

# A Simplified Numerical Treatment of a Transient Water Quality Model

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## Introduction

Recent concern about the environment, has motivated a lot of interest in water quality modelling. Developments towards practical models are mainly due to Masden et. al. [1975], and Braun et al.[1974] among others. The first attempts to solve numerically the convection-dispersion (hitherto known as the CD equation) can be attributed to researchers like Price et. al. [1966], Guymon et al. [1970]. None of these researchers has been able to incorporate all the phenomena influencing solute transport as mentioned by Borden et al [1986]. In some simulations certain phenomena are totally omitted, whereas in others, essential phenomena are lumped together and represented by a simplified mathematical relationship.

In this study we consider the BOD-DO dynamics as a mass transport problem in an aquatic medium. Therefore it is necessary to combine the transport process with reaeration/decay process in a global model. In this regard, we consider the following physical processes:

- i)axial convective transport of mass
- ii)axial dispersion of mass (3) interaction between BOD and DO
- iii)reaeration and decay.

## Transport Model

Mathematical description of BOD-DO dynamics involves a set of coupled convective-dispersive equations. In the present study we adopt the approach described by Bear[1972] to write a set of one-dimensional CD equations for the BOD-DO dynamics with the inclusion of chemical reaction rates:

$$\frac{\partial B}{\partial t} + \frac{\partial (uB)}{\partial x} = \frac{\partial}{\partial x} \left( E_B \frac{\partial B}{\partial x} \right) - K_B B + L_B + \sum_{j=1}^M \frac{Q_j B_j^*}{A_j} \delta(x - x_j) \quad (1)$$

$$\frac{\partial DO}{\partial t} + \frac{\partial (uDO)}{\partial x} = \frac{\partial}{\partial x} \left( E_D \frac{\partial DO}{\partial x} \right) - K_B B + R_D + K_R (DO^{SAT} - DO) + \sum_{j=1}^M \frac{Q_j DO_j^*}{A_j} \delta(x - x_j) \quad (2)$$

where B : BOD concentration

DO: DO concentration

$DO^{SAT}$  : saturation DO concentration

$E_B$  : BOD dispersion coefficient

$E_D$  : DO dispersion coefficient

$K_B$  : BOD decay rate

$L_B$  : BOD distributed source

$K_R$  : Rearation rate

$R_D$  : DO distributed source

$u$  : stream velocity

$x$  : axial distance

$t$  : time

$Q_j$  : volumetric flowrate at  $j$

$DO_j^*, B_j^*$  : concentration of inflow loads BOD/DO at  $j$

$x_j$  : position of loading

$A_j$  : cross-sectional area of the stream or pipe at the load point

$M$  number of concentrated loads.

Equations (1) and (2) come from the averaging of a point equation over a cross-sectional area of a stream. The differential operator defined by both equations are not self-adjoint. Therefore the problem has no variational formulation and the FEM is formulated by applying the Galerkins procedure. Without any loss of generality we can specify:

$$c = \sum_{i=1}^N c_i \varphi_i(x) \quad (3)$$

where  $c$ ; approximate concentration

$N$ : number of nodes

$c_i$  : approximate value of  $c$  at node  $i$

$\varphi_i$  : interpolating function

Galerkin's procedure requires the minimization of the weighted residual with respect to the spatial dependence for each node  $i$ . The weighted residual is defined as

$$R_i = \int_{\Omega} L(c) \varphi_i(x) \quad (4)$$

where  $L$  is a differential operator. We elect to choose a linear approximation for the specie concentration inside each element, i.e.

$$c = c_{m1} + (c_{m2} - c_{m1}) \frac{(x - x_{m1})}{l_m} \quad (5)$$

where  $l_m = x_{m2} - x_{m1}$  is the length of an element  $m$ .

According to the definition of the interpolating function, contribution to the weighted residual only happens at the nodal points and since the second differential of the dependent variable is no longer defined, because of the linearity of the interpolating functions, we have to apply integration by parts to equation (4). A detailed analysis of the implementation of this procedure can be found in Zienkiewicz [1991].

The system of matrix equation resulting from the overall equation takes the form:

$$[\Phi]^* \left[ \frac{dc}{dt} \right] - [K][C] + [\omega] = [0] \quad (6)$$

where  $\Phi$  is the coefficient of the time term,  $K$  is the capacitance matrix and  $\omega$  takes care of all the sources and sink terms in the formulation. The solution of this system of linear algebraic equations yields the concentration profile at each node. It is worthwhile to point out that due to the presence of the first derivative of  $c$  in the differential equation, the coefficient matrix is not symmetric, but it is banded, this allows the use of a banded solver which reduces the processing time considerably.

Most finite element algorithms employ a mixed formulation in the discretization of space and time domains. While the space domain is handled by the FEM procedure, the finite difference is often used to approximate the time coordinate. While this approach could be effective for a vast array of problems; it could lead to stability problems where there are singularities and sudden changes in the time domain. Resolving the time term by an integral procedure would prove far superior to the differential approach of the finite difference technique in terms of robustness in handling singularities and stability considerations. Equation (6) represents a first order differential equation in matrix form. As pointed out, we will adopt a one step Galerkins procedure to resolve its transient component.

Applying the FEM to equation (6) between  $t = 0$  and  $t = t_f$  yields:

$$[R_t] = \int_0^{t_f} \left( [\Phi]^* \left[ \frac{dc}{dt} \right] - [K]^* [C] + [\omega] \right) \eta_t \quad (7)$$

where  $\eta_t$  is the time approximating function. Galerkins procedure requires that

$$[R_t] = 0 \quad (8)$$

A linear approximation of the dependent variable with respect to time yields:

$$[c] = [c_0] + ([c_f] - [c_0]) \frac{t}{t_f} \quad (9)$$

where  $[c_0]$  and  $[c_f]$  are approximate values of the dependent variable at  $t = 0$  and  $t = t_f$  respectively. Substituting equation (9) into equation (7) yields:

$$\int_0^{t_f} \left( [\Phi] \left( [c_f] - [c_0] \right) \frac{1}{t_f} + [\omega] - [K]^* [c_0] - [K]^* \left( [c_f] - [c_0] \right) \right) \frac{t}{t_f} = 0 \quad (10)$$

performing the required integration yields:

$$[\zeta_A] [c_f] = [\zeta_B] [c_0] - [\omega] \quad 27 \quad (11)$$

where:

$$[\zeta_A] = \frac{[\Phi]^*}{t_f} - \frac{2}{3} [K]^* \quad 28 \quad (12)$$

$$[\zeta_B] = \frac{[\Phi]^*}{t_f} + \frac{1}{3} [K]^* \quad 29 \quad (13)$$

If we generalize for an interval  $\Delta t = t_m - t_{m-1}$  30 we obtain:

$$[\zeta_A]^M [c_m] = [\zeta_B]^M [c_{m-1}] - [\omega]^M \quad 31 \quad (14)$$

with:

$$[\zeta_A] = \frac{[\Phi]}{\Delta t} - \frac{2}{3} [K]^M \quad 32 \quad (15)$$

and:

$$[\zeta_B]^M = \frac{[\Phi]^*}{\Delta t} + \frac{1}{3} [K]^M \quad 33 \quad (16)$$

Equation (14) can be put in the form:

$$[\zeta_A] [c_m] = [\psi]^* \quad 34 \quad (17)$$

where  $[\psi]^*$  35 is a vector of known quantities. Equation (17) represents a time marching procedure that will generate the concentration profile starting from an initial condition. Since the BOD concentration appears as a variable in both equations, equation (1) must be solved first. Once  $B(x,t)$  is known,  $K_B$  36 is then considered a source term function of  $x$  and  $t$ .

Since the approximation of the BOD concentration is linear in  $x$ , and  $t$ , the arithmetic mean of BOD concentration is used to evaluate the DO source term which is used for the solution of equation (2).

For transient variation, the DO source terms are calculated by:

$$S_{DO} = -K_{BM}^n \frac{(B_M^n + B_M^{n-1})}{2} + R_{DM}^n + K_{RM}^n DO^{SATn} \quad 37 \quad (18)$$

A numerical scheme such as the one proposed here must be tested for convergence to be

proven reliable. To accomplish this, comparisons were made between analytical and numerical solutions which should allow for the mathematical validation of the method. We consider the following differential equation which incorporates sources and sinks, whose analytical solution is known

$$\frac{D^2 C}{dx^2} - 2C + 0.5 = -\delta(x) \quad -5 \leq x \leq 15 \quad (19)$$

The differential equation is solved straightforwardly to obtain:

$$\begin{aligned} C &= 0.005053e^{-x} + \frac{1}{3}e^{2x} + 0.25 \quad -5 \leq x < 0 \\ C &= 0.33839e^{-x} + 0.25 \quad 0 \leq x \leq 15 \end{aligned} \quad (20)$$

The solution displayed in table 1 shows an excellent agreement between the analytical and numerical results.

## Model Application and Conclusions

The model is applied to simulate the concentration profiles of BOD and DO in a river network. Data for coefficients and stream dimensions were taken from O'Laoghaire [1978] and the values of the dispersion coefficients are within the range suggested by Beltaos [1980] (Table 2). The physical configuration of the river network and the node numeration are shown in fig.1. Two wastewater treatment plants provide the source of concentrated loads of BOD to the system. Note that no specifications were made for the downstream. This implies that we are assuming that the last reach is long enough for the flux of concentration to be zero. The network was simulated with 250 nodes.

The initial concentrations are given by:

$$\text{IC: BOD} = 0.5 \text{ g/m}^3 \text{ } ^{40} \quad , \quad \text{DO} = 7.0 \text{ g/m}^3 \text{ } ^{41}$$

at all points in the stream network. In addition, we impose a requirement which specifies that the concentration of BOD in the waste load from the wastewater treatment plant will increase from  $300 \text{ g/m}^3$  <sup>42</sup> to  $350 \text{ g/m}^3$  <sup>43</sup>. Furthermore at  $t=10$  days a new wastewater treatment plant will go into operation according to the characteristics shown below:

$Q_i (\text{m}^3/\text{d})=5000$   $A_i (\text{m}^2)=500$   $\text{BOD}_i^* (\text{g/m}^3)=150$   $\text{DO}_i^* (\text{g/m}^3)=0.44$  . The plant is located at  $x = 20000\text{m}$  and  $y = 4580\text{m}$ .

Fig. 2 shows the dynamic BOD profiles at various points along the x axis of the stream reach. It clearly portrays the problem specifications. The net effect of the new treatment plant is to increase the BOD concentration. The model is sensitive enough to reflect the high concentration gradient brought about by the sudden changes in solution profiles at  $t=10$  days, and the effects of the already existing ones. We can observe the sudden rise of BOD concentration due to the imposition of BOD load by WWTP1 (wastewater treatment plant 1) located 10 kilometers from the origin. The effect of the fresh water source due to an inflowing stream located 20 kilometers from the source is to bring down the level of BOD. This downward trend in BOD concentration could have continued had it not been for the imposition of a third plant almost at the source of the inflowing stream. The cup shaped portion of fig. 2 characterizes the high concentration gradient brought about by this sudden load change and the overall effect of the WWTP2. The rest of the curve displays an exponential decay in response to the no flux boundary condition at the downstream.

Fig. 3 displays the DO concentration. We observe that the changes introduced at  $t=10$  days reduce the minimum DO concentration from  $5.2 \text{ g/m}^3$  <sup>45</sup> to  $4.5 \text{ g/m}^3$  <sup>46</sup>. The implication of this to the environment should be obvious.

The second example deals with the simulation of BOD-DO dynamics with the following physical properties:

$$u = 1, E_B = E_D = 1, L_B = 0.5, K_B = 2.0, E_B = 1.0, R_D = -0.2, K_R = 1.5 \text{ and } DO^{SAT} = 3.0.$$

$$\text{Boundary Conditions: } B(x=-5, t) = DO(x=-5, t) = 1.0 g/m^3 \quad 47$$

$$\frac{\partial B}{\partial x}(x=15, t) = \frac{\partial DO}{\partial x}(x=15, t) = 0 \text{ g/m}^3 \quad 48 \quad (21)$$

Initial Conditions:

$$BOD(x, 0) = DO(x, 0) = 1.0 g/m^3 \quad 49 \quad (22)$$

A concentrated load is imposed at  $x = 0$ , and  $t = 0.75$  days with the following magnitudes.

$$\left( \frac{Q_1 B_1^*}{A_1} \right)_B = 1.0 g/m^3 \quad 50$$

$$\left( \frac{Q_1 DO_1^*}{A_1} \right)_{DO} = 0.5 g/m^3 \quad (23)$$

Fig. 4 illustrates the DO dynamics for this example. Observe the effect of an introduction of concentrated load on the DO profile at  $t = 0.75$  days and  $x = 0$  meters. it brings up the level of DO especially at those points closest to the point of introduction. The gradient of the DO concentration is highest around the region very close to the point of loading. The same could be said of the BOD profile of fig. 5. The results react satisfactorily to the problem specifications. Furthermore the point  $x = 0$  shows a considerable sensitivity to concentrated loads.

This study has explored the use of a simultaneous space-time finite element discretization for the solution of coupled equations of BOD-DO dynamics for a river network. The model was numerically checked by comparing the results obtained from the solution of a differential equation with those obtained analytically. Based on the results obtained from simulation tests, the model could be said to be reliable, and to have the potential of modelling transient water quality constituents in an aquatic system.

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Table 1: Comparison of Numerial and Analytical Results.

Node	C	C exact
1	1.000	1.000
2	0.774	0.775
3	0.616	0.617
4	<b>0.306</b>	0.507
5	0.419	0.420
6	0.375	0.376
7	0.338	0.339
8	0.313	0.314
9	0.297	0.298
10	0.288	0.290
11	0.288	0.290
12	0.300	0.304
13	0.337	0.340
14	0.411	0.420
15	0.525	0.588
16	0.366	0.374
17	0.291	0.296
18	0.265	0.267
19	0.275	0.256
20	0.252	0.252
21	0.251	0.261
22	0.250	0.250
23	0.250	0.250
24	0.250	0.250
25	0.250	0.250
26	0.250	0.250
27	0.250	0.250
28	0.250	0.250
29	0.250	0.250
30	0.250	0.250

Table 2: Stream data and Coefficients

REACH	E (m <sup>2</sup> /d)	u(m/d)	l <sub>R</sub> (m)	K <sub>B</sub> (d <sup>-1</sup> )	L <sub>B</sub> (g/m <sup>3</sup> d)	K <sub>R</sub> (d <sup>-1</sup> )	DO(SA T) g/m <sup>3</sup>	R <sub>D</sub> g/m <sup>3</sup> d
1	3*10 <sup>6</sup>	10000	10000	0.45	0.15	0.45	10.0	0.20
2	3*10 <sup>6</sup>	10000	10000	0.45	0.15	0.45	9.8	0.20
3	9*10 <sup>5</sup>	6000	10000	0.60	0.30	0.30	9.5	0.00
4	2*10 <sup>6</sup>	8000	5000	0.50	0.60	0.60	8.8	0.10
5	2*10 <sup>6</sup>	8000	30000	0.50	0.60	0.60	8.8	0.10

**Upstream specifications:**

Reach no.1: B(mg/l) = 1.5 , DO(mg/l) = 8.8

Reach no. 2: B(mg/l) = 0.8, DO(mg/l) = 9.0

**Concentrated loads:**

Treatment plant no. 1 :  $Q_i$  (m<sup>3</sup>/d)= 11350,  
 $A_i$  (m<sup>2</sup>)=300 ,  $BOD_i^*$  (g/m<sup>3</sup>) ,  $DO_i^*$  (g/m<sup>3</sup>)=0 51

no. 2 :  $Q_i$  (m<sup>3</sup>/d) = 80000  
 $A_i$  (m<sup>2</sup>)=500 ,  $BOD_i^*$  (g/m<sup>3</sup>)=200 ,  $DO_i^*$  (g/m<sup>3</sup>) =0 52

Fig.1: Node Numeration and Coordinate System.

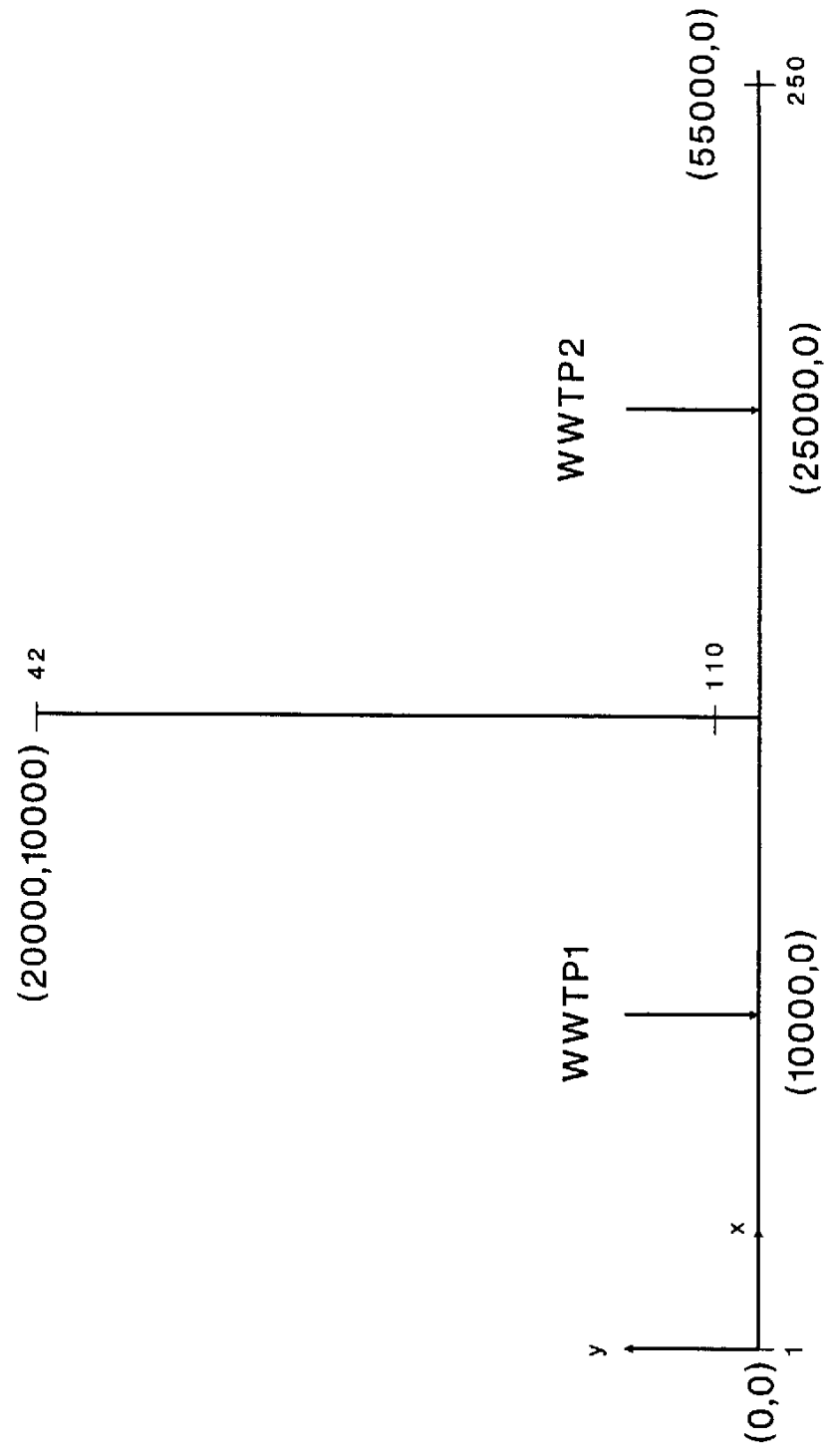


Fig.2: Dynamic BOD profiles

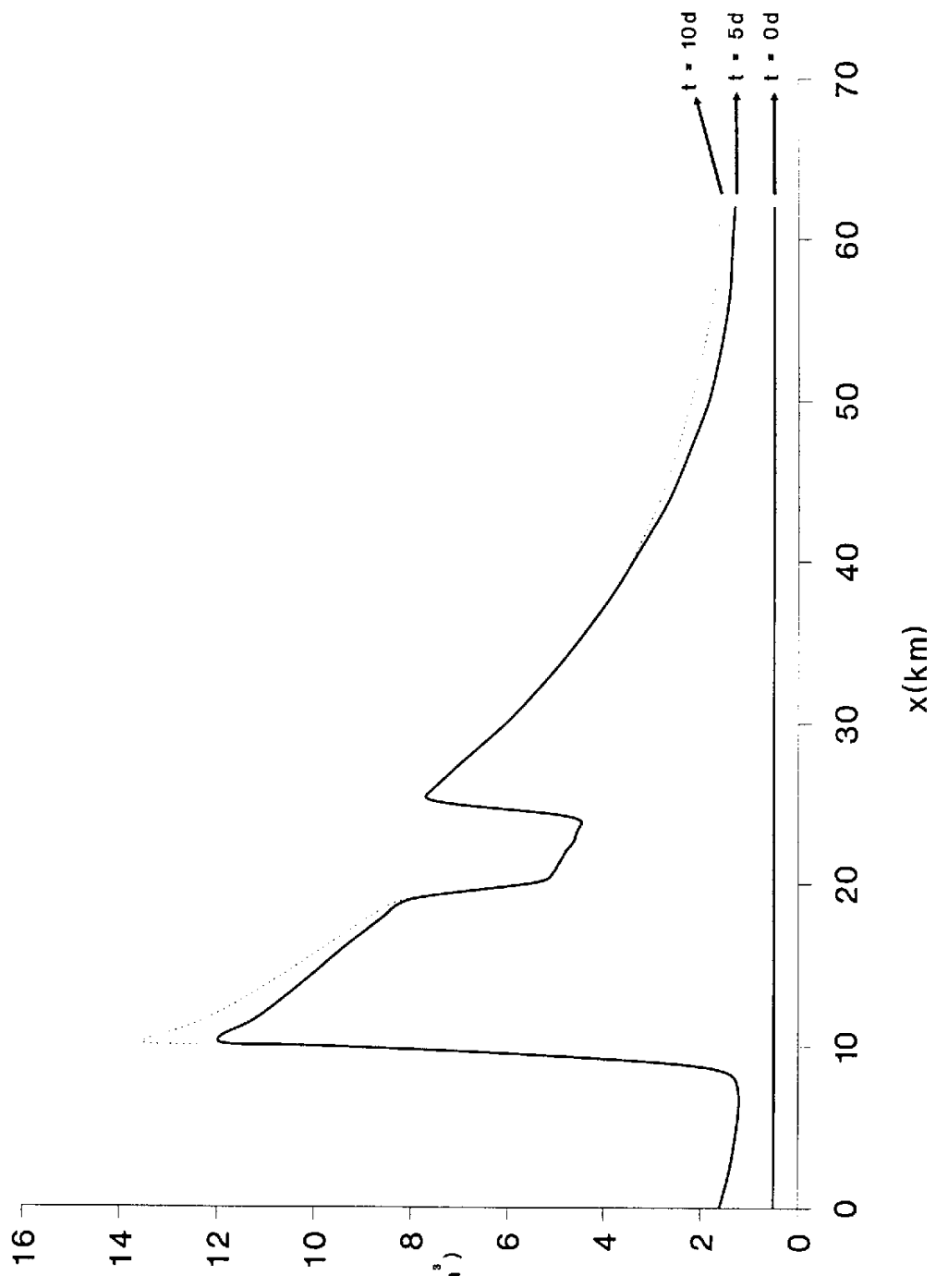


Fig.3: Dynamic DO Profiles

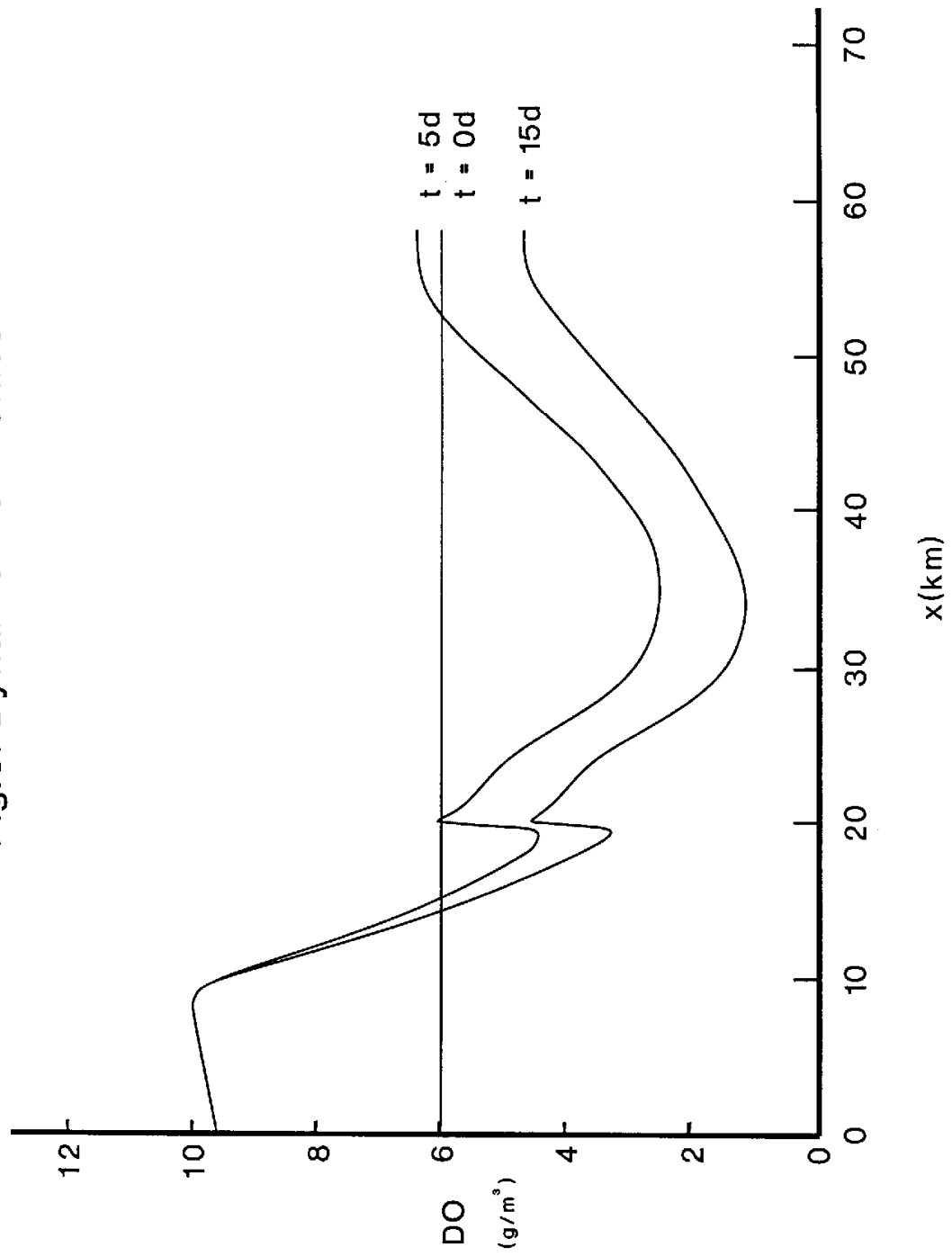


Fig.4: DO Dynamics

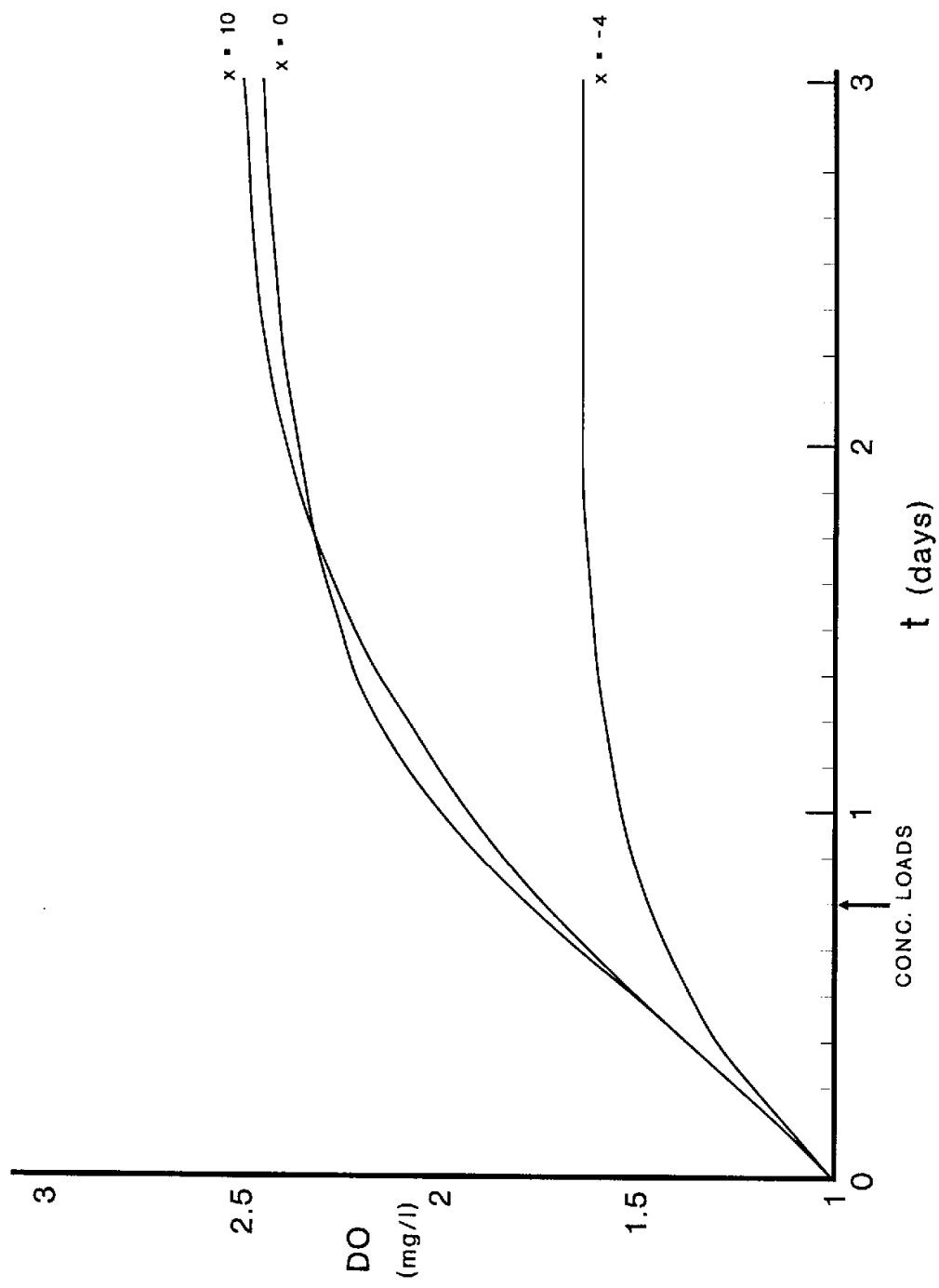


Fig.5: BOD DYNAMICS

