SIMPLIFIED DEVELOPMENT OF OXYGEN SAG MODEL*

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ABSTRACT

A dissolved oxygen sag equation is developed by use of the Laplace transform and the convolution integral for a stream in which the biochemical oxygen demand (BOD) deoxygenation rate is described as a second-order reaction. The Laplace transform method simplifies the mathematical solution of the model equation by avoiding difficult-to-evaluate integrals. The dissolved oxygen sag equation incorporates exponential integral functions which are calculated by exact or approximate series. The time at which the minimum dissolved oxygen concentration occurs is calculated numerically. The dissolved oxygen sag model is applied using BOD data collected from Douglas Fir needles in stream water. The Douglas Fir needles had a small reaction rate constant which results in the stream being able to carry a BOD load without exhausting its dissolved oxygen supply. The model is useful in calculating Total Maximum Daily Loads (TMDL) of streams.

INTRODUCTION

Water quality modeling in a river has developed from the pioneering work of Streeter and Phelps [1], 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 [2-4]. 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 [5], although these items represent sources of loads on streams and are important in Total Maximum Daily Load (TMDL) studies.

Several investigators 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 [6-10]. Butts and Kothandaraman 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 [11]. In spite of these results, they did not develop a DO sag equation which included a second-order BOD model. Adrian and Sanders developed an analytical solution for the DO sag equation which incorporated a second-order BOD reaction but their development involved integration of cumbersome equations [12]. 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.

DO SAG MODEL FORMULATION

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

$$\frac{dC}{dt} = k_s\,(C_s - C) - k_2 f(t) \tag{1}$$

where C is the DO concentration (g/m^3), C_s is the saturation value for DO (g/m^3), k_s is the reaeration rate (day^{-1}), t is flow time (days), k_2 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 [7, 8, 13] express the second order BOD equation as

$$L = \frac{L_0}{1 + k_2\, L_0\, t} \tag{2}$$

where L is the BOD yet to be satisfied (g/m³), t is time (days), k_2 is the second order rate constant having units of volume/mass-time (such as m³/g-day), while L_o is the initial ultimate first stage BOD. The term f(t) in Equation (1) for a second-order BOD reaction is given by the square of Equation (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/m³), as a function to time. The relationship $L = L_o - y$ can be substituted into Equation (2), which is then rearranged to obtain

$$y = \frac{k_2\, L_o^2\, t}{1 + k_2\, L_o\, t} \tag{3}$$

which Woodward attributes by personal communication to H. A. Thomas [13]. Examples are available of calculating the parameters k_2 and L_o from linearized forms of Equation (3) [7, 11, 14]. A preferable procedure for determining k_2 and L_o is to find their values such that the best fit in the least squares sense is obtained using Equation (3) and the measured values of y versus t [15-18].

Adrian and Sanders applied an integrating factor to Equation (1), after it had been modified to include f(t) equal to the square of Equation (2), then integrated several rather unwieldy expressions to obtain the DO concentration [12]. The Laplace transform method which is presented below is easier to follow than the previous solution.

Equation (1) is modified by noting $f(t) = L^2$, given by Equation (2), then the Laplace transform of modified Equation (1) is

$$p\overline{C} - C_o + k_s\overline{C} = \frac{k_s C_s}{p} - \frac{1}{k_2}\, \mathcal{L}\,(1/(a + t)^2) \tag{4}$$

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_o 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 [19]:

$$\mathcal{L}\left\{\frac{1}{(a + t)^2}\right\} = \frac{1}{a} + pe^{ap}\, Ei(-ap) \tag{5}$$

in which the term Ei(-ap) signifies the exponential integral with argument (−ap). Equation (4) is rearranged to show the Laplace transform of the DO concentration

$$C = \frac{C_0}{p + k_s} + \frac{k_s C_s}{p\,(p + k_s)} - \frac{1}{k_2\,(p + k_s)}\left[\frac{1}{a} + pe^{ap}\, Ei(-ap)\right] \tag{6}$$

The inverse transform of Equation (6) is expressed as

$$C(t) = C_0 e^{-k_s t} + C_s (1 - e^{-k_s t}) - \frac{1}{k_2} e^{-k_s t} * \frac{1}{(a+t)^2} \tag{7}$$

where the * notation means $\exp(-k_s t)$ is convoluted with $1/(a+t)^2$ [19]. In other words,

$$e^{-k_s t} * \frac{1}{(a+t)^2} = \int_0^t \frac{e^{-k_s(t-\tau)}}{(a+\tau)^2} d\tau = e^{-k_s(a+t)} \int_a^{a+t} \frac{e^{k_s x}}{x^2} dx \tag{8}$$

where τ and x are dummy variables of integration and the change in variable $x = a + \tau$ has been introduced. Gradshteyn and Ryzhik show [20]:

$$\int \frac{e^{k_s x}}{x^2} dx = -\frac{e^{k_s x}}{x} + k_s \, Ei(k_s x) \tag{9}$$

Thus, Equation (7) is expressed as

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

$$- \frac{k_s}{k_2} e^{-k_s(a+t)} \left(Ei[k_s(a+t)] - Ei[k_s a] \right) \tag{10}$$

Equation (10) is identical to the DO sag equation derived by Adrian and Sanders [12]. 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 (1).

The DO deficit, $D = C_s - C$, g/m^3, is commonly used instead of C. Equation (10) is rearranged to

$$D = D_o \exp(-k_s t) + L_o \exp(-k_s t) - \frac{L_o}{1 + k_2 L_o t}$$

$$+ \frac{k_s}{k_2} \exp\left[-\left(\frac{k_s}{k_2 L_0} + k_s t \right) \right] \left[Ei\left(\frac{k_s}{k_2 L_0} + k_s t \right) - Ei\left(\frac{k_s}{k_2 L_0} \right) \right] \tag{11}$$

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

The Exponential Integral

The exponential integral Ei(x) is tabulated in mathematical tables [21]. However, in Equations (10) and (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 [21]:

$$Ei(x) = \gamma + \ln(x) + \sum_{n=1}^{\infty} \frac{x^n}{n \cdot n!} \tag{12}$$

where γ = Euler's constant = 0.577215. . . . 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 [21]:

$$Ei(x) = \frac{e^x}{x}\left(\frac{0!}{x^0} + \frac{1!}{x^1} + \frac{2!}{x^2} + \ldots + \frac{n!}{x^n}\right) = \frac{e^x}{x} \sum_{m=0}^{m=n} \frac{m!}{x^m} \tag{13}$$

The asymptotic expansion is a divergent series if $n \to \infty$, 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 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 [22]. It is not permissible to differentiate an asymptotic expansion [20]. In DO sag modeling, both small and large values of x are encountered. Equation (12) has been recommended for use instead of Equation (13) when x <5 due to error in the asymptotic expansion, but when x ≥5 either Equation (12) or (13) could be used if one was aware that Equation (12) may require n to be large to converge [12]. Examples presented later will show how large n may be for Equation (12) to converge.

Two Forms of the Oxygen Sag Equation

Combining Equation (10) with the asymptotic expansion, Equation (13), yields

$$C(t) = C_s + (C_0 - C_s)\exp(-k_s t) + \frac{L_0}{1 + k_2 L_0\, t} - L_0 e^{-k_s t}$$

$$\tag{14}$$

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

This expression is a computationally tractable approximate form of Equation (10) which is suitable when the term $k_s/(k_2 L_o)$ is greater than 5. N and M are selected as the nearest integers to the arguments of the exponential integrals by using the roundoff function, where

$$M = \text{round}\,[k_s/(k_2 L_o)] \tag{15}$$

$$N = \text{round } [k_s/(k_2 L_o) + k_s t] \tag{16}$$

A form of the DO sag equation that is always applicable is obtained by combining Equation (10) with the convergent series, Equation (12). The result is

$$C(t) = C_0 e^{-k_s t} + C_s (1 - e^{-k_s t}) + \frac{L_0}{1 + k_2 L_0 t} - L_0 e^{-k_s t} \tag{17}$$

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

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 (10). The derivative of Equation (10) when dC/dt = 0 is

$$0 = k_s \left(C_s - C_0 + \frac{1}{k_2 a} \right) \exp(-k_s t) - \frac{1}{k_2 (a+t)^2} - \frac{k_s}{k_2 (a+t)} \tag{18}$$

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

This equation is solved for the root t_c by a numerical root finding method in a software package such as MATHCAD™ with Equation (12) or (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 (14) or (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 Equation (14) or (17) and record the value of the minimum DO concentration and the time to which it corresponds.

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 in which needles from Douglas Fir in samples prepared with stream water are tested for BOD [5]. The second-order reaction rate coefficient of 0.000440 m^3/g-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 g/m^3 and the reaction rate coefficient remains unchanged (due to the small rate constant the 5 day BOD would be about 82 g/m^3). Ponce carried the BOD test out for 90 days yet found no evidence of nitrification [5]. His data for Douglas Fir are presented in Table 1. The DO saturation value in the application is 9.08 g/m^3 and the initial DO value is 7 g/m^3. 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 (18). These data are input into Equations (14) and (17) for comparison while the results are tabulated in Table 2. The value of $k_s/(k_2L_0)$ was calculated as 13.63 by Equation (15), so M was set to 14, and N calculated from Equation (16) varied with t as shown in Table 2. The time t_c = 3.3 day was calculated using Equation (18) with the exponential integral calculated by Equation (13) instead of Equation (12) due to the reduced number of calculations using Equation (13) when M or N are larger than 5 or 6. The DO concentration was 3.516 g/m^3 at the critical time. The error was calculated by finding the difference between C(t) from Equations (14) and (17). Negligible error was found in using Equation (14), which contained the approximate series expression. The complete DO sag curve is shown in Figure 1 using both Equations (14) and (17). The DO sag curve is of interest in TMDL studies.

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 (10), contains exponential integrals which are evaluated

Table 1. BOD Data for Douglas Fir Needles [5][a,b]

Time (day)	Oxygen consumed (g/m^3)	Time (day)	Oxygen consumed (g/m^3)
0	0	45	432
5	252	60	440
10	312	90	460
20	408		

[a]Each value of oxygen consumed is an average of four samples.
[b]Nonlinear least squares analysis yields rate coefficient k_2 = 0.000440 m^3/(g day) and ultimate BOD L_0 = 481.445 g/m^3 for second order BOD.

Table 2. Comparison of DO Concentrations for
Second Order BOD Reaction

t days	C eq. (17) (Exact)	C eq. (14) (Approximate)	N eq. (16)	$C_{exact} - C_{approx}$ Error
0	7.000	7.000	14	0.000
1	4.781	4.782	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

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 (18). Other simulations have shown the asymptotic series should not be used to calculate the DO concentration in Equation (10) or the critical time in Equation (18) at which the minimum DO occurs if the values of M or N from Equations (15) and (16) are less than five. Also, other simulations have shown that when N is less than 7 a plot of Equation (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 (16). It has been recommended that Equation (14) not be used for M or N less than 5 [12]. 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 (12), the exact series for the exponential integral, to find the number of terms to sum. One hundred and fifty terms were used in the calculations in this article, 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 1 shows that the small
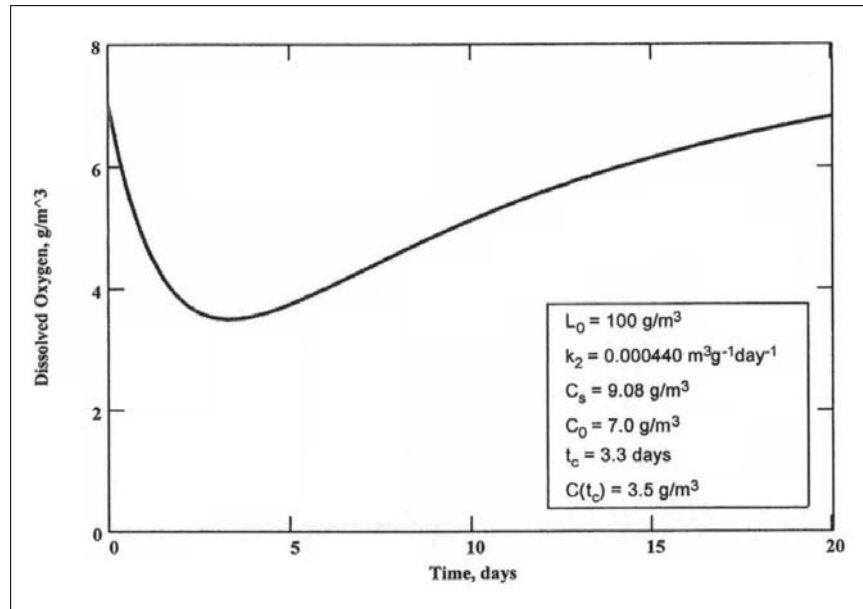
Figure 1. Dissolved oxygen sag curve for a stream which receives BOD loading from Douglas Fir needles. The BOD reaction is second-order. The time at which the minimum dissolved oxygen concentration occurs is 3.3 days and the minimum dissolved oxygen concentration is 3.5 g/m^3.

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 streams.

NOMENCLATURE

C = dissolved oxygen concentration, g/m^3

C_o = dissolved oxygen concentration when t = 0, g/m^3

C_s = saturation value of dissolved oxygen, g/m^3

$\overline{C}$ = Laplace transform of dissolved oxygen concentration

D = dissolved oxygen deficit, $(C_s - C)$, g/m^3

D_o = dissolved oxygen deficit at time zero, g/m^3

$Ei(x)$ = exponential integral of x

k_2 = second-order biochemical oxygen demand rate constant, m^3/g-day

k_s = reaeration rate constant, day^{-1}

L   = biochemical oxygen demand yet to be satisfied, g/m^3
L_o = initial ultimate biochemical oxygen demand, g/m^3
M   = integer value limit in a series summation
N   = integer value limit in a series summation
n   = integer numbers
p   = parameter in Laplace transform
t   = time
t_c = time when the minimum dissolved oxygen concentration occurs, day
y   = amount of oxygen consumed at any time $(L_o – L)$, g/m^3
γ   = Euler's constant = 0.577215...

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