

# **CHAPTER -4**

**DEVELOPMENT OF OXYGEN SAG MODEL  
(SIMPLIFIED FORM)**

# CHAPTER 4

## DEVELOPMENT OF OXYGEN SAG MODEL (SIMPLIFIED FORM)

### 4.1 Introduction

Water quality modeling in a river has been developed from the pioneering work of Streeter and Phelps (1925) who developed a balance between the dissolved oxygen supply rate from reaeration and the dissolved oxygen consumption rate from stabilization of an organic waste in which the biochemical oxygen demand (BOD) deoxygenation rate was expressed as an empirical first order reaction, producing the classic dissolved oxygen sag (DO) model. When the dispersion process is considered, the governing equation becomes a partial differential equation. However, the effect of dispersion on BOD and DO in small rivers is negligible (Li 1972; Thomann, 1974; McCutcheon, 1989). The minimum value of the DO concentration has been of particular significance in wastewater treatment design calculations and to regulatory agencies. By contrast the BOD decay characteristics of leaves and logging debris are relatively unknown (Ponce, 1974), although these items represent sources of loads on streams and are important in Total Maximum Daily Load (TMDL) studies. Several investigators (Thomas, 1957; Young and Clark, 1965; Clark and Viessman, 1965; Nemerow, 1974; Tebbutt and Berkun, 1976) presented data showing that second order rather than first order reactions frequently describe the stabilization of wastewaters, but none of these authors incorporated a second order BOD reaction into the DO sag equation. Butts and Kothandaraman (1970) analyzed stream samples from the Illinois River and found that the majority of these samples' BOD decay was described better by a first order reaction model, while a minority of the samples' BOD decay was described by a second order reaction model. In spite of these results they did not develop a DO sag equation which included a second order BOD model. Adrian and Sanders (1998) developed an analytical solution for the DO sag equation which incorporated a second order BOD reaction but their development involved integration of cumbersome equations. The Laplace transform method provides a user friendly approach to solution of differential equations. The purpose of this study is to demonstrate application of the Laplace transform method to

develop a DO sag equation for a river in which a second order relationship describes the BOD decay of the loading to the river.

## **4.2 LAPLACE TRANSFORMATION:**

Firstly the reason behind to use such a procedure is strongly motivated by real engineering problems. There, typically we encounter models for the dynamics of phenomena which depend on rates of change of functions, eg velocities and accelerations of particles or points on rigid bodies, which prompts the use of ordinary differential equations (ODEs). Ordinary calculus can be used to solve ODEs, provided that the functions are nicely behaved—which means continuous and with continuous derivatives. Unfortunately, there is much interest in engineering dynamical problems involving functions that input step change or spike impulses to systems—playing pool is one example. Now, there is an easy way to smooth out discontinuities in functions of time: simply take an average value over all time. But an ordinary average will replace the function by a constant, so it is used a kind of moving average which takes continuous averages over all possible intervals of  $t$ . This very neatly deals with the discontinuities by encoding them as a smooth function of interval length  $s$ . The amazing thing about using Laplace Transforms is that it can be converted a whole ODE initial value problem into a Laplace transformed version as functions of  $s$ , simplify the algebra, find the transformed solution  $f(s)$ , then undo the transform to get back to the required solution  $f$  as a function of  $t$ . Interestingly, it turns out that the transform of a derivative of a function is a simple combination of the transform of the function and its initial value. So a calculus problem is converted into an algebraic problem involving polynomial functions, which is easier. There is one further point of great importance: calculus operations of differentiation and integration are linear. So the Laplace Transform of a sum of functions is the sum of their Laplace Transforms and multiplication of a function by a constant can be done before or after taking its transform.

**4.2.1 The transform concept and definition:**

An improper integral of the form  $\int_{-\infty}^{+\infty} K(s,t)F(t)dt$  is called integral transform of F(t)

if it is convergent. Sometimes it is denoted by f(s) or T{F(t)}. Thus

$$f(s) = T\{F(t)\} = \int_{-\infty}^{+\infty} K(s,t)F(t)dt \text{ -----(A)}$$

The function K(s,t) appearing in the integrand is called kernel of the transformation. Here s is a parameter and is independent of t, s may be real or complex number.

If it is taken as  $K(s,t) = \begin{cases} e^{-st}, t \geq 0 \\ 0, t < 0 \end{cases}$  and  $K(s,t)=0$  when  $t < 0$  then the equation (A)

becomes  $f(s) = T\{F(t)\} = \int_0^{+\infty} e^{-st} F(t)dt$ , this transform is known as Laplace

transformation where F(t) is a piecewise continuous over every finite interval in the range  $t \geq 0$  and of exponential order as  $t \rightarrow \infty$ .

This transformation can also be written as  $f(s) = L\{F(t)\} = \int_0^{+\infty} e^{-st} F(t)dt$ , where L is

called Laplace transformation operator. The Laplace transform is said to exist if the integral in right hand side is convergent for some value of s.

**4.3 DO Sag Model Formulation**

The differential equation describing the DO concentration in a river subject to a BOD reaction is

$$\frac{dC}{dt} = k_1(C_s - C) - k_2 f(t) \text{ -----4.1}$$

where C is the DO concentration, g/m<sup>3</sup>, C<sub>s</sub> is the saturation value for DO, g/m<sup>3</sup>, k<sub>1</sub> is the reaeration rate, day<sup>-1</sup>, t is flow time, days, k<sub>2</sub> is the rate constant in the BOD expression,

and  $f(t)$  is a function that expresses the BOD concentration as a function of time. The form of the BOD function is related to the expression selected to describe the BOD reaction. The units of the rate constant  $k_2$  depend on the BOD function. Several investigators (Young and Clark, 1965; Clark and Viessman, 1965; Woodward, 1953) express the second order BOD equation as

$$L = \frac{L_0}{1 + k_2 L_0 t} \quad \text{-----4.2}$$

where  $L$  is the BOD yet to be satisfied,  $g/m^3$ ,  $t$  is time, days,  $k_2$  is the second order rate constant having units of volume/mass-time, such as  $m^3/g\text{-day}$ , while  $L_0$  is the initial ultimate first stage BOD. The term  $f(t)$  in equation (4.1) for a second order BOD reaction is given by the square of equation (4.2) which enables the differential equation for the DO concentration to be formed.

Conventional BOD tests give values of  $y$ , the amount of DO consumed by a sample,  $g/m^3$ , as a function to time. The relationship  $L = L_0 - y$  can be substituted into equation (4.2) which is then rearranged to obtain

$$y = \frac{k_2 L_0^2 t}{1 + k_2 L_0 t} \quad \text{-----4.3}$$

Examples are available of calculating the parameters  $k_2$  and  $L_0$  from linearized forms of equation (4.3) (Young and Clark, 1965; Butts and Kothandaraman, 1970; Weber and Carlson, 1965). A preferable procedure for determining  $k_2$  and  $L_0$  is to find their values such that the best fit in the least squares sense is obtained using equation (4.3) and the measured values of  $y$  versus  $t$  (Marske and Polkowski, 1972; Bates and Watts, 1988; Borsuk and Stow, 2000).

Adrian and Sanders (1998) applied an integrating factor to equation (4.1), after it had been modified to include  $f(t)$  equal to the square of equation (4.2), then integrated several rather unwieldy expressions to obtain the DO concentration. The Laplace transform method which is presented below is easier to follow than the previous solution.

Equation (4.1) is modified by noting  $f(t) = L_2$ , given by equation (4.2), then the Laplace transform of modified equation (4.1) is

$$p\bar{C} - C_0 + k_s\bar{C} = \frac{k_s C_s}{p} - \frac{1}{k_2} \mathcal{L}\left\{1/(a+t)^2\right\} \quad \text{-----4.4}$$

where  $a = 1/(k_2 L_0)$ ,  $p$  is the parameter in the Laplace transform, the Laplace transform of  $C(t)$  is designated by the overbar,  $C_0$  is the initial DO concentration, and  $\mathcal{L}\{1/(a+t)^2\}$  is the Laplace transform of  $1/(a+t)^2$ , which for  $a > 0$  is (Nemerow, 1974)

$$\mathcal{L}\left\{\frac{1}{(a+t)^2}\right\} = \frac{1}{a} + p e^{ap} Ei(-ap) \quad \text{-----4.5}$$

in which the term  $Ei(-ap)$  signifies the exponential integral with argument  $(-ap)$ .

Equation (4.4) is rearranged to show the Laplace transform of the DO concentration

$$\bar{C} = \frac{C_0}{p+k_s} + \frac{k_s C_s}{p(p+k_s)} - \frac{1}{k_2(p+k_s)} \left[ \frac{1}{a} + p e^{ap} Ei(-ap) \right] \quad \text{-----4.6}$$

The inverse transform of equation (4.6) is expressed as

$$C(t) = C_0 e^{-k_s t} + C_s (1 - e^{-k_s t}) - \frac{1}{k_2} e^{-k_s t} * \frac{1}{(a+t)^2} \quad \text{-----4.7}$$

where the  $*$  notation means  $\exp(-k_s t)$  is convoluted with  $1/(a+t)^2$  (Churchill, 1958). In other words

$$e^{-k_1 t} \frac{1}{(a+t)^2} = \int_0^t \frac{e^{-k_1(t-\tau)}}{(a+\tau)^2} d\tau = e^{-k_1(a+t)} \int_a^{a+t} \frac{e^{k_1 x}}{x^2} dx$$

-----4.8

where  $\tau$  and  $x$  are dummy variables of integration and the change in variable  $x = a + \tau$  has been introduced. Gradshteyn and Ryzhik (1980) show

$$\int \frac{e^{k_1 x}}{x^2} dx = -\frac{e^{k_1 x}}{x} + k_1 Ei(k_1 x)$$

-----4.9

Thus, equation (4.7) is expressed as

$$C(t) = C_0 e^{-k_1 t} + C_s (1 - e^{-k_1 t}) + \frac{1}{k_2(a+t)} - \frac{e^{-k_1 t}}{k_2 a} - \frac{k_1}{k_2} e^{-k_1(a+t)} \{Ei[k_1(a+t)] - Ei[k_1 a]\}$$

-----4.10

Equation (4.10) is identical to the DO sag equation derived by Adrian and Sanders (1998). However, the Laplace transform method is easier to apply and involves fewer steps than the earlier method which used an integrating factor and several transformations of variables to integrate equation (4.1).

The DO deficit,  $D = C_s - C_0$  g/m<sup>3</sup>, is commonly used instead of  $C$ . Equation (4.10) is rearranged to

$$D = D_0 \exp(-k_1 t) + L_0 \exp(-k_1 t) - \frac{L_0}{1 + k_2 L_0 t} + \frac{k_1}{k_2} \exp\left[-\left(\frac{k_2}{k_2 L_0} + k_1 t\right)\right] \left[ Ei\left(\frac{k_1}{k_2 L_0} + k_1 t\right) - Ei\left(\frac{k_1}{k_2 L_0}\right) \right]$$

-----4.11

where  $D_0$  is the DO deficit,  $g/m^3$ , when  $t = 0$ .

### 4.3.1 The Exponential Integral

The exponential integral  $Ei(x)$  is tabulated in mathematical tables (Abramowicz and Stegun, 1965). However, in equations (4.10) and (4.11) it is convenient to calculate the exponential integral directly from its series expansion. There are two series expansions for the exponential integral, one convenient to use for small values of the argument,  $x$ , and the other convenient to use for larger values of  $x$ . The first series expansion is (Abramowicz and Stegun, 1965)

$$Ei(x) = \gamma + \ln(x) + \sum_{n=1}^{\infty} \frac{x^n}{n \cdot n!}$$

-----4.12

where  $\gamma = \text{Euler's constant} = 0.577215\dots$  This series converges for all values of  $x$ , however, it converges slowly for large values of  $x$ . An alternative method for calculating  $Ei(x)$  for large values of  $x$  is to use an asymptotic expansion series (Abramowicz and Stegun, 1965)

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

-----4.13

The asymptotic expansion is a divergent series if  $n \rightarrow \infty$ , yet the difference between the true value of  $Ei(x)$  and the sum of a finite number of terms in the truncated series may be very small especially when  $x$  is large. Kaplan (1952) presents a simple, practical rule for selecting  $n$ : the best approximation of the asymptotic expansion series to  $Ei(x)$  occurs when  $n$  is the closest integer to  $x$ . It is not permissible to differentiate an asymptotic

expansion (Gradshteyn and Ryzhik, 1980). In DO sag modeling both small and large values of  $x$  are encountered. Equation (4.12) has been recommended for use instead of equation (4.13) when  $x < 5$  due to error in the asymptotic expansion, but when  $x \geq 5$  either equation (4.12) or (4.13) could be used if one was aware that equation (4.12) may require  $n$  to be large to converge (Adrian and Sanders, 1998). Examples presented later will show how large  $n$  may be for equation (4.12) to converge.

### 4.3.2 The Oxygen Sag Equation(Two Forms)

Combining equation (4.10) with the asymptotic expansion, equation (4.13), yields

$$C(t) = C_s + (C_0 - C_s)\exp(-k_s t) + \frac{L_0}{1 + k_2 L_0 t} - L_0 e^{-k_2 t} - \frac{k_s}{k_2} \left[ \frac{k_2 L_0}{k_s (1 + k_2 L_0 t)} \sum_{n=0}^N n! \left( \frac{k_2 L_0}{k_s (1 + k_2 L_0 t)} \right)^n - \frac{k_2 L_0}{k_s} \exp(-k_s t) \sum_{n=0}^M n! \left( \frac{k_2 L_0}{k_s} \right)^n \right]$$

-----4.14

This expression is a computationally tractable approximate form of equation (4.10) which is suitable when the term  $k_s / (k_2 L_0)$  is greater than 5.  $N$  and  $M$  are selected as the nearest integers to the arguments of the exponential integrals by using the round off function,

where

$$M = \text{round} [k_s / (k_2 L_0)] \text{-----}(4.15)$$

$$N = \text{round} [k_s / (k_2 L_0) + k_s t] \text{-----}(4.16)$$

A form of the DO sag equation that is always applicable is obtained by combining equation (4.10) with the convergent series, equation (4.12). The result is

$$C(t) = C_0 e^{-k_s t} + C_s (1 - e^{-k_s t}) + \frac{L_0}{1 + k_2 L_0 t} - L_0 e^{-k_s t} - \frac{k_s}{k_2} e^{-\frac{k_s(1+k_2 L_0 t)}{k_2 L_0}} \left\{ \ln(1 + k_2 L_0 t) + \sum_{n=1}^{\infty} \frac{\left[ \frac{k_s(1+k_2 L_0 t)}{k_2 L_0} \right]^n}{n \cdot n!} - \sum_{n=1}^{\infty} \frac{\left[ \frac{k_s}{k_2 L_0} \right]^n}{n \cdot n!} \right\}$$

-----4.15

### 4.3.3 Minimum DO Concentration

The minimum DO concentration will occur either at  $t = 0$  or at the time called the critical time,  $t_c$ , when  $dC/dt = 0$  in equation (4.10). The derivative of equation (4.10) when  $dC/dt = 0$  is

$$0 = k_s \left( C_s - C_0 + \frac{1}{k_2 a} \right) \exp(-k_s t) - \frac{1}{k_2 (a+t)^2} - \frac{k_s}{k_2 (a+t)} + \frac{k_s^2}{k_2} \exp[-k_s (a+t)] \{ Ei[k_s (a+t)] - Ei[k_s a] \}$$

-----4.16

This equation is solved for the root  $t_c$  by a numerical root finding method in a software package such as MATHCAD™ with equation (4.12) or (4.13) used to evaluate the exponential integrals. If  $t_c$  is negative, then the minimum DO concentration occurs at  $t = 0$  where  $C(0) = C_0$ . A positive  $t_c$  is substituted into equation (4.14) or (4.17) to calculate the minimum DO concentration. The value of  $N$  is not known a priori so a few trials may

be needed to find the value of  $N$  that is consistent with  $t_c$ . An alternative procedure to find the minimum DO and  $t_c$  is to apply a series of times in equations (4.14) or (4.17) and record the value of the minimum DO concentration and the time to which it corresponds.

#### 4.4 Application of the DO Sag Equation

The DO sag equation for a second order BOD demand is illustrated in an example developed from data presented by Ponce (1974) in which needles from Douglas Fir in samples prepared with stream water are tested for BOD. The second order reaction rate coefficient of  $0.000440 \text{ m}^3/(\text{g}\cdot\text{day})$  is calculated from BOD test data. Assume that the streamflow and temperature are such that after mixing with the Douglas Fir needles the ultimate first stage BOD is  $100 \text{ g/m}^3$  and the reaction rate coefficient remains unchanged (due to the small rate constant the 5 day BOD would be about  $82 \text{ g/m}^3$ ). Ponce (1974) carried the BOD test out for 90 days yet found no evidence of nitrification. His data for Douglas Fir are presented in Table 3.1.

Table 4.1. BOD Data for Douglas Fir Needles (Ponce, 1974)<sup>1,2</sup>.

Time [Day]	Oxygen Consumed [g/m <sup>3</sup> ]	Time [Day]	Oxygen Consumed [g/m <sup>3</sup> ]
0	0	45	432
5	252	60	440
10	312	90	460
20	408		

1 Each value of oxygen consumed is an average of four samples.

2 Nonlinear least squares analysis yields rate coefficient  $k_2 = 0.000440 \text{ m}^3/(\text{g day})$  and ultimate BOD  $L_0 = 481.445 \text{ g/m}^3$  for second order BOD.

The DO saturation value in the application is 9.08 g/m<sup>3</sup> and the initial DO value is 7 g/m<sup>3</sup>. The reaeration rate is 0.6/day. The DO concentrations are calculated at daily intervals for the first seven days using the exact and the approximate equations for the exponential integral, and the minimum DO concentration is found using equation (4.18). These data are input into equations (4.14) and (4.17) for comparison while the results are tabulated in Table 3.2. The value of  $k_3/(k_2L_0)$  was calculated as 13.63, by equation (4.15), so M was set to 14, and N calculated from equation (4.16), varied with t as shown in Table 4.2. The time  $t_c = 3.3$  day was calculated using equation (4.18) with the exponential integral calculated by equation (4.13) instead of equation (4.12) due to the reduced number of calculations using equation (4.13) when M or N are larger than 5 or 6. The DO concentration was 3.516 g/m<sup>3</sup> at the critical time. The error was calculated by finding the difference between C(t) from equations (4.14) and (4.17). Negligible error was found in using equation (4.14) which contained the approximate series expression.

The complete DO sag curve is shown in Figure 4.1 using both equations (4.14) and (4.17). The DO sag curve is of interest in TMDL studies.

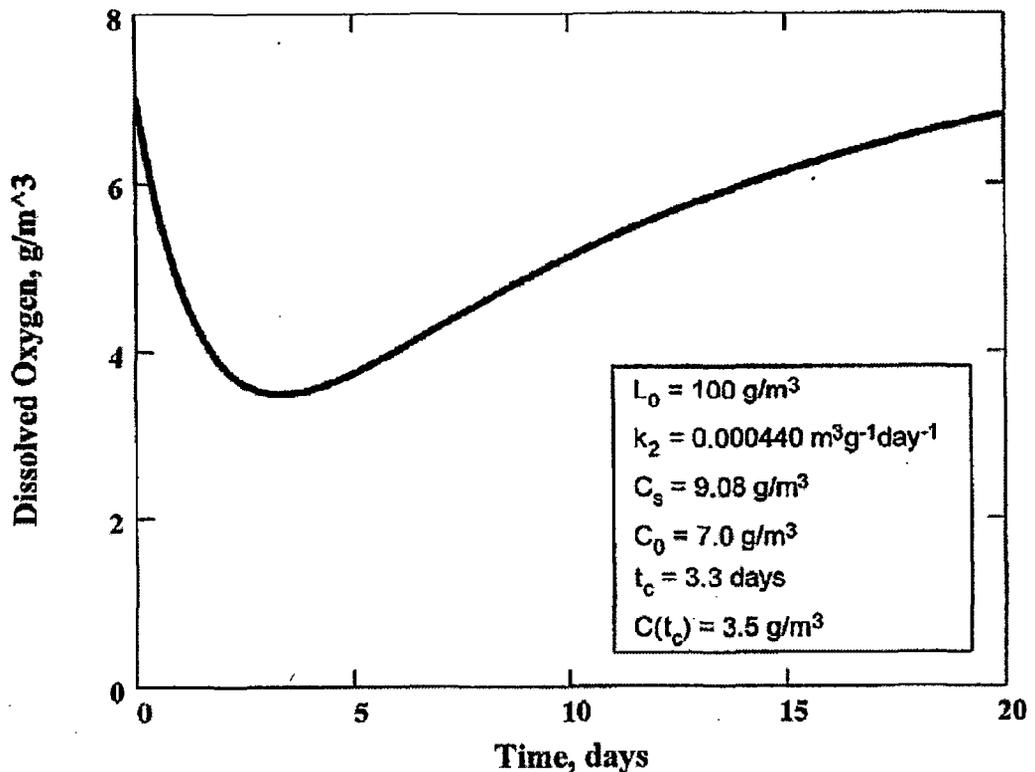
Table 4.2. Comparison of DO Concentrations for Second Order BOD Reaction

t days	C Eq.(3.17) (Exact)	C Eq.(3.14) (Approximate)	N Eq.(3.16)	$C_{\text{exact}} - C_{\text{approx}}$ Error
0	7.000	7.000	14	0.000
1	4.781	7.782	14	- 0.001
2	3.819	3.819	15	0.000
3	3.516	3.516	15	0.000
3.3 = $t_c$	3.500	3.500	16	0.000
4	3.549	3.549	16	0.000
5	3.746	3.746	17	0.000
6	4.014	4.014	17	0.000
7	4.305	4.305	18	0.000

#### 4.5 Conclusions

A DO sag equation for a stream has been developed in which the biochemical oxygen demand is evaluated as a second order reaction. The differential equation for the DO sag model was solved by applying the Laplace transform method. The DO sag model, equation (4.10), contains exponential integrals which are evaluated by either an exact series or an approximate asymptotic series. The location of the minimum DO concentration is found by calculating the time at which  $dC/dt = 0$  in equation (4.18).

Other simulations have shown the asymptotic series should not be used to calculate the



**Figure 4.1**

DO Sag curve for a stream which receives BOD loading from Douglas Fir Needles. The BOD Reaction is Second Order. The time at which the minimum DO concentration occurs is 3.3 days and the minimum DO concentration is  $3.5 \text{ G/M}^3$ .

DO concentration in equation (4.10) or the critical time in equation (4.18) at which the minimum DO occurs if the values of M or N from equations (4.15) and (4.16) are less than five. Also, other simulations have shown that when N is less than 7 a plot of equation (4.14) may produce a rough appearing DO sag curve which may have a jump or a sudden change in slope each time N takes on a different integer value in equation (4.16). It has been recommended that equation (4.14) not be used for M or N less than 5 (Adrian and Sanders, 1998). The example presented in this study in which Douglas Fir needles produced BOD, showed that the DO sag model which incorporated an asymptotic series was virtually identical in its predictions with  $M = 14$  and N ranging from 14 to 18 to predictions using the exact series. It is necessary to experiment with equation (4.12),

the exact series for the exponential integral, to find the number of terms to sum. 150 terms were used in the calculations in, although more terms may have been needed for calculations at larger times. Thus, the DO sag equation for second order BOD is not suitable for calculation without a computer. Figure 4.1 shows that the small value of the BOD reaction rate constant results in the stream being able to carry a large BOD concentration from Douglas Fir needles without having the DO concentration being exhausted. The result is of interest in TMDL studies involving waste load allocation to stream.