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Mathematical Modelling of Water Quality and Engineering of Pili River Stream in Nagpur District of Maharashtra

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ABSTRACT

The working plan deals with the preliminary proposal for mathematical modelling of water quality and engineering of Pili River stream located in Nagpur District of Maharashtra (India). The total length of Pili River within the city is about 16.7 Kilometres. Its width varies from 20-40 meters and depth ranges from 2 to 4.5 meters. There has been growing concern for maintenance of water quality and ecosystem along Pili River at both Legislative and Judiciary levels. Therefore it is need of the day to rejuvenate its water quality and habitat. Urbanization had created ecological threat due to immense dumping of domestic wastewater. General background information about natural characteristics of the selected stations along the Pili River and main source of pollution was made for a better understanding of this problem. The calculation was divided into three stages, and the problem was solved using the so-called "combined catch-up / feedback method". Computer memory space is saved as well as calculations speeds up using this method. The complicated hydraulic conditions in stream networks make it very difficult to estimate parameters. While the present developed model can be used for varied stream networks, it is necessary to estimate the parameters of the model according to the local measurements.

I. INTRODUCTION

Criteria for Water Pollution Control

There are different kinds of criteria that are currently used for water pollution control in India, waste water criteria, natural water body criteria, and organic waste discharge criteria (Deininger, 1973). If the waste water control criteria were worked out according to the local economic conditions and the technological level, they would be convenient as they are very concise (Rinaldi and Soncini, 1979). But they fail to link the pollution of waste-water sources with the local environmental conditions, *i.e.*, they do not take the environmental impacts of pollution into account.

The criteria for the quality of natural water bodies are based on the requirements of the water users. They represent the behalf of the water users, but fail to take the real situation into account. The third kind of criteria is mainly for organic waste discharge. These criteria should take into account the distribution of pollution sources, the amount of pollution, the available treatment capacity, the self-purification capacity of the natural water bodies, the demands of water users regarding quantity and quality and other factors of an aquatic ecosystem (James, 1978).

The variables of the water pollution control problem which is a dynamic system control problem, can be divided into three classes (Thomani, 1972):

1. User demands
- Areal distribution of users
- Water quality desired by users
- Water quantity desired by users
- Future new users, their demands regarding water quality and quantity
- Variations of water demands (quality and quantity) in the future
- Basic and maximum demands (quality and quantity) during different periods

2. Pollution sources
- Distribution of main sources of pollution
- Main categories of pollution
- Amounts of pollution from the various sources
- Capacity of pollution control and waste-water treatment
- Probable future status of pollution sources
- Probable amounts and categories of pollution in the future
- Probable control levels and treatment capacity

3. Self-purification capacity
- Structure of the channels in a stream network
- Hydrological and aquatic conditions in streams
- Present water quality
- Probable unfavourable hydrological conditions in the future
- Probable water quality under most unfavourable hydrological and aquatic conditions
- Required treatment of waste influents to meet the desires of the users under different hydrological and aquatic conditions
- Sewage treatment needed to meet the basic requirements of users under most unfavourable hydrological and aquatic conditions

The third class of variables is decisive for defining the criteria. It combines the pollution sources with the desired water quality and the demands of the water users. Once the desired water quality has been determined, the self-purification capacity is the key factor defining the waste discharge criteria. The mathematical model described below is a powerful tool for this purpose.

Mathematical Modelling of Self-purification Processes in Pili River Stream Networks

The basic principle of founding mathematical models on the water quality in tidal stream networks is the principle of matter equilibrium. i.e., the variant rare of flux of materials on the surface of the system equilibrate the variance of the concentration of the materials inside the system.

The factors that cause the variance of matter concentration inside the system are of physical, chemical and biological origin. Physical factors include convection, turbulent diffusion (or dispersion in one-dimensional problems), settlement (or resuspension) of solid particles and dilution by mixing.

Chemical reactions which cause the variance of the concentration of pollutants include solubility equilbria and acidic reaction. Principally, they cause a shift in pH value and alkalinity, which affects the dissociation of carbonates.

Some people refer to adsorption as a physical reaction; others, as a chemical reaction.

The decomposition of organic pollutants by microbe is the main cause for polluted rivers to be deprived of oxygen. It involves two stages. At the first stage, the organic matter is oxidized by the bacteria. The rate of this reaction is assumed to be proportional to the concentration of the remaining organic matter, measured in terms of oxygen. This reaction may be expressed as Eq. (1).

$$\frac{dL}{dt} = -K_1 L \quad (1)$$

where

L = concentration of organic matter in terms of BOD [mg/l]

t = time

K_1 = coefficient defining the reaction velocity $[day^{-1}]$

The second stage is nitrification, i.e., oxidation by bacteria of ammonium salts. The rate of this reaction can be expressed as Eq. (2)

$$\frac{dL_N}{dt} = -K_N t \quad (2)$$

Where

L_N = concentration of nitric organic pollutants in terms of nitrification biochemical oxygen demand BOD_N [mg/l]

K_N = coefficient defining the velocity of the nitrification reaction.

<u>Decomposition of Sedimental Sludge at the Bottom of Rivers</u>

The organic matter in the sedimental sludge is decomposed by microbes under anaerobic conditions, which results in the generation of reductive gases such as organic acids, methane, carbon dioxide, hydrogen, etc. These gases are released into the water body or into the interface between water and sediment and combine with the oxygen contained in the water.

<u>Reoxygenation</u>

$$K_3 = f(u, d, \varphi) \quad (7)$$

Water may absorb oxygen from the atmosphere when the dissolved oxygen (DO) is below saturation. The rate at which oxygen is absorbed, or the rate of reaeration, is proportional to the degree of under saturation and may be expressed as in Eq. (3)

$$\frac{dD}{dt} = K_2 (D_2 - D) = K_2 D_d \quad (3)$$

where

D = concentration of dissolved oxygen [mg/l]

D_s = saturation concentration of DO at definite temperature.

K_2 = reaeration coefficient $[day^{-1}]$.

t = time

D_d = dissolved oxygen deficit.

The photosynthesis of aquatic plants is another source of DO in water bodies. The rate of oxygen generation can be obtained from Eq. (4) and Eq. (5).

$$P(t) = P_m \sin \frac{(t - t_{sr})}{t_{ss} - t_{sr}} \qquad t_{sr} < t < t_{ss} \quad (4)$$

$$P(t) = 0 \qquad t_{sr} > t > t_{ss} \quad (5)$$

where

P_m = maximum rate of oxygen generation of aquatic plants during photosynthesis.

t_{sr} = time of sunrise.

t_{ss} = time of sunset.

Another factor affecting the material equilibrium is settling / resuspension. JANSA and AKERLINDH have shown that a term for deoxygenation due to BOD of sediment may be added to the model equations :

$$\frac{dL_b}{dt} = K_3 \,.\, L_s \,.\, e^{-K}3^{t} \quad (6)$$

where

L_b = concentration of organic matter in settled sludge in terms of BOD at time t

L_s = total BOD of settling sludge.

K_3 = coefficient of sedimentation.

Factors affecting the sedimentation rate are flow velocity U, depth of water body d and particle diameter φ :

For elaborating a mathematical model of stationary streams, it is sufficient to take these factors into account. But in a Pili River stream network it is necessary to include the tidal action and the particular flow conditions as these two factors govern the distribution and concentration of pollutants. Most coefficients are not constant. In a Pili River stream network, flows vary in direction and velocity, but not in a periodic manner as is the case for single estuaries or single tidal streams. In contrast to estuaries, there is no stratification and no crosswise circulating currents. Waters running in stream networks move forward, backward and around, but do not follow definite rules. At the nodes of the stream network, water discharge takes place depending on the geometric characteristics of the channels, the structure of the stream beds, as well as the water levels in the upstream and downstream reaches. There is no constant coefficient for the same amount of discharge. Flow velocities vary considerably, from high velocities in one direction to high velocities in the other direction. The uneven distribution of velocities over the cross-sections of the streams plays an important role in the distribution of pollutants.

Therefore, the unsteadiness of the concentration field, the transportation caused by variable flow velocities, dispersion, and the regulative function of the nodes on the assignment of water discharges in stream networks need to be taken into account. Dispersion may be expressed as Eq. (8).

$$I_x = -E_x \frac{d^2L}{dx^2} \quad (8)$$

where

E_x = coefficient of dispersion $[L^{-2}]$

L = length.

x = longitudinal distance.

The negative sign means that dispersion is directed towards the lower concentration.

Advection may be expressed as Eq. (9)

$$I_{o_a} = U \frac{dL}{dx} \quad (9)$$

Based on the above assumptions, the mathematical model of the water quality in tidal stream networks may be expressed as the following equations :

When $i \neq i,1$

$$\frac{aH}{at} + \frac{1}{B}\frac{aQ}{ax} = 0 \quad (10)$$

$$\frac{aU}{at} + U\frac{aU}{ax} + g\frac{aH}{ax} + g\frac{U\,|U|}{c^2\,d} = 0 \quad (11)$$

$$\frac{a(AL)}{at} + \frac{a(AUL)}{ax} = \frac{a}{ax}\left(A.E_x\frac{AL}{ax}\right) - \sum_{io=1}^{P_0} K_{io}.A.L.+S \quad (12)$$

When $i = i,1$

$$\sum_{i=1}^{P_1} Q_{j_1}, i_1 = 0 \quad (13)$$

$$H_{j_{1,1}} = H_{j_{1,2}} = \cdots = H_{j_1,i_1} = \cdots = H_{j_1,P_1} \quad (14)$$

$$\frac{aL}{at}.V_{j_1} = \Delta F_{j_1} \quad (15)$$

Initial conditions, j = 0

$$H\ (i,0) = h\ (i) \quad (16)$$

$$U\ (i,0) = u\ (i) \quad (17)$$

$$L\ (i,0) = l\ (i) \quad (18)$$

Marginal conditions, i = f

$$H\ (i,j) = h\int (f,j) \quad (19)$$

$$L\ (i,j) = l\int (f,j) \quad (20)$$

The equations (10) to (20) constitute the mathematical model of the water quality in tidal stream networks. For water quality simulation using the concentration of dissolved oxygen as indicator, the modeling equations should be hydraulic coupled equations and BOD-DO coupled equations.

$$\frac{aH}{at} + \frac{1}{B}\ \frac{aQ}{ax} = 0 \quad (21)$$

$$\frac{aU}{at} + U\frac{aU}{ax} + g\frac{aH}{ax} + g\ \frac{U\ |U\,|}{e^2\ \ d} = 0 \quad (22)$$

$$\frac{a(A.L)}{at} + \frac{a(AUL)}{ax} = \frac{a}{ax}\left(A.E_x.\frac{aL}{ax}\right) - \sum_{io=1}^{P_0} K_{io}.A.L.+S \quad (23)$$

$$\frac{a(A.D)}{at} + \frac{a(AUD)}{ax} = \frac{a}{ax}\left(A.E_x.\frac{aD}{ax}\right) + K_2.A.(D_s - D) \qquad i \neq i,1$$

$$- \sum_{io=1}^{P_0} K_{io}.A.L.+S_1 \quad (24)$$

$$\sum_{i1=1}^{P_1} Q_{j_1}, i1 = 0 \quad (25)$$

$$H_{j_{1,1}} = H_{j_{1,2}} = \cdots = H_{j_1,i_1} = \cdots = H_{j_1,P_1} \qquad i = i,1 \quad (26)$$

$$\frac{aL}{at}.V_{j_1} = \Delta F_{j_1} \quad (27)$$

$$\frac{a0}{at}.V_{j_1} = \Delta D_{j_1} \quad (28)$$

Marginal conditions, i = f

$$H\ (i,j) = h\ 1\ (f,j) \quad (29)$$

$$L\ (i,j) = l\ 1\ (f,j) \quad (30)$$

$$D\ (i,j) = d\ 1\ (f,j) \quad (31)$$

Initial conditions, j = 0

$$H\ (i,0) = h\ (i) \quad (32)$$

$$U\ (i,0) = u\ (i) \quad (33)$$

$$L\ (i,0) = l\ (i) \quad (34)$$

$$D\ (i,0) = d0\ (i) \quad (35)$$

where

Eq. (21)	=	so-called continuity equation
Eq. (22)	=	momentum equation
Eq. (23)	=	equation of pollution conservation
Eq. (24)	=	equation of DO conservation
B	=	average width of cross sections, for narrow and wide channels it approximately equals the width of the water surface [m]
A	=	area of the cross section through which waters flow [m^2]
Q	=	water discharge [m^3/e]
c	=	coefficient expressing the roughness of the stream bed. Chezy coefficient
d	=	hydraulic radius; for wide and narrow rivers it usually approximates the average depth of the water in the channels
K_{i0}	=	coefficients defining the decay velocities of pollutants. For organic pollutants, these coefficients define the oxidation velocity (K_1), settling/resuspension velocity (K_3), etc.
s	=	other sources or sinks, including branch influents, etc.
p_p	=	amount of coefficients
io	=	ordinal number
i1	=	ordinal numbers of cross sections located in the areas of stream network nodes
j1	=	ordinal numbers of the nodes of a stream network
V_{j1}	=	water volume at node j1 of the stream network
ΔF_{j1}	=	net flux of pollutants at node j1
h 1(f,j)	=	water levels at marginal sections
l 1(f,j)	=	concentration of pollutants in marginal sections
h(i)	=	original water level of a section
u(i)	=	original flow velocity in a section
l(i)	=	original concentration of pollutants in a section
f	=	ordinal numbers of marginal sections
i	=	ordinal numbers of segments of the stream network
j	=	ordinal numbers of time steps
m	=	total number of time steps
n	=	total number of segments of the stream network
d1 (f,j)	=	concentration of dissolved oxygen in marginal sections
d0 (i)	=	original concentration of a section
D_{j1}	=	net flux of dissolved oxygen at node j1
S_1	=	other source or sink of dissolved oxygen
K_2	=	coefficient defining the rate of reaeration of waters in the stream network

For the above model, it is assumed that the carbonaceous oxygen demand resulting from organic matter degradation is the main factor influencing the dissolved-oxygen balance.

If other factors exert a secondary oxygen demand, such as nitrifying bacteria by the oxidation of ammonia, appropriate equation, which have the same form as Eq. (23) need to be added and appropriate terms need to be added to the equation defining the equilibrium of dissolved oxygen.

Numerical Solution of the Mathematical Model

It we have all coefficients we need and we know the initial and marginal conditions, the equations of the mathematical model can be solved. But it is difficult to find an analytical solution. We need a proper numerical method.

Normally, in natural waters, the flow field is independent of the concentration field unless the concentration of pollutants is so high that it causes marked variations of water density and water viscosity.

The concentration field, however, is not independent of the flow field. Therefore, it is possible to solve the flow first and then the concentration field.

In the same way, the concentration field of organic pollution is independent of that of dissolved oxygen as long as there is dissolved oxygen in the water.

Therefore, we can use the recurrence relations of equations to simplify the calculation. That means we can calculate the flow field first, then, using the results of the flow field as a known condition, we can solve the concentration field of organic pollution and then the concentration field of dissolved oxygen.

In order to speed up the calculation and to save computer storage capacity, the following disposals are adopted: For each time sequence, the equations are solved in combination, while for each time span, the equations are solved by a recurrence method. The processes of the calculation are provided in detail below.

The first step is the calculation of the flow field. The relative equations are the following :

$$\frac{aH}{at} + \frac{1}{B}\ \frac{aQ}{ax} = 0 \tag{36}$$

$$i \neq i, 1$$

$$\frac{aU}{at} + U\frac{aU}{ax} + g\frac{aH}{ax} + g\ \frac{U\ |U|}{c^2\ \ d} = 0 \tag{37}$$

$$P_1$$

$$Q_{j1,i1}\ =\ 0 \tag{38}$$

$$i1=1 \qquad\qquad i = i, 1$$

$$H_{j_{1,1}} = H_{j_{1,2}} = \cdots = H_{j_1,i_1} = \cdots = H_{j_1,P_1} \tag{39}$$

Marginal conditions,

$$H\ (i,j) = h1\ (i,j) \quad i = f \tag{40}$$

Initial conditions,

$$H\ (i,0) = h\ (i) \quad j = 0 \tag{41}$$

$$U\ (i,0) = u\ (i) \quad j = 0 \tag{42}$$

Using finite differences of a four-point implicit pattern, we can transform the differential equations into finite difference equations if the time spans are all of the same magnitude and the space spans are different. The pattern of differences is shown in Fig. 1.

For the variable θ , we have the following formulas :

$$\overline{\theta} = \frac{1}{4}\left(\theta_{i-1}^{j-1} + \theta_i^{j-1} + \theta_{i-1}^{j} + \theta_i^{j}\right) \tag{43}$$

$$\frac{a\theta}{at} = \frac{1}{2t}\left(\theta_{i-1}^{j} + \theta_i^{j} - \theta_{i-1}^{j-1} - \theta_i^{j-1}\right) \tag{44}$$

$$\frac{a\theta}{ax} = \frac{1}{2\Delta x_1}\left(-\theta_{i-1}^{j} + \theta_{i}^{j} - \theta_{i-1}^{j-1} + \theta_{i}^{j-1}\right) \quad (45)$$

where

θ = average value of the values of four nodes of a network.

Substituting finite difference formulas for the differential terms, we obtain, for stream segment no. i , the following difference equations.

$$\begin{cases} \emptyset 1_{i-1} H_{j-1}^{j} + \emptyset 2_{i-1} U_{i-1}^{j} + \emptyset 3_{i-1} H_{i}^{j} + \emptyset 4_{i-1} U_{i}^{j} = \emptyset 5_{i-1} & (46) \\ \Psi 1_{i} H_{i-1}^{j} + \Psi 2_{i} U_{i-1}^{j} + \Psi 3_{i} H_{i}^{j} + \Psi 4_{i} U_{i}^{j} = \Psi 5_{i} & (47) \end{cases}$$

Making identical alterations to these two equations, we can obtain equations of the following type.

$$\begin{cases} H_{i-1}^{j} + a_{i-1} U_{i-1}^{j} + b_{i-1} H_{i}^{j} = R_{i-1} & (48) \\ U_{i-1}^{j} + a_{i} H_{i}^{j} + b_{i} U_{i}^{j} = R_{i} & (49) \end{cases}$$

For each stream segment not located in the node regions, we have coupled equations similarly to the above, where a, b, ∅, Ψ are factors.

For the segments located in the node area, we have equations like Eq. (38) and Eq. (39). Adding the equations of the marginal and initial conditions, we obtain closed and solvable equations.

For the total stream network, the equations are of the following type :

$$A \,.\, \underline{\overline{x}} = R \quad (50)$$

Take a stream network of the following type as an example.

We can see that the coefficient matrix is of the tridiagonal type with some coefficients being discrete. Equations of this type can be solved with the "combined catch-up/feedback method". This method includes two steps. The first step is the "catch-up process". Using the boundary conditions, and beginning with the first equation, one equation after the other is transformed together with the last equation by means of identical alternation to eliminate a variable. The second step is the "feedback process", conducted in opposite direction. Feeding the latest boundary condition into the last equation, we obtain the value of the last equation but one, we obtain the value of the last variables but one. In this way, one by one, we obtain the values of all variables. When making a catch-up step with the equations related to the nodes of the stream network, we must make an identical alternation with the equation having a discrete coefficient in order to bring the discrete co-efficient a step closer to the tridiagonal.

The second step of solving the equations of the model is the calculation of the concentration field of the organic pollutants.

The relevant equations are :

$$\begin{cases} \frac{a(AL)}{at} + \frac{a(AUL)}{ax} = \frac{a}{ax}\left(A.E_x.\frac{aL}{ax}\right) - \sum_{io=1}^{P_0} K_{10}.A.L.+S & i \neq i1 \quad (51) \\ \frac{aL}{at}.V_{j1} = \Delta F_{j1} & i = i1 \quad (52) \end{cases}$$

Marginal conditions,

$$L\ (i,j) = 1\ (f, j) \qquad i = f \quad (53)$$

Initial conditions,

L (i,0) = l (i) j = 0 (54)

The requisite hydraulic conditions and the relevant data on the structure of the channels are provided by the computation above.

Using finite differences of the four-point implicit pattern, the differential equation can be transformed into a finite difference equation. Fig. 4 shows the difference pattern. The time and space spans are the same as used for the calculation of the flow field.

For variable θ , we have the following formulae :

$$\frac{a\theta}{at} = \left(\theta_i^j - \theta_i^j\right)/\Delta t \quad (55)$$

$$\frac{a\theta}{ax} = \Delta x_{1+1} \frac{\Delta x_i}{(\Delta x_1 + \Delta x_{i+1})}\theta_{i+1}^j + \frac{\Delta x_{i+1} - \Delta x_i}{\Delta x_1 \bullet \Delta x_{i+1}} \theta_i^j - \frac{\Delta x_{i+1}}{\Delta x_i (\Delta x_i + \Delta x_{i+1})}\theta_{i-1}^j \quad (56)$$

$$\frac{a^2\theta}{ax^2} = \frac{4\left(\theta_{i+1}^j - 2\,\theta_i^j + \theta_{i-1}^j\right)}{(\Delta x_1 + \Delta x_{i+1})^2} \quad (57)$$

Using these formulas to replace the partial derivative terms of the differential equation and to put it in order, we obtain difference equations of the following type :

$$L_{i-1} + a_i' L_i + b_i' L_{i+1} = R_i' \quad (58)$$

where a_i' , b_i' and R_i' are coefficients.

For each two segments, we have an equation of this type. The segments between two cross sections that are related to the nodes of the stream network are the so-called false segments. For these segments we use the equilibrium equation to connect the flows in the relevant channels. With the marginal conditions added, the equations are closed and can be solved. The coefficient matrix of the equations is of the tridiagonal type, the coefficients of the equations for the false segments being discrete. These equations can be solved with the combined catch-up/feedback method mentioned above.

Here, the letter L could be the concentration of BOD, of NH_3-N, NO_3 –N, NO_2-N or any other oxygen consuming material. Taking into account several kinds of factors of the biochemical oxygen demand, we obtain several groups of equations of the same type as discussed above.

The third step deals with the calculation of the concentration of dissolved oxygen. The relevant equations are :

$$\frac{a(A.D)}{at} + \frac{a(A.U.D)}{ax} = \frac{a}{ax}\left(A.E_x.\frac{aD}{ax}\right) + K_2.A.(D_s - D) - \sum_{io=1}^{P_0} K_{io}.A.L. + S_1 \qquad i \neq i,1 \quad (59)$$

$$\frac{aD}{at}.V_{j1} = \Delta D_{j1} \qquad i = i,1 \quad (60)$$

Marginal conditions,

D (i,j) = d1 (f ,j) i = f (61)

Initial conditions,

D (i,0) = d0 (i) j = 0 (62)

These equations have the same structure as those for organic pollutants and can be solved in the same way.

Having completed all the three steps, we can turn to the calculation of the next time stage and repeat the three steps of calculation. In this way, steps by step, we obtain the results of all variables at different times and places.

II. DISCUSSION AND CONCLUSION

Mathematical models of water quality are powerful tools to study pollution processes in rivers, especially in tidal stream networks (Fu, 1982). It is impossible to assess the present and future conditions of the water quality in a tidal stream network without mathematical models. By using the models, we can provide planers, managers and decision-makers with sufficient and concrete information, especially information for hypothetical cases. However, models cannot do the work of planners, managers and decision-makers.

The mathematical model of water quality in tidal stream networks has universal significance and can be used for various tidal stream networks (Rich, 1981). When applying the model to a given stream network, it is necessary to incorporate the cross sections of this system, to evaluate the coefficients and to calibrate the model using the information available on the system under study.

The information obtained by measurements and monitoring is most important in developing a mathematical model of water quality (Zhang, 1982). Since there are many channels in a stream network, a sufficient number of measuring points is needed to obtain reliable information. Measurements should be made, and samples taken, continuously and simultaneously at all points. It is not easy to obtain sufficient information. But if the model is well founded, it is considerably easier to study and manage the water resources in stream networks. Measurements should always be taken over two full tides in order to avoid being hoodwinked by false mathematical phenomena in the early period of calculation (Zhan, 1981).

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