A water quality simulation model for river systems

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Abstract
An interactive river water quality model has been developed for simulating the fate and transport of pollutants through a river system using C++ on a microcomputer. At present, it helps a user predict the variation of BOD, DO, nitrogen, phosphorus and toxic substances as these move through a river system. The submodels have been validated with data readily available in the literature. The use of model has been illustrated with the help of a number of case studies.

INTRODUCTION

Mathematical modeling of water quality presents a special challenge to the systems analyst because it demands integration of so many disciplines. It has significantly contributed in the decision support process by providing the tools for estimating and evaluating the temporal and spatial economic, environmental, or ecological impacts of water quality plans and management policies.

Many of the water quality models in use are extensions of two simple equations proposed by Streeter and Phelps in 1925 for predicting the biochemical oxygen demand (BOD) for various bio-degradable constituents, and the resulting dissolved oxygen concentration (DO) in rivers (Thomann, 1972). More complex multi-constituent water quality models have also been proposed and have been applied to predict the physical, chemical and biological interactions of many constituents and organisms found in natural water bodies. Water quality models can be used to evaluate steady state conditions, for which the values of the water quality and quantity variables do not change with time. They can also be used to evaluate dynamic or time varying conditions. One-dimensional models of river system assume complete vertical and lateral mixing. Two dimensional models may assume lateral mixing as in stratified estuaries or lakes, or vertical mixing as in relatively shallow and wide rivers.

The aim of the present study is develop an interactive model for simulating the fate and transport of pollutants through river systems. The main objectives of the present study were i) to study the behavior of river pollutants along the river flow direction once they are discharged into the river, ii) to develop river quality sub-models for Dissolved Oxygen, Nitrogen, Phosphorus and Heavy metals to predict their concentration profiles along the river flow and iii) to develop case studies for checking the validity of the proposed sub-models with those established in the literature.

THE RIVER WATER QUALITY MODEL

The proposed model is capable of simulating one dimensional steady state behaviour of pollutant transport in the river system. Keeping the model simple, interactive and easy to

use with limited available data was the main driving force behind the proposed model. Since, it should suitable for multi constituents normally discharged in the river systems, the structure of model has been kept as modular so that more submodels can be added easily once they have been developed subsequently. At present, it consists of 4 submodels, viz. BOD-DO submodel, Nitrification submodel, Phosphorus submodel and Heavy metal submodel. Each of submodels is discussed below.

BOD-DO Submodel

The need for the BOD-DO model of any river is well known. The impact of low DO (Dissolved Oxygen) concentrations or of anaerobic conditions is reflected in an unbalanced ecosystem, fish mortality, odors and other aesthetic nuisances.

The DO problem has its origin with the input of waste into a water body. Nevertheless, water has a carrying capacity, which is the maximum concentration of pollutant that could be taken care of by the nature itself. But, when an oxygen demanding waste having pollutant concentration greater than the carrying capacity of the water body, a need to monitor the DO-BOD profile, arises. Reaeration from the atmosphere and DO in the incoming tributaries or effluents have been included as sources of DO and the oxidation of carbonaceous waste material and oxidation of nitrogenous waste material have been considered as sinks.

The net equation for DO deficit is

$$dD/dt = k_1 L_t - k_2 D + 4.57\, k_{23}\, N_2 \tag{1}$$

The solution for the differential equation is

$$
\begin{aligned}
D = & \, k_1 L_0\, (\exp(-k_1 t) - \exp(-k_2 t))/(k_2 - k_1) - D_0 \exp(-k_1 t) \\
& + 4.57\{k_{12} k_{23}\, (((1 - e^{-k_{11} t})/k_{11}) - ((1 - e^{-k_{22} t})/k_{22}))/(k_{22} - k_{11}) N_{01} \\
& + k_{23}/k_{22}\, (1 - e^{-k_{22} t})\, N_{02}\}
\end{aligned} \tag{2}
$$

where D is oxygen deficit, C_s is oxygen concentration at saturation level, C is oxygen concentration at any time t, L is amount of carbonaceous material at any time t, k_1 is rate of BOD exertion, k_2 is the rate of reaeration, N_1 is conc. of Organic N, N_2 is conc. of NH_3-N, N_3 is conc. of NO_2^-,NO_3^--N, k_{12} is rate of decomposition of Organic N to NH_3, k_{11} is rate of decomposition of Organic N to NH_3 and its settling, k_{23} is rate of oxidation of NH_3 to NO_2^-,NO_3^-, k_{22} is rate of oxidation of NH_3 and the rate of uptake of NH_3 by aquatic plants.

When CBOD of the waste is very high, then DO would approach complete depletion and anaerobic conditions would result. The end of the anaerobic reach is given by

$$x_f = x_i + U(k_1 L_i - k_2 C_s)/k_1 k_2 C_s \tag{3}$$

From the end of anaerobic reach, the original equation of oxygen deficit can be used with L_o- ultimate BOD at the end of anaerobic reach (L_f) and initial deficit, $D_0 = C_s$.

Nitrification Submodel

When the waste is discharged into the river, it contains nitrogen mostly as Organic N and very small amounts of NH_3-N and (NO_2^-, NO_3^--N). The nitrogen concentrations in the river at various points along the flow direction are to be monitored. The conditions for nitrification include the presence of nitrifying bacteria, optimum pH in the alkaline range (pH=8), DO concentration is more than 1 mg/L. Organic N $\rightarrow$ NH_3 $\rightarrow$ NO_2^-, NO_3^-

So, the formation of nitrate may utilize DO and therefore deplete the oxygen resources of the water body if the conditions are favourable for nitrification.

If N_1 is conc. of Organic N, N_2 is conc. of NH_3-N, N_3 is conc. of NO_2^- and NO_3^--N, k_{12} is rate of decomposition of Organic N to NH_3, k_{11} is overall loss co-eff of organic N due to settling of particulate forms and hydrolysis and bacterial decomposition of NH_3, k_{23} is rate of oxidation of NH_3 to NO_2^-,NO_3^-, k_{22} is rate of oxidation of NH_3 and rate of uptake of NH_3 by aquatic plants, k_{33} is rate at which NO_2^-, NO_3^- is lost due to uptake by aquatic plants or through denitrification, then nitrification kinetics can be described by following equations -

$$dN_1/dt = -k_{11}N_1 \tag{4}$$
$$dN_2/dt = k_{12}N_1 - k_{22}N_2 \tag{5}$$
$$dN_3/dt = k_{23}N_2 - k_{33}N_3 \tag{6}$$

Solutions for the above differential equations are

$$N_1 = N_{01} e^{-k_{11}t} \tag{7}$$
$$N_2 = \{k_{12}N_{01} (e^{-k_{11}t} - e^{-k_{22}t})/ (k_{22}-k_{11}) \} - N_{02} e^{-k_{22}t} \tag{8}$$
$$N_3 = k_{12}k_{23}N_{01}\{(e^{-k_{11}t} - e^{-k_{33}t})/ (k_{33}-k_{11}) - (e^{-k_{22}t} - e^{-k_{33}t})/ (k_{33}-k_{22})\}/(k_{22}-k_{11})$$
$$+ k_{23}N_{02} (e^{-k_{22}t} - e^{-k_{33}t})/ (k_{33}-k_{22}) + N_{03} e^{-k_{33}t} \tag{9}$$

where N_{01}, N_{02}, N_{03} are initial conc. of Organic N, NH_3-N, and NO_2^-, NO_3^--N respectively.

Phosphorus Submodel

The capacity of a naturally flowing stream to assimilate nutrients is important in determining nutrient loading to downstream receiving water bodies. Eutrophication may be slowed if inflow streams have insufficient self-purification ability. Self-production is understood to be the stream's capacity to decrease the mass transport of water contents within a given flow distance. If the phosphate concentration goes above 0.015mg/L in the stream, then eutrophication would occur. Thus, the phosphate-phosphorus concentration in the river is to be monitored. In the steady state, the phosphorus concentration is given by

$$V_x dP/dx = D_L \, \partial^2 P/\partial x^2 + R_A \tag{10}$$

where V_x is velocity in x direction, D_L is longitudinal dispersion coefficient, R_A is reactions, sources and sinks and P is orthophosphate concentration

The reactive and source/sink terms (R_A) for dissolved inorganic phosphorus are identified as R_1 is chemical precipitation, R_2 is biological uptake by algae, R_3 is regeneration by plankton, R_4 is biological uptake by macrophytes, R_5 is phosphorus input from GW and surface distributed inflows, R_6 is phosphorus input from direct rainfall, R_7 is release rate of phosphorus from sediments.

The chemical precipitation (R_1) is based on calcium phosphate $Ca_3(PO_4)_2$ kinetics (Ferguson, 1975).

$$dP/dt \propto P^3$$
$$= K_1P^3 \text{ i.e. } R_1 = K_1P^3 \tag{11}$$

The biological uptake (R_2) by algae is represented by Micahelis-Menton equation:

$$dP/dt = \mu_{max} (D_E/D_Z) * P/(K_p + P)$$

where μ_{max} is maximum growth rate possible with optimum conditions, D_E is euphotic depth, D_Z is river depth, K_p is Michaelis or half-saturation constant (0.001 and 0.010ppm).

$$\text{i.e. } R_2 = K_2 * P/(K_p + P) \tag{12}$$

Therefore, equation (1) leads to

$$V_x dP/dx = D_L \partial^2 P/\partial x^2 - R_1 - R_2 + R_3 - R_4 + R_5 + R_6 + R_7$$
$$= D_L \partial^2 P/\partial x^2 - K_1P^3 - K_2P/(K_p + P) + R_3 - R_4 + R_5 + R_6 + R_7$$
$$= D_L d^2 P/dx^2 - K_1P^3 - K_2P/(K_p + P) + K_\in \tag{13}$$

where $K_\in$ is sum of all the rates affecting phosphorus concentration.

Rearranging above, we get

$$D_L d^2 P/dx^2 - V_x dP/dx - [3K_1P_o^2 + K_2K_p/(K_p + P_o)^2]P = K_2P_o^2/(K_p + P_o)^2 - 2K_1P_o^3 - K_\in$$
$$\tag{14}$$

The above equation is of the form,

$$A d^2 P/dx^2 + B dP/dx + C P = D \tag{15}$$

The General Solution is

$$P = C_1 e^{m_1 x} + C_2 e^{m_2 x} + D/C \tag{16}$$

where $C_1 = [m_2 (D/C - P_o) + P_o'] / (m_1 - m_2)$, $C_2 = [m_1 (P_o - D/C) - P_o'] / (m_1 - m_2)$ and m_1, m_2 are the roots of the differential equation.

Heavy Metal Submodel

The release of chemicals into the water body such as rivers, streams in concentrations to be toxic is of intense concern in water quality. The uniqueness of the toxic substance problem lies in the potential impact on human health or to the aquatic ecosystem, either via ingestion of the chemical from the drinking water supply or via ingestion of the chemical from contaminated aquatic foodstuffs. Metals are an important category of toxic substances, which result from industrial activities such as electroplating, battery manufacturing, mining, smelting and refining.
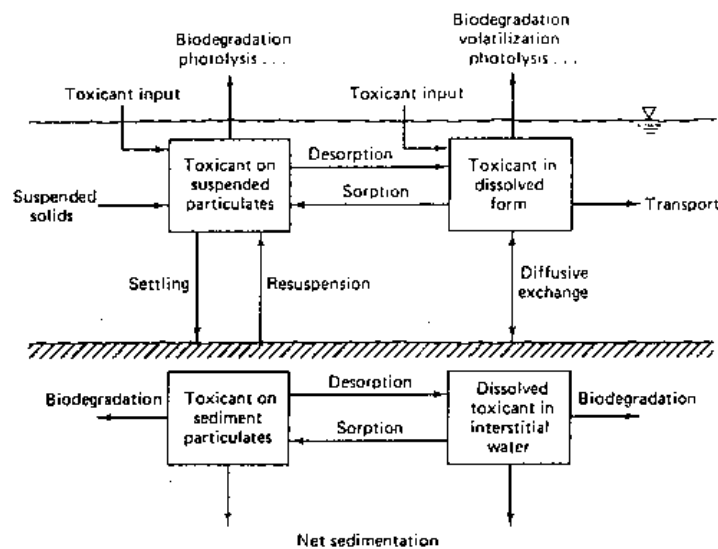
Figure 1. A schematic diagram showing various mechanisms involved with a toxic substance in river system.

The figure 1 shows the general features of the physio-chemical phases of the transport of a toxic substance in the river. The inputs include all sources such as municipal and indsutrial discharges, urban and agricultural runoff and atmospheric inputs. In the water column and sediment, the principal physical and chemical phenomena that take place are 1. Sorption and desorption between dissolved and particulate forms in the water column and sediment, 2. Settling and resuspension mechansims of particulates between the sediment and the water column., 3. Diffusive exchange between the sediment and the water column, 4. Loss of metal due to volatilization, photolysis, 5. Gain of metal due to chemical reactions, 6. Transport of metal due to advective flow transport and dispersive mixing, 7. Net deposition and loss of metal to deep sediments.

Toxicant forms: The metal toxicant can exist in two basic forms: the dissolved phase and the metal on the solids, both for either the water column or sediment. Let the dissolved form be denoted by cd' and the metal in the particulate form be defined by cp.

$$c_d' = M_T/L_w^3 \tag{16}$$

$$c_p = M_T/L_{w+s}{}^3 \tag{17}$$

where M_T is mass of the toxicant, $L_w{}^3$ is volume of water and $L_{w+s}{}^3$ is volume of solids plus water (the bulk volume).

The total toxicant concentration anywhere in the water body or sediment is

$$\begin{aligned} c_T &= c_p + \phi\, c_d' \\ &= c_p + c_d \end{aligned} \tag{18}$$

It may be noted that for water column $\phi = 1$ and for sediments, it varies from 0.7-0.8. The particulate form c_p is expressed as a mass of toxicant per bulk volume of solids and water. For a given concentration of solids, c_p can also be expressed as $c_p = rm$ where m is solids concentration ($M_s/L_{w+s}{}^3$) and r is toxicant concentration expressed on a dry weight solids basis (M_T/M_s).

Sorption-desorption: The particulate form and dissolved form of metal in the water body will be in continuous equilibrium because of the mechanism of sorption of the metal to the particulates and desoprtion from the particulates back into the dissolved phase. A simple kinetics relationship is given by the following equations-

$$dc_p/dt = k_u\, m\, c_d' - K\, c_p \tag{19}$$

where k_u is sorption rate ($L_w{}^3/M_s.T$) and K is desorption rate (1/T).

In terms of r, the equation become $dr/dt = k_u c_d' - K\, r$. The fast kinetics of sorption-desorption indicates that there will be a virtually continuous equilibrium of the dissolved and particulate forms depending on the local solids concentration. Now, a partition coefficient can be defined as

$$\begin{aligned} P' &= r/c_d' \\ (\text{or})\ P &= r/c_d \end{aligned} \tag{20}$$

Using the above relationship, c_p and c_d can be written as

$$c_p = f_d c_T \tag{21}$$
$$c_p = f_p c_T \tag{22}$$

where $f_d = (1+Pm)^{-1}$, m being the concentration of suspended solids.

Volatilization: Toxicant in dissolved from in the water column undergoes volatilization. The rate of loss of the toxicant due to this pressure is given by:

$$N_s = K_1\, (C_s - C_{si}) \tag{23}$$
$$= K_1\, (C_g/\, H_e - C_{si}) \tag{24}$$

where K_1 is liquid film mass transfer co-efficient (m/hr), H_e is Henry's law constant, $C_s = C_g/H_e$, C_g is vapour pressure concentration and C_{si} is dissolved toxicant concentration.

If C_{T1} is the toxicant in the water column, then toxicant in dissolved form in the water column $= f_{d1} * C_{T1}$

So, $N_s = K_1 (C_g / H_e - f_{d1} C_{T1})$ (25)

Specifically the assumptions that the river is in a steady state and that the bed sediment may remain suspended permit partial simplifications in the analysis. However, for the first estimates of the distribution of toxic substances in rivers, it is generally not feasible to carry out detailed time variable sediment transport modeling coupled to a chemical model. Therefore, in spite of the severity of the two aforementioned assumptions, the simplicity of the final results and resulting ease of the use urges consideration of the simplified approach for the first level toxic substances allocations in rivers.

Solids Balance: The water column solids in a river represent the balance between settling and resuspension. Assuming a reach of the river with constant parameters of settling, resuspension, and deposition, the mass balance equations in the water column and sediment are:-

$$u \frac{dm}{dx} = -\frac{v_s}{H} m + \frac{v_u}{H} m_s$$

$$u_s \frac{dm_s}{dx} = \frac{v_s}{H} m - \frac{v_u}{H} m_s - \frac{v_d}{H} m_s$$

where m is solids conc. in the water column, m_s is solids conc. in the sediment column, v_s is settling velocity of the particle, v_u is resuspension velocity of the particle fdrom the sediment to the water column, v_d is overall average net sedimentation velocity.

Heavy metals balance:

$$u \frac{dc_{T1}}{dx} = K_f (f_{d2} \frac{c_{T2}}{\phi_2} - f_{d1} c_{T1}) + k_1 (\frac{c_g}{H_e} - f_{d1} c_{T1}) - \frac{v_s}{H} f_{p1} c_{T1} + \frac{v_u}{H} f_{p2} c_{T2}$$

$$u_s \frac{dc_{T2}}{dx} = -K_f (f_{d2} \frac{c_{T2}}{\phi_2} - f_{d1} c_{T1}) + \frac{v_s}{H} f_{p1} c_{T1} - \frac{v_u}{H} f_{p2} c_{T2} - \frac{v_d}{H} f_{p2} c_{T2}$$

where c_{T1} is total metal in the water column, c_{T2} is total metal in the sediment column, K_f is diffusive exchange rate between metal in dissolved form in the water column and that in the sediment, k_1 is volatilization rate with c_g is vapor phase conc. and H_e is Henry's constant.

The four differential equations shown above reflect the concentration profiles of the suspended solids in the water column and in the sediment column, and the total metal concentration in the water column and in the sediment column.

The results of the numerical solution to the differential equation reflect a series of point inputs of heavy metal inputs along river flow direction. The profiles for the various concentrations give a picture of the concentration along the flow direction. This helps in monitoring the inputs so that the metal concentration does not go beyond the permissible standard.

USING THE MODEL

The model has been written in Turbo C++ on a microcomputer. By running the program, a screen giving the details of the project is seen. By pressing any key as indicated at the bottom right, screen 2 is printed which calls for option from the user. By pressing the number of any submodel, the user can execute that particular submodel. Each submodel can be executed by inputting the values in proper units as indicated along with the arrow at each point.

Case Study 1
A river with flow of 0.5 cu.m/s has Dissolved Oxygen concentration of 8.0 mg/L and a BOD5 of 3.0 mg/L. The deaeration and reaeration rates are 0.2/day and 0.6/day respectively. Along the river profile, two industrial wastes with the following characteristics are being discharged into the river. Find the DO concentration profile along the river flow direction.

	Q (m^3/s)	DO (mg/L)	BOD$_5$ (mg/L)	Dist. (km)	Organic N	NH$_3$	NO$_3^-$
Waste 1	0.2	3.0	80.0	65.0	8.0	0.01	0.01
Waste 2	0.25	2.0	30.0	130.0	5.0	0.001	0.001

Case Study 2 (Nitrification)
A river with flow of 0.5 cu.m/s has organic N concentration of 5mg/L, NH$_3$ -N of 0.05 mg/L and NO$_2^-$,NO$_3^-$ of 0.03 mg/L. The values of k_{11}, k_{12}, k_{22}, k_{23}, k_{33} may be assumed to be 0.11, 0.09, 0.14, 0.13, 0.16/day respectively. A municipal wastewater with discharge of 0.2cu.m/s has organic N concentration of 40 mg/L, NH$_3$ -N of 0.1 mg/L and NO$_2^-$, NO$_3^-$ of 0.05 mg/L. The river is to be monitored for a distance of 450km from the point where the wastewater is being discharged into it.

Case Study 3 (Phosphorus)
A river has flow of 0.5cu.m/s and flow velocity of 162 m/hr with no Phosphorus concentration. The value of $k_1 = 7.48 \times 10^{-10}$ (mg/l)$^{-2}$/hr and $k_2 = 4.296 \times 10^{-3}$ mg/l/hr. kP=0.005 mg/L and $k_E = 5.755 \times 10^{-3}$ mg/l/hr. The value of the dispersion co-efficient for the river is found to be 1532.52 m^2/hr. Now, a wastewater of 0.2 cu.m/s and Phosphorus conc. of 0.07 mg/L is being discharged as a point source. Evaluate the Phosphorus concentration profile along the river flow direction.

Case Study 4 (Heavy Metals)

For a river with flow as 0.5 cu.m/s, velocity as 0.045 m/s, settling velocity as 0.5 mm/s, resuspension velocity as 0.5 nm/s, overall net sedimentation velocity as 0.2 nm/s, the suspended solids concentration in the water column and in the sediment column are 9.2 mg/L and 4.0 g/L while the heavy metal concentrations are 0.02 mg/L and 0.001 mg/L in both the columns respectively.

A wastewater from an industry is discharged as a point source with waste discharge= 0.2 cu.m/s, mass of suspended solids (ss) in water column=70 mg/L, mass of ss in sediment column= 35 g/L, heavy metal concentration in water column=3.5 mg/L and in sediment column=0.035 mg/L. The diffusive exchange rate is 0.1 m/day while volatilisation rate is 3.38 m/day. He=0.0582 atm l/gm. Find the profile of various concentrations along the river flow direction.

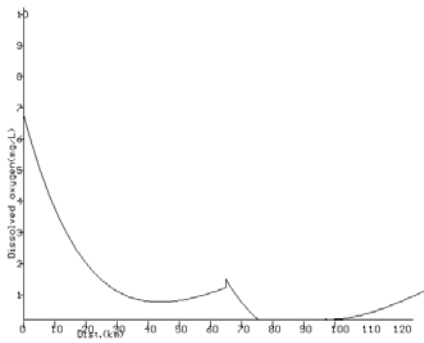Typical outputs for above case studies are shown in figures 2 to 5.
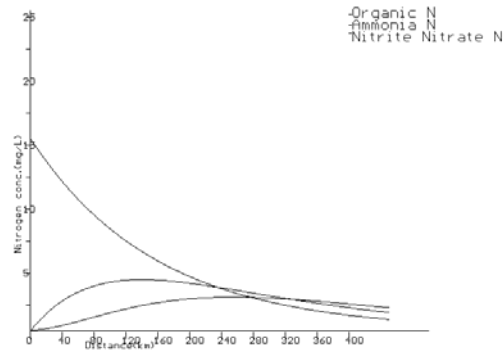

Figure 2. DO sag curve for case study 1.

Figure 3. Output showing concentration profiles of Organic N, NH$_3$-N, NO$_3$⁻-N for case study 2.
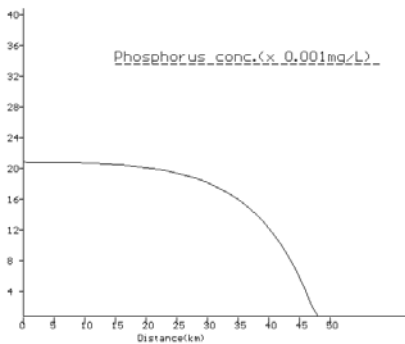

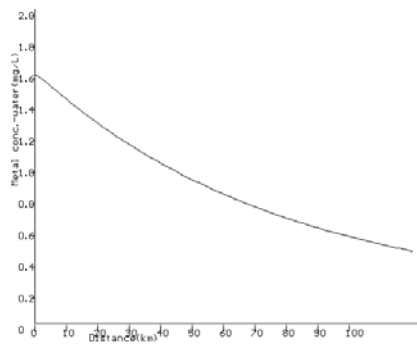**Figure 4 .Typical output for the case study 3.**

Figure 5. Metal concentration in the water column along the river profile for case study 4.

CONCLUSIONS

The presented program has four submodels viz., BOD-DO submodel, nitrification submodel, phosphorus submodel and heavy metal submodel. The proposed submodels have been checked for their validity by comparing the results with those available in the literature. The values for various constants and the data needed for executing the program were taken from the available literature. The various profiles exhibited by these submodels were found to be more or less accurate with the profiles predicted in the literature with an allowable error. Thus, this model comprising of various submodels can be used for predicting the behaviour of DO, nitrogen, phosphorus and heavy metal along the river flow direction.

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