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MODELING RIVER WATER QUALITY BY THE SUPERPOSITION METHOD

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ABSTRACT

A one-dimensional (1-D) advection-dispersion equation (ADE) with a first-order biochemical reaction was solved using the superposition method. Three sets of initial and boundary conditions were considered. The boundary condition of the model virtually can be any type of chemical or BOD concentration functions. Thus, the model accepts discrete and time-dependent input and produces a continuous concentration distribution over time and space. A simple and accurate equation was derived to calculate the upper-bound memory time of a given river. Since the model requires only a finite record-length, it can be easily updated. The model was compared with some analytical and numerical models and was found to be accurate, simple, and easy to apply.

Much work has been done on one-dimensional (1-D) modeling of chemical transport in a river or through a soil column. A multitude of solutions of the 1-D advection-dispersion equation (ADE) are available. Some of the solutions are numerical [1-3], and some are analytical [4-9]. Van Genuchten and Alves listed forty-four analytical solutions for the 1-D ADE for different initial and boundary conditions as well as for different orders of biochemical reactions [8]. Although these analytical solutions were originally obtained for 1-D subsurface flow, they can also be extended to 1-D surface flow by letting the retardation factor and medium porosity be unity, respectively.

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Although 1-D analytical models may not be adequate in many cases and 2-D or 3-D numerical models may, therefore, be employed [10], analytical solutions to 1-D flow cases are, nevertheless, useful. A survey of recent literature showed that the current 1-D analytical solutions often ignore two important and practical aspects in river quality simulation:

1. The concentration at a boundary, or at a pollutant source, is always time-dependent and its functional form is not known; and
2. Observations at a boundary are normally available in discrete form.

Thus, it is desirable to derive an analytical model considering these two aspects. A typical example of such a practical environmental problem is shown in Figure 1, that shows a river with an observation station at the upstream end near a pollutant source. Observations of the biochemical oxygen demand (BOD) are given in discrete form. A simple accurate model is needed to predict the BOD concentration distribution along the river. It may be even more important to know what the concentration profile would be if the pollutant source concentration was double or triple its present value tomorrow.

In this study, a simple analytical model was developed, with input being discrete and time-dependent, and output being continuous over time and space. The unit step function was used to represent the observed input series, and the superposition method was employed to obtain the solution to the 1-D advection-dispersion equation. In order to update the model as more observed data became available and to keep the length of the input series as short as possible, a simple equation was derived to calculate the upper-bound memory time of a given river reach.

MODEL DEVELOPMENT

Let there be a river reach with an observation station at the upstream end of the river reach or at a pollutant source, and with an average flow velocity u. The BOD or chemical concentration in the reach is assumed to be uniformly distributed through the flow cross-section so that a one-dimensional model may be applied. The BOD concentration values at the station can be taken at a fixed time interval, i.e., hourly, daily, or weekly. An example of the observations is shown in Figure 1.

The governing equation for the 1-D BOD concentration transport process in a river reach can be obtained by the mass-balance principle as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} - K_1 C, \tag{1}$$

where $D(L^2T^{-1})$ is the dispersion coefficient, $K_1(T^{-1})$ is the first-order decay constant, $C(ML^{-3})$ is the BOD concentration, $t(T)$ is the time, and $x(L)$ is the

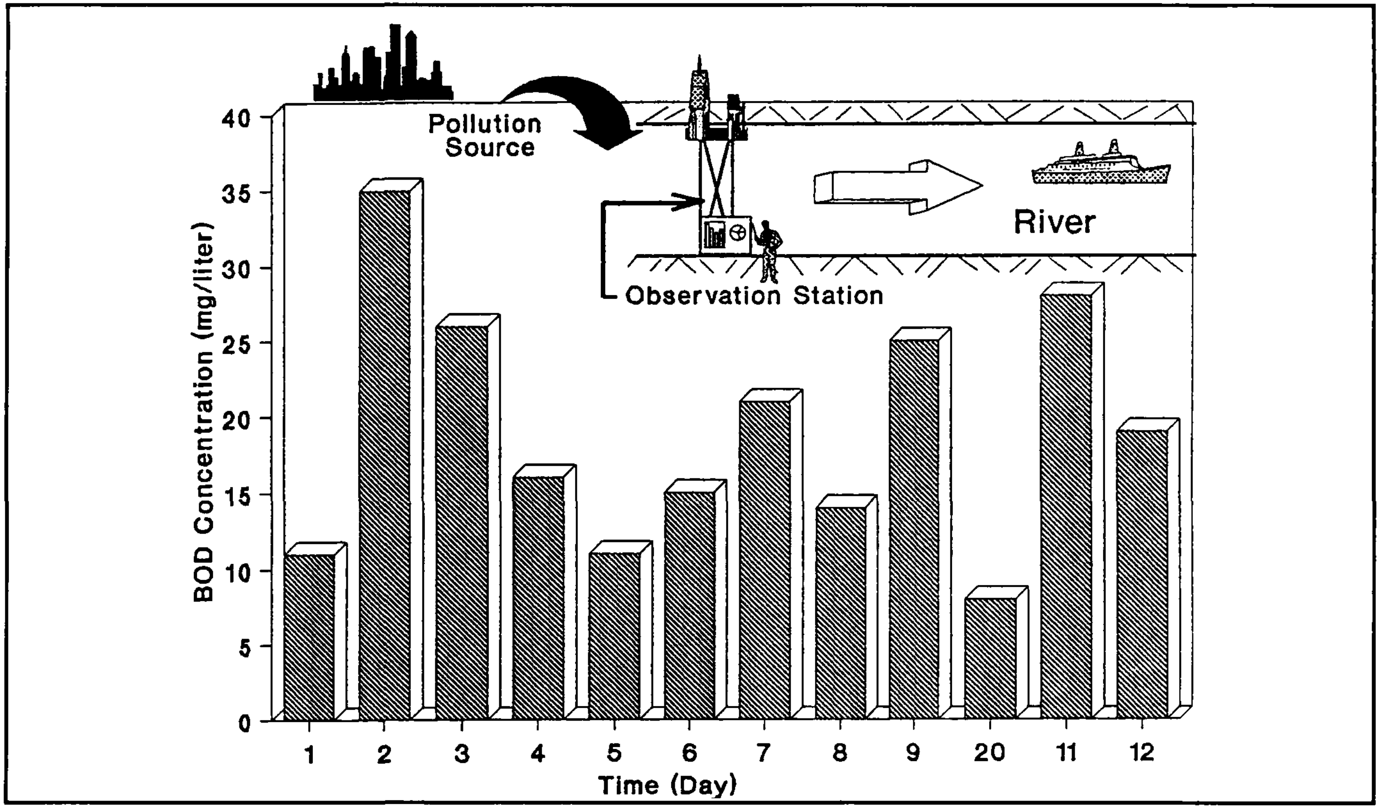


Figure 1. Example of readings at a station.

distance from the observation station. The following initial and boundary conditions may be used to solve equation (1):

$$C(x,0) = C_1 \tag{2}$$

$$C(0,t) = \sum_{i=0}^{n} \{ C[0,i\Delta T] - C(0,(i-1)\Delta T) \} \cdot H(t - i\Delta T) \tag{3}$$

$$\lim_{x \to \infty} C(x,t) = 0 \tag{4}$$

here n is the number of readings at the observation station (later, it will be shown that not all observations have to be considered as the maximum practical value of n is proportional to the memory length of the river), ΔT is the fixed observation time interval (T), C_1 is the initial BOD concentration along the river – a constant (ML^{-3}), $C(0,-\Delta T = 0$, and $H(t-i\Delta T)$ is the step function or the Heaviside function defined as

$$H(t-i\Delta T) = \begin{cases} 0, & t-i\Delta T < 0 \\ 1, & t-i\Delta T \geq 0 \end{cases} \tag{5}$$

For simplicity, let $C(0,-\Delta T) = 0$, and

$$\Delta C_i = C[0,i\Delta T] - C[0,(i-1)\Delta T], \; i = 0,1,2,...,n. \tag{6}$$

The upstream boundary condition given in equation (3) can be reduced to

$$C(0,t) = \sum_{i=0}^{n} \Delta C_i H(t-i\Delta T) \tag{7}$$

Solution to equation (1) with the boundary and initial conditions (2), (3), and (4) was obtained using the Laplace transform method. The derivation was, however, very lengthy. It was found later that the solution can be more easily obtained by the superposition method. If $\Delta C_i = 0$, i = 1, 2, . . . , n, and $C(0,0) = C_0$, where C_0 is some constant, then equation (7) reduces to

$$C(0,t) = C_0 \tag{8}$$

The solution of equation (1), along with the initial condition (2) and the boundary conditions (4) and (8), has been obtained by Van Genuchten and Alves [8]:

$$C(x,t) = C_1 \exp(-K_1 t)\left\{1 - \frac{1}{2}\, erfc\left[\frac{x-ut}{\sqrt{4Dt}}\right] - \frac{1}{2}\exp\left(\frac{ux}{D}\right) erfc\left[\frac{x+ut}{\sqrt{4Dt}}\right]\right\}$$
$$+ \frac{C_0}{2}\exp\left[\frac{ux}{2D} - \sqrt{\frac{\lambda}{D}}\,x\right] erfc\left[\frac{x}{\sqrt{4Dt}} - \sqrt{\lambda t}\right]$$

$$+\frac{C_0}{2}\exp\left[\frac{ux}{2D}+\sqrt{\frac{\lambda}{D}}x\right] erfc\left[\frac{x}{\sqrt{4Dt}}+\sqrt{\lambda t}\right] \tag{9}$$

where $\lambda = u^2/4D + K_1$, erfc[•] is the complementary error function, and exp[•] is the exponential function. If the boundary condition (8) changes to

$$C(0,t) = \Delta C_i H(t-i\Delta T) \tag{10}$$

and equations (1), (2), and (4) remain the same, then by comparison with equation (8) and using the definition of the step function, the corresponding solution can be obtained by replacing t in the second and third terms of equation (9) by (t-iΔT) and C_0 by $\Delta C_i H(t-i\Delta T)$,

$$c(x,t) = C_1 \exp(-K_1 t)\left\{1-\frac{1}{2} erfc\left[\frac{x-ut}{\sqrt{4Dt}}\right]-\frac{1}{2}\exp\left(\frac{ux}{D}\right) erfc\left[\frac{x+ut}{\sqrt{4Dt}}\right]\right\}$$
$$+\frac{\Delta C_i}{2}\exp\left[\frac{ux}{2D}-\sqrt{\frac{\lambda}{D}}x\right] H(t-i\Delta T)\cdot erfc\left[\frac{x}{\sqrt{4D(t-i\Delta T)}}-\sqrt{\lambda(t-i\Delta T)}\right]$$
$$+\frac{\Delta C_i}{2}\exp\left[\frac{ux}{2D}+\sqrt{\frac{\lambda}{D}}x\right] H(t-i\Delta T)\cdot erfc\left[\frac{x}{\sqrt{4D(t-i\Delta T)}}+\sqrt{\lambda(t-i\Delta T)}\right] \tag{11}$$

Because equations (1), (2), (4), and (7) are linear, the solution to equation (1) along with the boundary and initial conditions (2), (4), and (7) can be obtained by applying the method of superposition. This can be done by breaking up the given problem in equations (1) through (4) into n + 1 simpler problems:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2}-K_1 C$$

$$C(x,0) = C_1$$

$$C(0,t) = C(0,0)$$

$$C(\infty,t) = 0 \qquad \text{(problem 1)}$$

and

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2}-K_1 C$$

$$C(x,0) = 0$$

$$C(0,t) = \left\{C(0,i\Delta T) - C\left[0,(i-1)\Delta T\right]\right\} H(t-i\Delta T)$$

$$C(\infty,t) = 0$$

$$i = 1,2,\ldots,n, \quad \text{(problem 2 to problem } n+1\text{)}$$

Clearly, the sum of all these n + 1 problems is equivalent to the original problem. Solution to each of these problems is given by equation (11) where $C_1 = 0$ for problems 2 to n + 1. Summation of all of the n + 1 solutions yields the solution to the original problem defined by equations (1) to (4),

$$C(x,t) = C_1 \exp(-K_1 t) \left\{1 - \frac{1}{2} erfc\left[\frac{x-ut}{\sqrt{4Dt}}\right] - \frac{1}{2} \exp\left(\frac{ux}{D}\right) erfc\left[\frac{x+ut}{\sqrt{4Dt}}\right]\right\}$$

$$+ \frac{1}{2} \exp\left[\frac{ux}{2D} - \sqrt{\frac{\lambda}{D}}x\right] \sum_{i=0}^{n} \Delta C_i H(t - i\Delta T) \cdot erfc\left[\frac{x}{\sqrt{4D(t-i\Delta T)}} - \sqrt{\lambda(t - i\Delta T)}\right]$$

$$+ \frac{1}{2} \exp\left[\frac{ux}{2D} + \sqrt{\frac{\lambda}{D}}x\right] \sum_{i=o}^{n} \Delta C_i H(t - i\Delta T) \cdot erfc\left[\frac{x}{\sqrt{4D(t-i\Delta T)}} + \sqrt{\lambda(t - i\Delta T)}\right] \quad (12)$$

This equation is referred to as the new one-dimensional analytical model (N1AM). On the other hand, if the river is initially not contaminated so that the initial condition in equation (2) is given as

$$C(x,0) = 0 \quad (13)$$

then the solution of equation (1), subject to equations (4), (7), and (13), becomes

$$C(x,t) = \frac{1}{2} \exp\left[\frac{ux}{2D} - \sqrt{\frac{\lambda}{D}}x\right] \sum_{i=0}^{n} \Delta C_i H(t - i\Delta T) \cdot erfc\left[\frac{x}{\sqrt{4D(t-i\Delta T)}} - \sqrt{\lambda(t - i\Delta T)}\right]$$

$$+ \frac{1}{2} \exp\left[\frac{ux}{2D} + \sqrt{\frac{\lambda}{D}}x\right] \sum_{i=0}^{n} \Delta C_i H(t - i\Delta T) \cdot erfc\left[\frac{x}{\sqrt{4D(t-i\Delta T)}} + \sqrt{\lambda(t - i\Delta T)}\right] \quad (14)$$

For the simplest case, if the initial and boundary conditions are given by equations(4), (8), and (13), then equation (14) further reduces to

$$C(x,t) = \frac{C_0}{2} \exp\left[\frac{ux}{2D} - \sqrt{\frac{\lambda}{D}}x\right] erfc\left[\frac{x}{\sqrt{4Dt}} - \sqrt{\lambda t}\right]$$

$$+ \frac{C_0}{2} \exp\left[\frac{ux}{2D} + \sqrt{\frac{\lambda}{D}}x\right] erfc\left[\frac{x}{\sqrt{4Dt}} + \sqrt{\lambda t}\right] \quad (15)$$

Thus, equation (12) is the general solution and solutions given by equations (14) and (15) are special cases.

MEMORY TIME OF A RIVER

It may be noted that as the number of observations increases, application of equation (12) or (14) becomes cumbersome. However, some of the past observations may have no effect on the current BOD profiles. Thus, a segment of a river may have a finite memory with regard to the BOD input concentration at the upstream end of the segment. To make the discussion clear, recall that the slug input problem applying to a 1-D static pond is defined as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - K_1 C \tag{16}$$

$$C(x,0) = \frac{M}{A}\sigma(x) \tag{17}$$

$$C(x,t)_{x \to \infty} = 0 \tag{18}$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0} = 0, \tag{19}$$

where M is the total amount of pollutant mass (slug input), and A is the flow cross-sectional area of the river. The solution of this slug input problem can be easily obtained using the Laplace transform:

$$C(x,t) = \frac{M/A}{\sqrt{4\pi Dt}}\exp\left(\frac{x^2}{4Dt} - K_1 t\right) \tag{20}$$

At this point, the river memory length is defined. For a given error tolerance or significant level α, the river memory length, T_m, is the time period taken by the solute mass from the time t = 0 when it is introduced into the river at the upstream end instantaneously to the time that 100 (1 - α)% of the solute mass has disappeared from the river reach L due to advection, dispersion, and biochemical reactions (see Figure 2). Advection, dispersion, and decay reduce the amount of solute mass in the reach. Therefore, if the first-order decay term is neglected, then the computed memory length will be longer and form an upper bound. By neglecting the first-order decay term in equation (20), the upper-bound of the memory length of a given river segment can be written as

$$\frac{C(x,t)}{M/A} = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \tag{21}$$

Equation (21) has the form of a normal distribution with mean $\mu_x = 0$ and standard deviation $\sigma_x = (2Dt)^{0.5}$. Since the advection and dispersion mechanisms are not interactive for equation (1), the superposition method can be invoked to find the upper bound of the memory time. That is, a slug mass is poured into the river at the upstream end at time t = 0, and will be moved to position $x = X_m$ at time T_m with changed shape. This simultaneous process can be considered to be superposition of two steps. First, the slug input is moved to position $x = X_m$ due to advection, and second, the rectangular input shape changes to a normal-distributed shape due to dispersion. Referring to Figure 2, the memory time T_m can be defined as

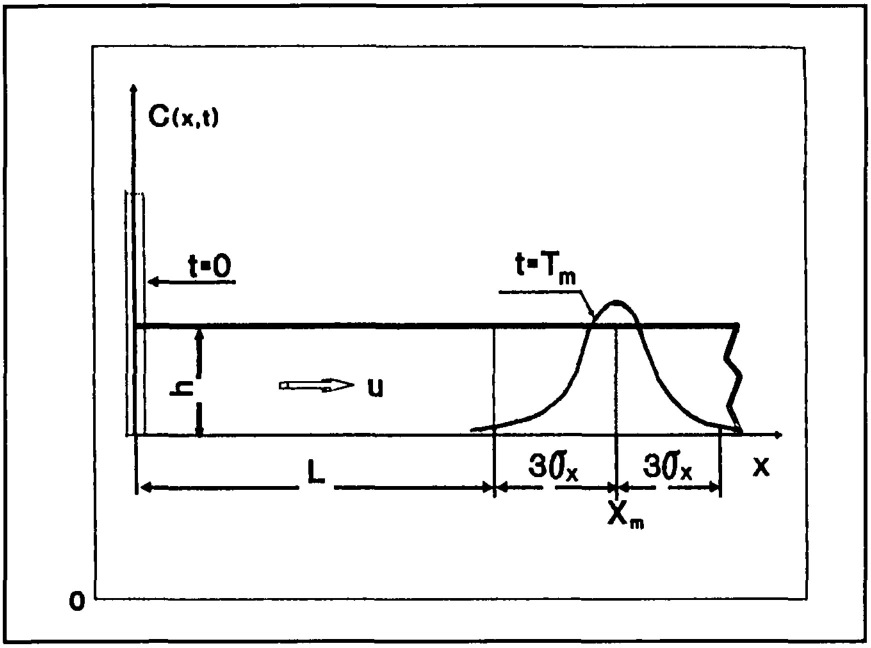


Figure 2. Estimation of river memory time by superposition method.

$$T_m = \frac{x_m}{u} \tag{22}$$

where X_m is the distance at which 100 (1 – α)% of the slug mass observed at the upstream end at t = 0 has disappeared from the river reach at time T_m. Let the error level (or significance level) be α = 0.001 which occurs three standard deviations away from the mean. Then

$$X_m = L + 3\sigma_x = L + 3\sqrt{2DT_m} \tag{23}$$

Substituting equation (23) into equation (22) and solving for T_m, one gets

$$T_m = \frac{uL + 9D + [(uL + 9D)^2 - L^2u^2]^{1/2}}{u^2} \tag{24}$$

T_m in equation (24) is the upper bound of the memory time for a given river for a given error tolerance of 0.001, because the first-order decay term is neglected in the calculation.

As an example, assume a river reach is L = 1.865 miles. The memory time for D = 50 ft^2/sec and u = 1 mile/day, is 142.4 hours and for u = 5 miles/day and D = 50 ft^2/sec is 15.37 hours. Thus, the value of n, defined in the boundary condition

(3), can be set to the next nearest integer of the computed $T_m/\Delta T$. It is seen from equation (24) that the upper bound of the memory time of a river is determined by the average river velocity, dispersion coefficient, and the river reach length. The model can be updated with the most recently recorded data at a finite memory time.

For assumed future BOD values at the observation station, the model can also be used to predict the river quality profiles. Since the basic solution given by Van Genuchten and Alves is an accurate solution for the initial and boundary conditions specified, it is expected that this model will retain the same accuracy if the observations are accurate and the observation interval is small enough [8]. Computations in the following two examples show that when $\Delta T = 1$ hour, the model yields rather accurate results as compared with some analytical solutions and numerical solutions.

PARAMETER ESTIMATION

The model has two parameters, D and K_1. These parameters can be estimated with observations using the Powell search method [11], which is a nonlinear optimization method and uses only the objective function values. The objective function can be defined as

$$F(D,K_1) = \frac{1}{n+m} \sum_{i=1}^{n} \sum_{j=1}^{m} [\, C(x_j,t_i) - C_0(x_j,t_i)]^2 \tag{25}$$

where $C(x_j,t_i)$ and $C_0(x_j,t_i)$ are the computed and observed BOD concentration values, respectively, at x_j and t_i, m is the number of observation points along the river, and n is the number of readings at each observation point. Given some initial values of D and K_1, the value of C(x,t) can be computed using equation (12). The nonlinear optimization technique can then find the set of parameters that minimize the objective function (mean square errors) given in equation (25).

ILLUSTRATIVE EXAMPLES

Example 1

As a comparison, the parameters used by Dresnack and Dobbins in their example 1 and their results obtained using a finite difference method, referred to as the DDM model, were used here [12]. In their example 1, they considered three different cases for the dispersive coefficient, D = 0, 150 and 1290 ft^2/sec, and gave $K_1 = 0$, u = 16 mile/day and the upstream boundary was $C(0,t) = 37 + 13\cos(2\pi t)$ PPM. The computed results, using N1AM, equation (12), for $\Delta T = 1$ hr, are given in Table 1. The computed BOD values, which are out best interpolated values from Figure 7 by Dresnack and Dobbins, are also given in Table 1. These results

Table 1. Comparison of Computed BOD Concentration Profiles between the DDM Model and the N1AM Model

Time (Hours)	X (Miles)	BOD Concentration (PPM)			
		Case 1		Case 2	
		N1AM	DDM	N1AM	DDM
120.00	4.00	35.34	37.0	35.85	37.0
120.00	8.00	24.62	24.5	27.37	27.5
120.00	12.00	38.73	37.0	37.38	37.0
120.00	16.00	48.95	48.8	44.19	44.2
120.00	20.00	35.35	37.0	37.07	37.0
120.00	24.00	25.48	25.5	31.65	32.0
120.00	28.00	38.60	36.5	36.69	36.5
120.00	32.00	48.13	48.0	40.97	40.8
120.00	36.00	35.48	36.5	37.43	36.5
120.00	40.00	26.28	25.9	34.10	34.6

Note: *Case 1*: D = 150 (sq. ft./sec.); *Case 2*: D = 1290 (sq. ft./sec.); DDM = finite difference Casemodel (Dresnack and Dobbins, 1968 [12]); N1AM = the new 1-D analytical model.

are plotted on Figure 3. It is seen from Table 1 and Figure 3 that the computed results by the two methods are almost identical, except slight deviations at the two ends of the given x range. Unfortunately, the BOD values between x = 0 and x = 4 miles were not given in Dresnack and Dobbins' paper and no comparison can be made for that practical range. In general, the analytical solution, equation (14), was found to be simple, accurate, and easy to apply as compared with the Dresnack and Dobbins model.

Example 2

To test the model of equation (12) with the analytical model of equation (15) under the boundary equation (8), let $K_1 = 0.25$/day, u = 16 mile/day, D = 50ft^2/sec, and $\Delta T = 1$ hour. Assuming the upstream BOD concentration is a constant, C(0,t) = 37 ppm. Computed results obtained by using equation (12) and (15) are virtually the same. BOD distribution profiles at t = 0.5, 1, 2, and 12 hours are plotted in Figure 4. It is clearly shown in Figure 4 that as t increases, the sharp front becomes widely spread due to the dispersion action and the maximum concentration declines linearly due to the first order reaction.

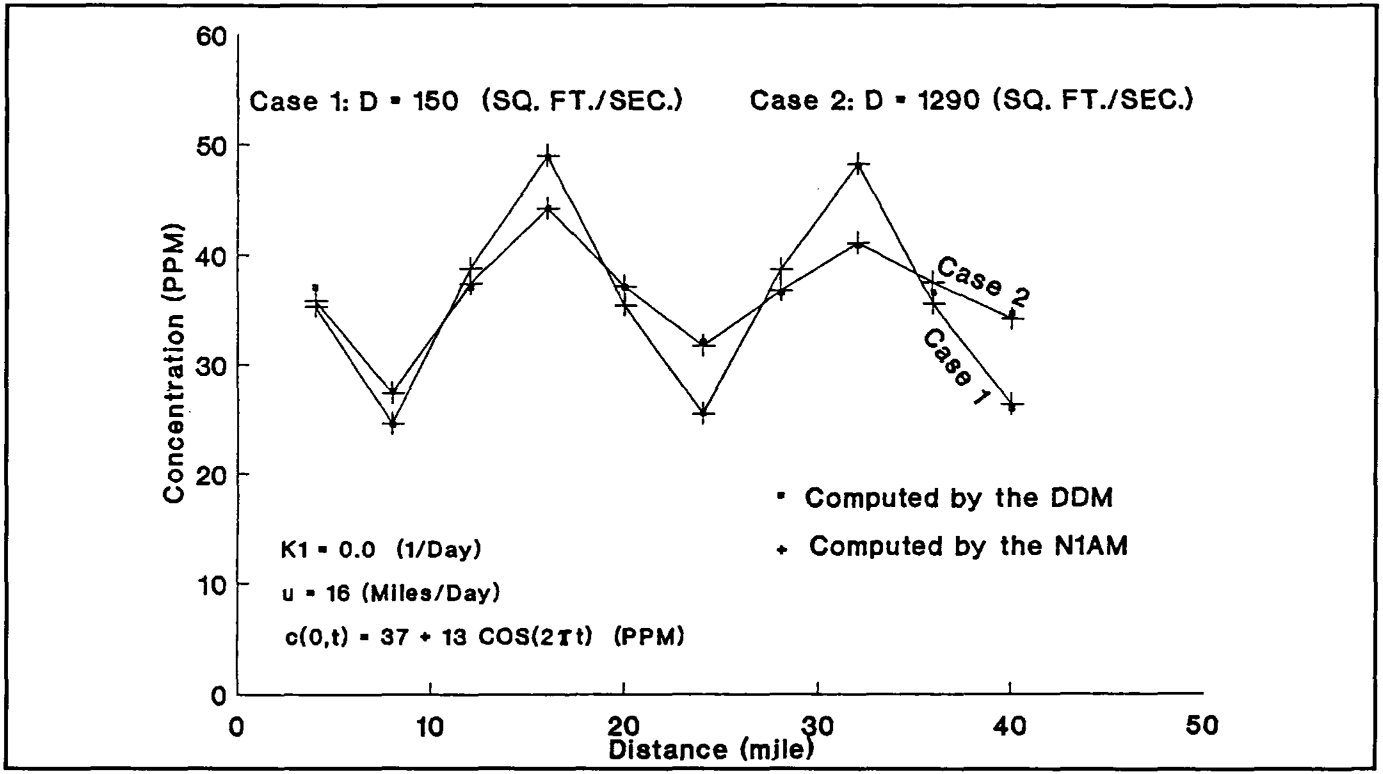
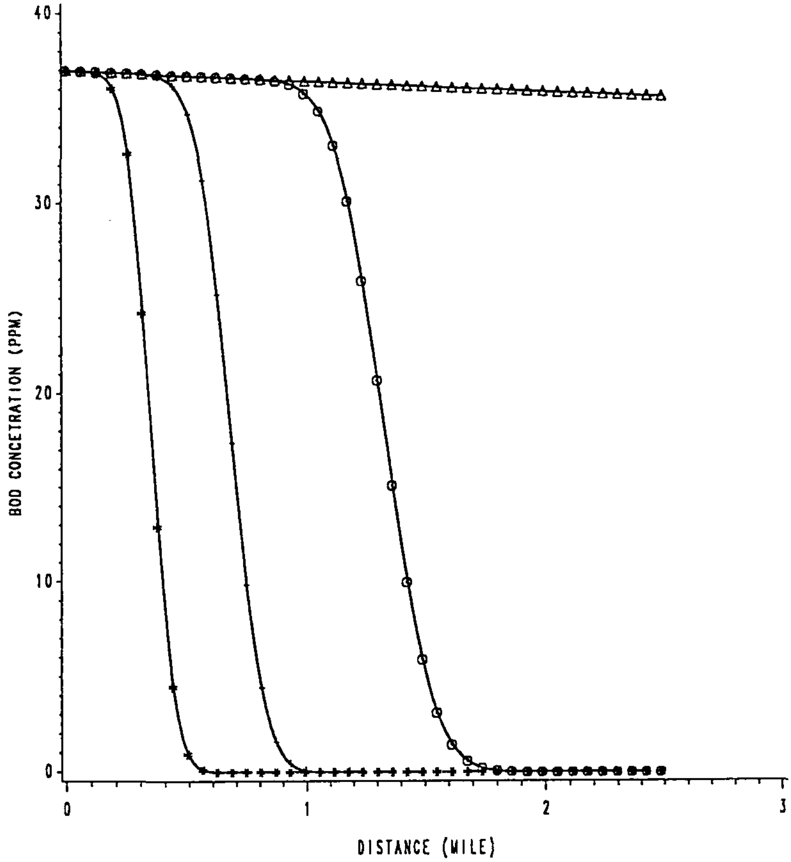


Figure 3. Computed concentration from Dresnack and Dobbins Model (DDM) [12] and the new one-dimensional analytical model (N1AM).

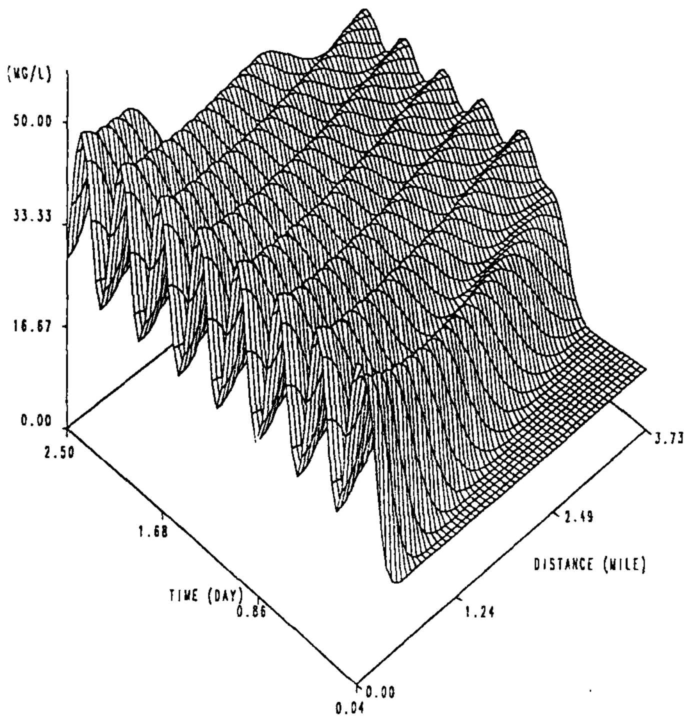


NOTE: TIME T = 0.5, 1, 2, 12 HOURS; U = 16 MILES/DAY; D = 50 FT^2/SEC; K_1 = 0.25 1/DAY; *T = 0.5; +T = 1; 0T = 2, ΔT = 12 HOURS.

Figure 4. BOD concentration profiles.

Example 3

To test the general model given by equation (12) and to illustrate the propagation of the source pollutant as a function of time and space, let K_1 = 0.25 day, D = 50 ft^2/sec, u = 5 mile/day, and ΔT = 1 hour. Assume sixty observations are available and are calculated by $C(0,t) = 37 + 13 \sin(6\pi t)$ (ppm), t is measured in days, and the initial BOD concentration is C_1 = 10 ppm. The BOD concentration values over time and space are plotted in Figure 5. If the average velocity changes to u = 1 mile/day and all other specifications are kept the same, then the BOD



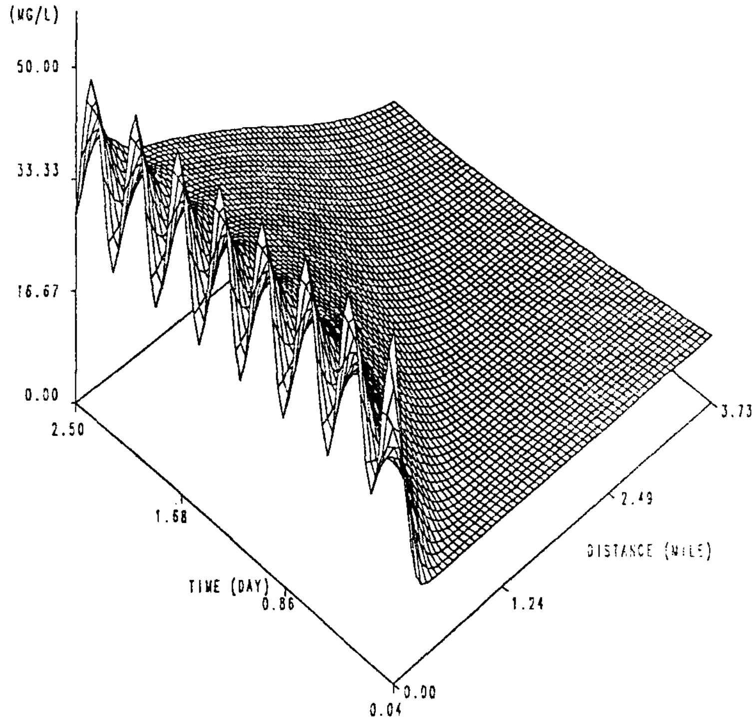
NOTE: K_1 = 0.25 1/DAY; D = 50 FT^2/SEC; U = 5 MILES/DAY; C_1 = 10 PPM, C(0,t) = 37 + 13 COS ($6\pi T$), PPM.

Figure 5. BOD concentration distribution.

concentration profiles are recalculated and plotted in Figure 6. Figures 5 and 6 clearly show that the advection velocity is the most important parameter affecting the BOD profiles in a given river. A memory time was not calculated in this example because the length of the river segment was not specified.

CONCLUSIONS

The model can be easily updated when new observations become available. This can be done through computer programming. Once a new observation is obtained, the first observation value in the previous input series will be dropped, and the new value inserted at the end of the series (a stack), and a new river quality profile for that time can be computed. On the other hand, by assuming some future



NOTE: K_1 = 0.25 1/DAY; D = 50 FT^2/SEC; U = 1 MILE/DAY; C_1 = 10 PPM, C(0,t) = 37 + 13 COS ($6\pi T$), PPM.

Figure 6. BOD concentration distribution.

BOD values at the upstream end, the future river quality profiles can be computed by using the assumed values. This would be very useful for predicting the effects of planned future activities.

The following conclusions are drawn from this study:

1. With the use of the method of superposition, a general solution to the 1-D advection-dispersion equation (ADE) was obtained and is given by equation (12). The solution can be applied to any type of Dirichlet boundary condition, especially for discrete time-dependent input values at the upstream boundary.

2. The analytical model can be used to simulate 1-D river quality problems accurately.
3. An upper-bound memory length of a river is defined. The finite memory definition permits easy updating of the N1AM model with availability of new information and easy forecasting of BOD profiles in a river for any planned future activities.

LIST OF SYMBOLS

A = cross-section area of a river (L^2)
ΔC = difference of BOD concentration between two observations (ML^{-3})
ΔT = constant interval between two observations (T)
σ_x = standard deviation of the variable x (L)
μ_x = mean of the variable x (L)
C = BOD concentration (ML^{-3})
C_0 = constant BOD concentration at the upstream end (ML^{-3})
C_1 = constant BOD concentration at t = 0 (ML^{-3})
D = dispersion coefficient (L^2T^{-1})
K_1 = first-order decay coefficient (T^{-1})
k = time step (T)
M = mass of the slug input (M)
n = number of observations
L = length of a river reach (L)
t = time (T)
T_m = memory time of a given river (T)
u = constant average velocity (LT^{-1})
x = distance from the upstream end (L)
X_m = memory length of a given river (L)
exp = exponential function
erfc = complementary error function

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