

Mathematical Modeling and Simulation for Predicting DO Condition in Rivers

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Abstract- The use of mathematical models to assess the pollution level in water bodies is widely accepted by environmental engineers as well as the managers involved in planning of the existing water resources. Various one dimensional models that are developed so far are applicable only after complete mixing of the pollutant across the cross-section is over which may take longer time for rivers with large width. Such type of situation is not represented effectively by various existing one dimensional models. Moreover, many of these one dimensional models do not account for the settle able part of Biochemical Oxygen Demand (BOD) that invariably takes place when partially treated/untreated waste enters these water bodies. A model that is not more complicated than a one dimensional model but rationally predict the Dissolved Oxygen(DO) conditions in almost 80% of mixing period is presented which can be used in conditions when partially treated/untreated waste is discharged in water body.

Keywords- Mathematical Model; DO; BOD; Water Pollution

I. INTRODUCTION

Clean water is absolutely essential for a healthy living. Pollution of river bodies has become a major global problem that is more critical in developing nations of the world due to inadequate measures to protect the surface water quality. All kinds of wastes (domestic, industrial, agricultural and others) are often discharged into the surface water bodies like lagoons, rivers and streams with little or no regard to their assimilative capacities. A wide variety of water quality variables is affected by various human activities while interacting with the water bodies. Dissolved oxygen (DO) of the river is one such parameter that is often used to measure the effect of pollution on the river. The biodegradable contaminants in water are quantified in terms of BOD, a parameter most related to DO. Both these parameters together are useful in tracing the pollution conditions and natural purification abilities of river and in determining permissible level of organic pollutants discharged in to the water bodies.

The DO conditions in a river are provided by appropriate mathematical models relating the BOD-DO concentrations after the discharge of organic pollutants in a water body.

River water quality modelling has a long history that dates back to the pioneering work of Streeter and Phelps [1]. The classical Streeter and Phelps (S-P) model describes the bacterial decomposition of organic carbon characterized by BOD and its impact on DO conditions. The S-P model does

not, however, account for the settle able BOD which constitutes a significant portion of the total BOD inputs through the wastewater outfalls into a river. Moreover, the assumption that advection is the only relevant transport mechanism, unnecessarily restricts the model's validity in the present era of excellent computing capabilities of digital computers.

Bhargava [2-5] presented a model for accurate prediction of DO due to disposal of waste containing settle able as well as dissolved part of BOD. The model suggest that settle able part of BOD is removed obeying the linear settling law along with simultaneous first order exponential decay of non settle able and dissolved portion of BOD.

Various one dimensional models predicting DO conditions in rivers are cited in literature [6-13] but these models are not valid in initial period. These models are capable to predict the concentration of BOD and DO only after the mixing length is over, a fact that is usually ignored and the model is used to calculate the BOD and DO values immediately after the point of discharge of pollutant. In reality, mixing takes some time to complete which may be longer for rivers with large width.

Apart from this limited factor, various models developed to date assume the pollutant to be in dissolved form only which is again an irrational assumption for the situations where a significant amount of the organic pollutant is in settle able form. Such situation arises particularly in developing countries where untreated/partially treated wastewater is discharged into the rivers due to ignorance/negligence of the people or costly equipments for wastewater treatment. In reality, a part of BOD in the wastewater is always in settle able form. Further, another part present in a colloidal form converts into a settle able form due to coagulation and flocculation attainable in the rivers [2].

Tyagi et al [14] developed a one-dimensional model that takes into account the effect of both types of BOD (settleable as well as dissolved) on river's DO, but this model is also applicable only after the mixing length is over. Various complex two-dimensional models [15-18] are also available but they need a considerable amount of hydraulic data which in many cases is not available and has to be assumed. Rough estimation of parameters may lead to a partial loss of accuracy gained through the multi-dimensional models.

An enhanced one dimensional model is proposed by Reichert and Wanner [19] that is capable of predicting substance distribution for about 80% of the initial period. In the presented work, the model presented by Reichert and Wanner is modified to predict BOD-DO conditions in river due to a discharge of organic waste containing both types of BOD namely settle able and dissolved types.

II. MODEL DEVELOPMENT

The cross-section of the river is divided into two zones namely advective zone in the centre of the river and stagnant zone along the two banks where the velocity is almost zero. A mathematical model is developed for the above stated river system based on the following assumptions:

- The entire BOD is in two forms namely settleable as well as dissolved forms. The dissolved part of BOD is decaying according to first order kinetics while the settle able part is being removed by linear law.
- The size of stagnant zone is αA_T and it consists of two parts located near the river banks while the size of advective zone is $(1-\alpha) A_T$, where A_T is the area of cross-section of the river and α is fraction of wetted cross-sectional area of the stagnant zone however for the sake of simplicity we are taking $\alpha A_T = A_s$ and $(1-\alpha) A_T = A$.
- No transverse gradient exists within any of the two zones but there is exchange of mass between the two zones (viz. advective and stagnant) which is related to the difference in the respective concentration.
- In stagnant zone, only exchange of mass with the advective zone and reaction are considered.
- In advective zone, advection, reaction and exchange of mass are considered.
- The effect of reaeration, modeled according to Henry's law, is considered in both the zones.
- The whole pollutant is being released into the advective zone only.

On the basis of the above assumptions the following equations representing the BOD mass balance equation in advective zone and stagnant zones are developed as follows:

A. Advective Zone

$$L = \begin{cases} L_o \left(1 - \frac{v}{d} \cdot \frac{x}{u} \right); & x < x_1 \\ 0 & ; x \geq x_1 \end{cases} \quad (1)$$

$$0 = -u \frac{dB_d}{dx} - kB_d - \frac{\gamma}{A} (B_d - B') \quad (2)$$

$$0 = -u \frac{dC}{dx} - mL - kB_d - \frac{\gamma}{A} (C - C') + k_r (C_s - C) \quad (3)$$

B. Stagnant Zone

$$0 = \frac{\gamma}{A_s} (B_d - B') - kB' \quad (4)$$

$$0 = \frac{\gamma}{A_s} (C - C') - kB' + k_r' (C_s' - C') \quad (5)$$

Where L = concentration of settleable BOD in advective zone; L_0 = concentration of initial settle able BOD in advective zone; u = average cross-sectional velocity in the advective zone (L/T); v = settling velocity of settle able BOD in advective zone (L/T); x = distance in flow direction (L); d = depth of stream in advective zone (L); x_1 = distance in advective zone where settle able part is completely removed; B' = concentration of BOD in stagnant zone (M/L³); B_d = concentration of dissolved BOD in advective zone (M/L³); γ = exchange coefficient per unit length (L²/T); k = decay rate of dissolved BOD (T⁻¹); A = cross-sectional area of the advective zone; A_s = cross-sectional area of the stagnant zone; k_r = coefficient of reaeration in advective zone (T⁻¹); m = removal rate of settle able BOD in advective zone (T⁻¹); k_r' = coefficient of reaeration in stagnant zone (T⁻¹); C = concentration of DO in advective zone (M/L³); C' = concentration of DO in stagnant zone (M/L³); C_s' = concentration of DO at saturation level in stagnant zone (M/L³); C_s = concentration of DO at saturation level in advective zone (M/L³);

The BOD in an advective zone is considered in two parts settle able as well dissolved and it is evaluated separately in Eq. 1 and Eq. 2. Eq. 1 gives the decay of settle able BOD while Eq. 2 represents the decay of dissolved BOD respectively with distance downstream. Eq. 1 suggests that the settle able part gets removed at a distance $x = x_1$ after which this does not take any oxygen from the river. This distance will be longer for deeper rivers and for smaller flocculated particle size. The combined effect of both the parts of BOD on DO is given by Eq. 3.

Since it is assumed that the settle able part gets settled at the outfall itself due zero velocity in stagnant zone, Eq. 4 gives the concentration of dissolved BOD only. Eq. 5 represents the effect of BOD on DO in stagnant zone.

C. Boundary Conditions

The associated boundary conditions reflecting the release of the pollutants according to assumption mentioned above:

$$B_d = B_{o-d} \text{ and } C = C_s \text{ at } x = 0$$

III. METHOD OF SOLUTION

Eq. 1 is solved independently and the value of L is obtained at various distances downstream. To solve Eq. 2 we need the value of B' which is obtained from Eq. 4 and Eq. 4 gives the value of B' in terms of B_d which when substituted

in Eq. 2 gives a first order differential equation in B_d which is solved by variable separable method. Solution of Eq. 3 requires the value of B_d , L and C' in terms of x . The values of L and B_d are supplied by Eq. 1 and Eq. 2 respectively. However, Eq. 5 is used to get the value of C' in terms of C . Since Eq. 5 contains B' also, solution of Eq. 4 is required prior to the solution of Eq. 5. After substitution of the values of L , B_d and C' in Eq. 5 we get a Leibnitz linear differential equation of first order in C .

The above mentioned steps are shown here for further clarification.

For $x < x_1$, solving Eq. 4 we get

$$B' = \frac{\gamma/A_s}{\left(\gamma/A_s + k\right)} B_d$$

or

$$B' = \frac{\beta'}{(\beta' + k)} B_d, \text{ where } \beta' = \frac{\gamma}{A_s}$$

(6)

Using Eq. 6 in Eq. 2 we get

$$0 = -u \frac{dB_d}{dx} + [-kB_d] - \beta' \left(B_d - \frac{\beta'}{(\beta' + k)} B_d \right)$$

where $\beta = \frac{\gamma}{A}$

Or

$$\frac{dB_d}{\partial x} = -\frac{k + \delta}{u} B_d \text{ where, } \delta = \frac{\beta k}{(\beta' + k)}$$

Or

$$\frac{dB_d}{\partial x} = -\mu B_d$$

Where $\mu = \frac{k + \delta}{u}$

(7)

Using the boundary condition $B_d = B_{o-d}$ at $x = 0$, Eq. 7 can be solved as

$$B_d = B_{o-d} \exp(-\mu x) \quad (8)$$

Therefore the total BOD in the advective zone is represented by the following equation:

$$\begin{cases} B = B_d + L & x < x_1 \\ = B_d & x \geq x_1 \end{cases} \quad (8a)$$

Using Eq. 8 in Eq. 6, we get

$$B' = \eta B_{o-d} \exp(-\mu x), \text{ where } \eta = \frac{\beta'}{\beta' + k} \quad (9)$$

Using Eq. 9 in Eq. 5

$$C = \frac{\beta'}{\beta' + k'} C - \frac{k\eta}{\beta' + k'_r} B_{o-d} \exp(-\mu x) + \frac{C'_s k'_r}{\beta' + k'_r} \quad (10)$$

Using Eq. 10 in Eq. 3, we get

$$\left. \begin{aligned} \frac{dc}{dx} + \frac{k_r + \xi}{u} C = & -\frac{kB_{o-d}}{u} \exp(-\mu x) \left(1 + \frac{\eta\beta}{\beta' + k'_r} \right) \\ & + \frac{mL_o v}{u^2 d} x + \frac{k_r C_s + \xi C_s - mL_o}{u} \end{aligned} \right\} \quad (11)$$

Where $\xi = \frac{\beta k'_r}{(\beta' + k'_r)}$

Eq. 11 is a Leibnitz linear equation with integrating factor equal to $\exp\left(\frac{(k_r + \xi)}{u} x\right)$

Solving Eq. 11 with boundary conditions $C = C_s$ at $x=0$ we get:

$$C = -\left(k\eta B_{o-d} \right) \left[\exp(-\mu x) - \exp\left(-\frac{(k_r + \xi)}{u} x\right) \right] + \frac{mL_o v x}{u d (k'_r + \xi)} - \frac{mL_o v}{d (k'_r + \xi)^2} \left[1 - \exp\left(-\frac{(k'_r + \xi)}{u} x\right) \right] + \frac{k_r C_s + \xi C'_s - mL_o}{(k_r + \xi)} \left[1 - \exp\left(-\frac{(k'_r + \xi)}{u} x\right) \right] + C_s \exp\left(-\frac{(k'_r + \xi)}{u} x\right), \quad (12)$$

where $\nu = \frac{(\beta' + k'_r + \eta\beta)}{(\beta' + k'_r)(k_r + \xi - \mu u)}$ and $x < x_1$

Using Eq. 12 in Eq. 10 we can get the value of C' .

When, $x \geq x_1$ omitting the term corresponding to settle able part from Eq. 10 and using in Eq. 3 we get

$$\frac{dc}{dx} + \frac{(k_r + \xi)}{u} C = -\frac{kB_{o-d}}{u} \left(\frac{(\beta' + k'_r + \eta\beta)}{(\beta' + k'_r)} \right) \exp(-\mu x) + \frac{k_r C_s + \xi C'_s}{u} \quad (13)$$

Integrating factor for Eq. 13 is given by

$$\exp\left(\frac{(k_r + \xi)}{u} x\right)$$

Solution of Eq. 13 with boundary conditions given by $C = D$ at $x = x_1$, we get

$$C = -\left(k_v B_o - d\right) \exp(-\mu x) - \exp\left(\frac{\left(k_r + \xi\right)\left(x_1 - x\right)}{u} - \mu x_1\right) + \frac{k_r C_s + \xi C'_s}{\left(k_r + \xi\right)} \left[1 - \exp\left(\frac{\left(k_r + \xi\right)\left(x_1 - x\right)}{u}\right)\right] + D \exp\left(\frac{\left(k_r + \xi\right)\left(x_1 - x\right)}{u}\right) \quad (14)$$

Using value of C from Eq. 14 in Eq. 11, we get the value of C' for $x \geq x_1$.

The total BOD (TB) and total DO (TD) at any point x are then calculated by following equations:

$$TC = (1 - \alpha) C + \alpha C' \quad (15)$$

$$TC = (1 - \alpha) C + \alpha C' \quad (16)$$

IV. CASE STUDY

To analyse the capabilities of the presented model, it is applied to Uvas Creek for which some of the physical parameters with their values are taken from Reference [9] and outlined in Table 1. To predict the concentration of DO in considered river system, some kinetic and chemical parameters are appropriately taken from the Literatures [2-5] and their values are given in Table 2. Comparison of BOD and DO predicted by one dimensional model by Tyagi et al [14] and presented model are shown in Fig. 1 and Fig. 2 respectively.

TABLE I
PARAMETERS ESTIMATED BY BENCALA AND WALTER FOR UVAS CREEK, CALIFORNIA

Sr. No.	Parameter	Value	Units
1	Q	0.013	m^3/s
2	A	0.36	m^2
3	A_s	0.64	m^2
4	u	2800	m/day

TABLE II
CHEMICAL AND KINETIC PARAMETERS

Sr. No.	Parameter	Value	Units
1	k	3	day^{-1}
2	$k_r' = k_r = m$	10	day^{-1}
3	B_d	16	M/L^3
4	L_o	12	M/L^3
5	γ	8957.95	L^2/day

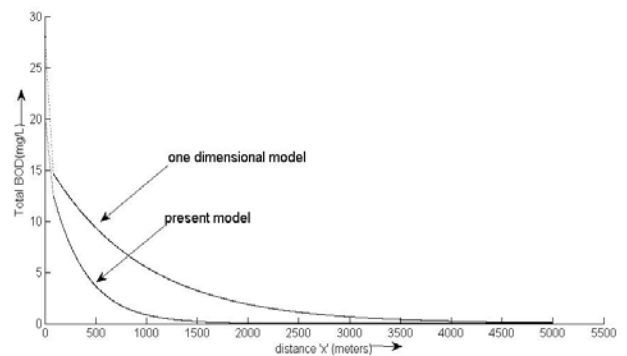


Fig. 1 Concentration of BOD predicted by present model & one dimensional model in advective zone.

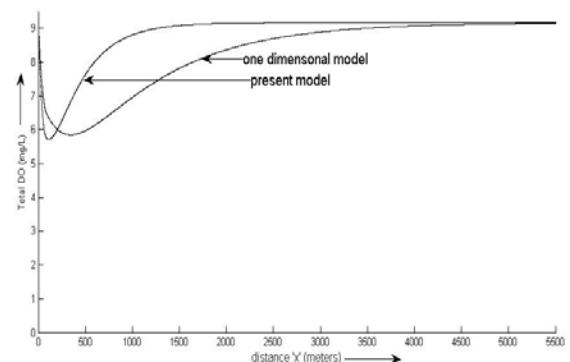


Fig. 2 Concentration of Total DO as predicted by present model & one dimensional model in advective Zone.

Fig. 1 represents a comparison of Total BOD predicted by presented model and One Dimensional Model. It is observed that Concentration of Total BOD obtained from presented Model is less than that predicted by one dimensional Model with the distance downstream. The reason is removal of settle able part at a rate faster than that for one dimensional model. The assimilation of BOD is therefore more and consequently the remaining BOD would be less with distance downstream.

Fig. 2 represents the comparison of DO predicted by presented model and one dimensional model. It is observed from the two DO sag curves that the critical point in case of DO predicted by presented model is shifted towards the source and its magnitude is lesser than the one predicted by one dimensional model, however, the recovery of DO is faster in case of present model. Since more assimilation of BOD at a faster rate would require more DO present in the river, the rate of oxygen depletion would be more and critical point (point at which DO is minimum) occurs earlier and consequently less DO shall remain in the river upto a certain point. The recovery of DO from atmosphere shall be faster in case of deeper sag (Henry's law) as is being observed in DO sag curve for presented model.

Table 3 gives the comparison of location and magnitude of critical DO deficit based on the prediction by the presented model and one dimensional model. It is observed from Table 3 that critical DO predicted by presented model is shifted towards origin as compared to One Dimensional Model. Since all the factors affecting the river's DO being same everywhere, the greater demand would consume more DO and

consequently the DO would decrease with increased amount of BOD exertion.

TABLE III
COMPARISON OF LOCATION AND MAGNITUDE OF CRITICAL CONCENTRATION OF DO

Sr. No.	Model	Distance (meters)	Critical concentration of DO(mg/L)
1	One dimensional model	348	5.85
2	Present model	108	5.72

V. CASE STUDY

To further advocate the robustness of presented model, it is applied to a real life data presented by Bhargava [3] for the Indian holy river Ganges along Kanpur. This data was collected at several points downstream of the sewage outfall points at some major urban centres (Kanpur). The values for BOD and DO concentration predicted by the presented model are plotted along with the observed values for BOD and DO.

Fig. 3 represents a comparison of BOD as predicted by the present model with the observed BOD values. Similar plots for DO are prepared in Fig. 4.

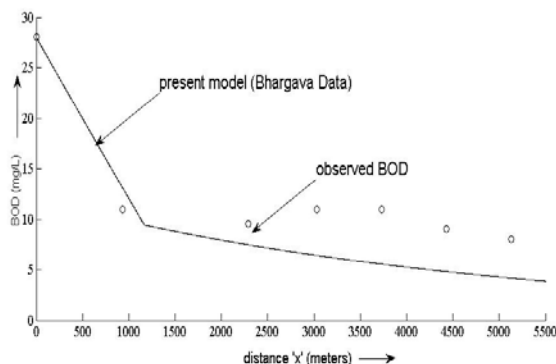


Fig. 3 Comparison of predicted BOD by the present model with the observed values

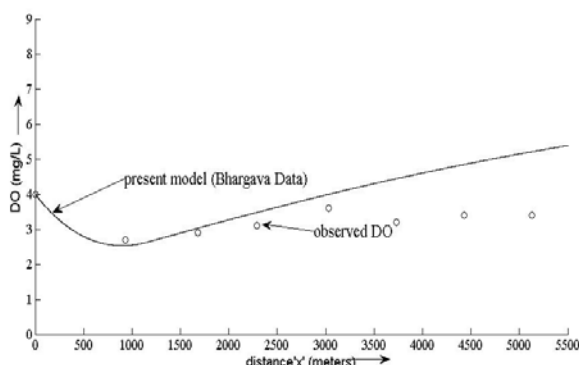


Fig. 4 Comparison of predicted BOD by the present model with the observed values

It is observed from Fig.3 and Fig.4 that the values of BOD and DO predicted by the present model agrees fairly well with the observed values of BOD and DO respectively.

Table 4 gives a comparison of the occurrence as well as the concentration of critical DO as predicted by Tyagi's one dimensional model, Bhargava's model and Presented model with the observed location and magnitude of the critical concentration of DO. It is observed from the table that the prediction by presented model is closer to the observed location and magnitude of critical concentration of DO.

TABLE IV
COMPARISON OF LOCATION AND MAGNITUDE OF CRITICAL CONCENTRATION OF DO

Sr. No.	Model	Distance (meters)	Critical Con. of DO(mg/L)	Error % in Con. Of critical DO
1	One dimensional model	1060	2.3	14.8
2	Bhargava Model	1050	2.297	14.9
3	Present model	901	2.53	6.3
4	Observed values	933	2.7	

VI. CONCLUSION

In this paper, a model is presented that effectively address the situation and accurately predict the condition of DO in rivers when partially treated/untreated waste is discharged into the rivers. The robustness of the model is established by two case studies using the data already published in the literature.

In Case Study-I, due to non availability of relevant data required for analysis of present model, a partially real data is taken for Uvas creek, California and the values of BOD and DO concentration predicted by one dimensional model and presented model are plotted. It is established that the decision based on prediction made by one dimensional model may be erroneous in situations where partially treated /untreated waste enters a river.

To show the robustness of the presented model, a real life data for the river Ganges (INDIA) is used to compare the concentration of DO predicted by the presented model, Bhargava's model, one dimensional model and observed DO values. A very good agreement of the DO concentration as predicted by the presented model with the observed values shows that the DO conditions in rivers can be predicted more accurately by the presented model in the situation when partially treated/untreated waste enters a river.

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