004). The steady-state DO model developed Streeter and Phelps (1925), which predicts DO concentration in streams using first order BOD kinetics, is well understood and accepted (Mulligan and Brown, 1998). Modifications have included accounting for sedimentation (Thomas, 1948), benthic addition of BOD (Thomann, 1974), effects of algae (Beck and Young, 1975), and dispersion (Dresnack and Dobbins, 1968). The effect of dispersion on BOD and DO concentration in small rivers is negligible (McCutcheon, 1989). Few studies have examined the effect that BOD reaction orders which were other than first order have on the DO behavior in a stream. Respirometry is a versatile method for measuring the BOD reaction characteristics of a wide variety of wastewaters and stream samples (Young and Cowan, 2004). Multiorder BOD data (Hewitt, et al, 1979) encouraged development of a DO sag equation for the three-halves order BOD reaction and a multiorder BOD reaction (Adrian, *et al.*, 1999; Adrian, *et al.*, 2004), although tedious mathematical expositions were plentiful. The purpose of this investigation is to review the relationships which describe a three-halves order BOD reaction, then to incorporate these BOD relationships into the differential equation for DO for a stream. Because of its ease in application the Laplace transform method is selected to solve the DO sag equation. Also, a methodology for locating the minimum DO concentration in a stream is developed, and examples are presented to illustrate application of the models.

5.2 Three-halves Order BOD Equation:

The three-halves order BOD equation is given by (Adrian *et al.*, 1999; Hewitt *et al.*, 1979)

$$\frac{dL}{dt} = -k_{3/2} L^{3/2} \text{-----5.1}$$

where L is the BOD remaining, g/m³, at time t, and k_{3/2} is the three-halves order rate constant having units of (m³/g)^{1/2}/day. Equation (5.1) is integrated, combined with L₀ – y = L and rearranged to

$$y = L_0 - \frac{4}{k_{3/2}^2 (T + t)^2} \text{-----5.2}$$

where $T = 2 / k_{3/2} L_0^{1/2}$ is a time constant having units of days and L₀ is the carbonaceous BOD remaining at time zero. By comparison, the first order BOD equation is (Adrian *et al.*, 2004)

$$L = L_0 e^{-k_1 t} \text{-----5.3}$$

where k₁ is the first order BOD rate constant with units of day⁻¹. The conventional BOD test or respirometry gives values of y_i, the BOD exerted, or the amount of oxygen consumed by a sample at time, t_i (Young and Cowan, 2004). Parameters k_{3/2} and L₀ are estimated from the measured y_i and t_i values with a nonlinear least squares procedure as those values which minimize the root mean squared error objective function

$$RMSE(k_{3/2}, L_0) = \sqrt{\frac{1}{N-2} \sum_{i=1}^{i=N} \left[y_i - L_0 + \frac{4}{k_{3/2}^2 \left(\frac{2}{k_{3/2} \sqrt{L_0}} + t_i \right)^2} \right]^2}$$

-----5.4

where $(N - 2)$ represents the number of degrees of freedom. The $RMSE(k_{3/2}, L_0)$ function is minimized by selecting the values of $k_{3/2}$ and L_0 for the data set consisting of the values of y_i on day t_i using an iterative technique, such as the Newton Raphson method or the Levenburg-Marquardt compromise (Bates and Watts, 1998). The RMSE methodology was applied to estimate the rate constant and ultimate BOD for samples taken from several New Jersey brooks and rivers (Hewitt *et al.*, 1979).

A Bayesian estimation method is available for calculating rate constants and ultimate BOD while providing the probability distribution of the parameters (Borsuk and Stow, 2000). Table 4.1 shows the rate constant, designated as $k_{3/2}$, and the ultimate BOD, L_0 , reported in two investigations in which river samples were analyzed in respirometers to determine how well the BOD data fit first order and three-halves order reactions. In data sets 1-7 the RMSE was smaller for the three-halves order BOD model than for the first order reaction (Hewitt *et al.*, 1979; Rodriguez, 1999).

5.3 Laplace Transform of Oxygen Sag Equation for Three-halves Order BOD Reaction

The differential equation for DO concentration in a stream with a three-halves order BOD reaction is found from conservation of mass combined with equation (5.2) expressed as L to yield

$$\frac{dC}{dt} + k_1 C = k_1 C_s - \frac{8}{k_{3/2}^2} \frac{1}{(T+t)^3}$$

-----5.5

Data Set	Location	Rate Constant		Ultimate BOD		RMSE	
		k ₁	k _{3/2}	L ₀	L ₀	First	Three-halves
		First Day ⁻¹	Three-halves (m ³ /g) ^{1/2} /day	First g/m ³	Three-halves g/m ³	First g/m ³	Three-halves g/m ³
1.	Mahananda River, Siliguri	0.237	0.0487	21.72	24.51	0.6870	0.6511
2.	Mahananda River, Siliguri	0.134	0.0259	19.50	23.00	0.2386	0.1883
3.	Mahananda River, Siliguri	0.101	0.0246	10.47	12.81	0.3491	0.1042
4.	Mahananda River, Malda	0.140	0.0322	14.96	17.43	0.3349	0.1248
5.	Mahananda River, Malda	0.217	0.0648	8.121	9.595	0.2106	0.1975
6.	Mahananda River, Malda	0.123	0.0411	5.648	6.870	0.0762	0.0681

Table 5.1. BOD Reaction Orders, Rate Constants, Ultimate BODs and Root Mean Square Errors for First and Three-Halves Order BOD Reactions from Mahananda river water quality data.

where C is the DO concentration, g/m³, and k_s is the reaeration rate constant, day⁻¹ (Adrian *et al.*, 1999). The DO concentration at time zero is C₀ and the saturation concentration is C_s. The Laplace transform of equation (5.7) yields (Oberhettinger and Badii, 1973)

$$p\bar{C} - C_0 + k_s\bar{C} = \frac{k_s C_s}{p} - \frac{8}{k_{3/2}^2} \mathcal{L}\left\{\frac{1}{(T+t)^3}\right\} \quad \text{-----5.6}$$

where the Laplace transform of C(t) is defined by

$$\mathcal{L}\{C(t)\} = \bar{C} = \int_0^{\infty} C(t) e^{-pt} dt \quad \text{-----5.7}$$

The inverse transform of equation (5.8) is found from Laplace transform tables and convolution (Oberhettinger and Badii, 1973)

$$C(t) = C_0 e^{-k_s t} + C_s (1 - e^{-k_s t}) - \frac{8}{k_{3/2}^2} e^{-k_s t} * \frac{1}{(T+t)^3} \quad \text{-----5.8}$$

where the symbol “*” means convolution

$$e^{-k_s t} * \frac{1}{(T+t)^3} = \int_0^t e^{-k_s(t-\tau)} \frac{1}{(T-\tau)^3} d\tau = k_s^2 e^{-k_s T} \int_{k_s T}^{k_s(t+T)} \frac{e^u}{u^3} du \quad \text{-----5.9}$$

with the change in variables $u = k_s(T + \tau)$. The integral in equation (5.11) is (Petit Bois, 1961; Abramowitz and Stegun, 1965)

$$\int_{k_s T}^{k_s(t+T)} \frac{e^u}{u^3} du = \left[-\frac{1}{2} e^u \left(\frac{1}{u^2} + \frac{1}{u} \right) + \frac{1}{2} \text{li}(e^u) \right] \Big|_{k_s T}^{k_s(t+T)}$$

-----5.10

where $\text{li}(e_u)$ is the logarithmic integral of e_u . The logarithmic integral is not commonly tabulated, but a related function, the exponential integral, is tabulated. The definition is $\text{li}(x) = \text{Ei}(\ln(x))$ for $x > 0$, where $\text{Ei}(\ln(x))$ is the exponential integral of $\ln(x)$ (Abramowitz and Stegun, 1965). After incorporating equations (5.11) and (5.12) into equation (5.8), the DO sag curve becomes

$$\begin{aligned} C(t) = & C_s - (C_s - C_0) e^{-k_s t} \\ & + \frac{4k_s^2}{k_{3/2}^2} \left[\left(\frac{1}{k_s^2 (T+t)^2} + \frac{1}{k_s (T+t)} \right) - e^{-k_s t} \left(\frac{1}{k_s^2 T^2} + \frac{1}{k_s T} \right) \right] \\ & - \frac{4k_s^2}{k_{3/2}^2} \{ e^{-k_s(T+t)} [E_i(k_s(T+t)) - E_i(k_s T)] \} \end{aligned}$$

-----5.11

This result, easily obtained by means of the Laplace transform and inversion using the convolution integral, agrees with a DO sag equation obtained by a more difficult procedure (Arian *et al.*, 1999). Equation (4.12) can be applied to rivers in a manner analogous to that used in applying the Streeter-Phelps DO sag equation (1925).

The exponential integral $\text{Ei}(x)$ which appears in equation (4.12) is calculated from its series expansion. There are two series expansions; one convenient for small values of argument x , and the other convenient for larger values of x . The first series expansion is (Abramowitz and Stegun, 1965).

$$E_i = \gamma + \ln x + \sum_{n=1}^{\infty} \frac{x^n}{nn!} \text{-----5.12}$$

where $\gamma = \text{Euler's constant} = 0.577215\dots$. This series converges for all values of x but may converge slowly for large values of x . For large values of x , an asymptotic expansion will converge more rapidly than equation (4.13) to an approximate value of $Ei(x)$

$$E_i = \frac{e^x}{x} \left(\frac{0!}{x^0} + \frac{1!}{x^1} + \frac{2!}{x^2} + \dots + \frac{n!}{x^n} \right) = \frac{e^x}{x} \sum_{m=0}^{n-1} \frac{m!}{x^m} \text{-----5.13}$$

where $n! = n(n - 1)(n - 2) \dots (3)(2)(1)$ and $0! = 1$. The asymptotic expansion is a divergent series, yet for a finite number of terms, the difference between the true value of $Ei(x)$ and the sum of a finite number of terms in the series may be small. For a fixed value of x , the closest approximation is obtained when n is the closest integer to x . The exact series expression should be used in DO modeling when $x < 5$ to reduce error (Adrian and Sanders, 1998).

5.4 Minimum DO Concentration

The time t_c at which the minimum DO concentration occurs is an important parameter which is found from equation (4.12) when $dC/dt = 0$. If $dC/dt \neq 0$, for $t > 0$, then the minimum DO concentration will occur when $t = 0$, for the case in which DO addition by reaeration is greater than the DO uptake rate by BOD. The derivative of equation (4.12), designated as $f(t_c)$, is

$$f(t_c) = k_s(C_s - C_0)e^{-k_s t}$$

$$+ \frac{4k_s^2}{k_{3/2}^2} \left\{ k_s e^{-k_s t_c} \left[\frac{1}{k_s^2 T^2} + \frac{1}{k_s T} \right] - \left[\frac{2}{k_s^2 (T + t_c)^2} + \frac{1}{k_s (T + t_c)^2} \right] \right\}$$

$$+ \frac{4k_s^2}{k_{3/2}^2} \left\{ k_s e^{-k_s (T + t_c)} [E_i(k_s (T + t_c)) - E_i(k_s T)] - \frac{1}{T + t_c} \right\}$$

The critical time occurs when $f(t_c) = 0$ which is found in root finding methods. An alternative to applying equation (4.15) is to find t_c directly from equation (4.12). In this case, one sets up equation (4.12) and uses a software package to calculate when $dC/dt = 0$. The derivative of equation (4.12) found by numerical methods and the corresponding time, t_c , are listed.

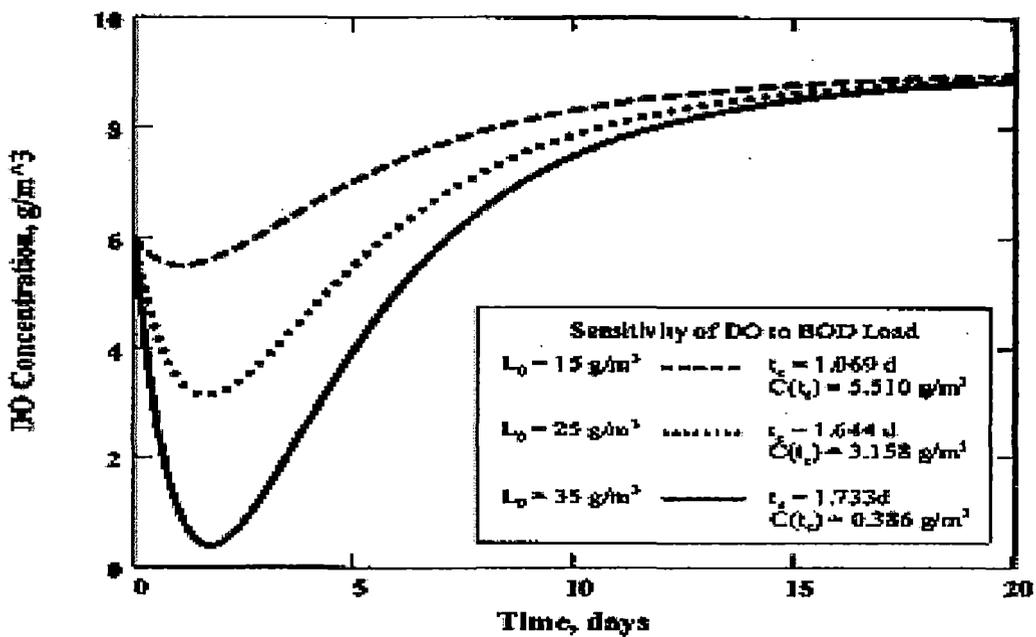


Figure 5.1. Effect of BOD Load on DO Sag Curves for Three-halves Order BOD Reaction

Data set 2 in Table 5.1 is for the river which has a three-halves order reaction rate coefficient of $0.0259 \text{ (m}^3/\text{g})^{1/2}/\text{day}$ and an ultimate first stage BOD of 23.0 g/m^3 (Hewitt et al., 1979). DO saturation is 9.2 g/m^3 , initial DO is 6.0 g/m^3 , and the reaeration rate constant is $0.6/\text{day}$. Time constant $T = 2 / (k_{3/2} L_0) = 16.101 \text{ day}$ and $k_1 T = 9.661$. The

corresponding rate constant and ultimate BOD for first order reaction are 0.134 day^{-1} and 19.50 g/m^3 (Hewitt *et al.*, 1979). The appropriate rate constant and ultimate BOD are input to equation (5.13) to obtain the DO concentrations which are shown in Table 5.2. Both equation (5.14) with 50 terms and equation (5.15) can be used to calculate $E_i(x)$.

5.5 Conclusions

1. Table 5.1 shows the three-halves order rate constant and ultimate BOD for seven analyses of BOD reaction data from six different locations of Mahananda rivers at Siliguri and Malda of North Bengal.
2. A DO sag equation developed for BOD consumption modeled as a three-halves order reaction is solved easily using the Laplace transform method and convolution. The DO sag equation contains exponential integrals which are evaluated from their series expressions. The exact series expression of an exponential integral may require summation of several hundred terms although 50 terms were adequate in the examples. The number of terms to include in an asymptotic expansion depends upon the magnitude of the argument. 14 terms were required in one example. An asymptotic expansion is not used to evaluate an exponential integral unless the argument is greater than five. The maximum error in the DO concentration was less than 0.79% on day 1.402 when comparing the two alternative methods of evaluating $E_i(x)$ when the argument was 9.661.
3. The minimum value of the DO concentration occurs at the critical time, t_c , which may be 0 if the reaeration rate is greater than or equal to the DO consumption rate, otherwise $t_c > 0$. t_c is calculated numerically from the DO sag equation by a root finding method. As the rate constant, $k_{3/2}$, increases both the minimum DO and t_c become smaller.