MATHEMATICAL MODELING FOR WATER QUALITY MANAGEMENT

by

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INTRODUCTION

It is estimated that by the year 2000, the population of the United States will reach 300 million people. It is also estimated that to reach a modest level of this nation's water quality goals will require an expenditure of from 2 to 5 billion dollars per year. To achieve these national water quality objectives in a most effective and economical way will require comprehensive planning and a thorough analysis of the complex alternatives for wastewater management. This need for planning was recognized by the federal regulations regarding construction grants for wastewater collection and treatment systems published July 2, 1970, which states that all such projects must be part of a comprehensive plan in order to be eligible for federal aid. To insure the selection of an optimum plan for wastewater management and to have the means of projecting future needs and identifying long-range plans, comprehensive planning must be based on sound mathematical models. Mathematical models can be utilized to analyze past data, assess present conditons and predict future requirements. Only through the use of mathematical modeling can optimal solutions be obtained to meet the set economic and social constraints.

Mathematical models used in water quality management studies may be classified into (a) water quality or mass distribution models and (b) management models. Figure 1 presents the relationship between water quality and management models as utilized in water quality management studies.

WATER QUALITY MODELS

Water quality models are usually used to predict the response of a water system to a certain waste input. This type of a model describes the temporal and spatial distribution of any substance, conservative or nonconservative, within a water body. For any combination of waste inputs, a water quality model can predict whether specific water quality goals can be met in the future. Water quality models have often been used to describe the temporal and spatial distribution of the dissolved oxygen in natural water systems and therefore define the assimilative capacity of such waters. In addition to dissolved oxygen, water quality models may be used to model phosphorus, coliform, phytoplankton, all forms of nitrogen, chloride, and metal ions.

Development of a water quality model is usually based on the principle of conservation of mass. The factors which affect the concentration of pollutants in a water system include dispersion, advection, and reactions. Dispersion and advection depend on the hydrodynamic characteristics of the natural water system while the reactions are a function of the pollutant being modeled. The magnitude of any of these factors, therefore, depends on both the water body and the pollutant being modeled.

A typical example of a one-dimensional water quality model follows:

$$\frac{1}{A(x,t)} \frac{\partial[C(x,t)\ A(x,t)]}{\partial t} = - \frac{1}{A(x,t)} \frac{\partial[Q(x,t)\ C(x,t)]}{\partial x} + \frac{1}{A(x,t)}$$

$$\frac{\partial}{\partial x} [E_{(x,t)}\ A_{(x,t)} \frac{\partial C(x,t)}{\partial x}] \pm \Sigma S \tag{1}$$

where:

$\frac{\partial[Q(x,t)\ C(x,t)]}{\partial x}$ = transport due to advection

$\frac{\partial}{\partial x} [E_{(x,t)}\ A_{(x,t)} \frac{\partial C(x,t)}{\partial x}$ = distribution due to dispersion

ΣS = sources and sinks. For dissolved oxygen, for example, sources will include reaeration and oxygen production by photosynthesis while oxygen utilization for the oxidation of carbonaceous and nitrogenous matter, respiration of aquatic plants, and oxygen demand of bottom deposits constitute the sink factors.

Equation (1) has been widely used to define the temporal and spatial distribution of conservative and non-conservative substances within the natural water systems. The steady-state form of equation 1, for example, was used for the modeling of dissolved oxygen within the fresh water streams and the tidal estuaries of the Pascagoula River Basin (1,2). The general equation used for the fresh water streams is as follows:

$$D = \frac{K_d L_o}{K_a - K_r} (e^{-K_r \frac{x}{U}} - e^{-K_a \frac{x}{U}}) \tag{2a}$$

$$+ \frac{K_n N_o}{K_a - K_n} (e^{-K_n \frac{x}{U}} - e^{-K_a \frac{x}{U}}) \tag{2b}$$

$$+ \frac{R}{K_a} (1 - e^{-K_a \frac{x}{U}}) \tag{2c}$$

$$- \frac{P}{K_a} (1 - e^{-K_a \frac{x}{U}}) \tag{2d}$$

$$+ \frac{S}{K_a} (1 - e^{-K_a \frac{x}{U}}) \tag{2e}$$

$$+ D_o \, e^{-K_a \frac{x}{U}} \tag{2f}$$

where D_o represents the initial dissolved oxygen deficit. Equation (5) was applied to model the dissolved oxygen distribution within the fresh water streams of the Pascagoula River Basin. The various parts of Equation (2) are defined as follows:

a. Dissolved oxygen deficit due to source of CBOD
b. Dissolved oxygen deficit due to source of NBOD
c. Dissolved oxygen deficit due to algal respiration
d. Dissolved oxygen deficit due to photosynthesis
e. Dissolved oxygen deficit due to bottom deposits
f. Initial value of dissolved oxygen deficit

For the tidal estuaries, however, the two-dimensional steady-state form of equation (1) was used. The two-dimensional model applied is as follows:

$$\begin{aligned}
& a_{i-1,j} \, C_{i-1,j} + [a_{i,j} - V_{i,j} \, (K_a)_{i,j}] \, C_{i,j} + a_{i+1,j} \, C_{i+1,j} \\
& + a_{i,j-1} \, C_{i,j-1} + a_{i,j+1} \, C_{i,j+1} - V_{i,j} \, (K_d)_{i,j} \, L_{i,j} \\
& - V_{i,j} \, (K_n)_{i,j} \, N_{i,j} + V_{i,j} \, P_{i,j} - V_{i,j} \, R_{i,j} \\
& - V_{i,j} \, S_{i,j} + W_{i,j} + V_{i,j} \, (K_a)_{i,j} \, C_s = V_{i,j} \, \frac{\Delta C_{i,j}}{\Delta t}
\end{aligned} \tag{3}$$

in which

$$\begin{aligned}
a_{i-1,j} &= Q_{i-\frac{1}{2},j} \, \alpha_{i-\frac{1}{2},j} + E'_{i-\frac{1}{2},j} \\
a_{i,j} &= (Q_{i-\frac{1}{2},j} \, \beta_{i-\frac{1}{2},j} - E'_{i-\frac{1}{2},j}) - (Q_{i+\frac{1}{2},j} \, \alpha_{i+\frac{1}{2},j} + E'_{i+\frac{1}{2},j}) \\
&\quad + (Q_{i,j-\frac{1}{2}} \, \beta_{i,j-\frac{1}{2}} - E'_{i,j-\frac{1}{2}}) - (Q_{i,j+\frac{1}{2}} \, \alpha_{i,j+\frac{1}{2}} + E'_{i,j+\frac{1}{2}}) \\
a_{i+1,j} &= -Q_{i+\frac{1}{2},j} \, \beta_{i+\frac{1}{2},j} + E'_{i+\frac{1}{2},j} \\
a_{i,j-1} &= Q_{i,j-\frac{1}{2}} \, \alpha_{i,j-\frac{1}{2}} + E'_{i,j-\frac{1}{2}} \\
a_{i,j+1} &= -Q_{i,j+\frac{1}{2}} \, \beta_{i,j+\frac{1}{2}} + E'_{i,j+\frac{1}{2}} \\
E' &= \frac{EA}{\ell}
\end{aligned}$$

Where C is the concentration of the dissolved oxygen; A is the cross-sectional area at the interface between two adjacent elements; E is the dispersion coefficient across the interface between two adjacent elements; $\bar{\ell}$ is the average length of two adjacent elements; Q is the fresh water flow across the interface between adjacent elements; V is the volume of any element; t is the time in units of tidal cycles; α and β are weighing factors ($\alpha + \beta = 1.0$); L is the ultimate carbonaceous BOD; N is the Nitrogenous BOD; K_a is the reaeration coefficient; K_d is the deoxygenation coefficient; P represents oxygen production by photosynthesis; R represents oxygen utilization through respiration of aquatic plants; S is the oxygen demand of bottom deposits; and W represents dissolved oxygen added through dilution.

Both models were verified against field data collected under various combinations of waste inputs, fresh water flow and temperature. Examples of the verification profiles are presented in Figures 2 and 3. The models are currently being used as planning tools to assess present water quality conditions and to project the effect of future municipal and industrial loads on the water quality in the receiving streams. Typical applications of the models to determine the levels of wastewater treatment that will meet the water quality criteria set for the receiving streams are presented in Figures 4 and 5.

The output from a water quality model usually serves as an input to a management model to determine the most effective solution to the water quality management problem - - - one which achieves the desired water quality objectives at a minimum cost. Thus it is evident that water quality models serve as the foundation for a comprehensive management and pollution abatement program for the entire basin.

MANAGEMENT MODELS

Management models utilize the output from the water quality along with specific constraints such as water quality criteria and cost functions, to predict the least cost alternative of waste collection, treatment and disposal in the region. These models basically use optimization techniques to evaluate the alternatives and select the optimum solution that meets the water quality goals. Both linear as well as nonlinear programming techniques may be utilized in solving optimization problems as applied to water quality management.

Management models may be classified into basin management models and regional management models. Basin management models are utilized to determine the optimum waste allocations or associated treatment levels of all waste sources along a river or an estuary. Regional models, however, are utilized to select the optimum plan for wastewater collection, treatment and disposal within a region. Such optimization techniques will provide information regarding treatment plant capacities and locations, waste sources to be served, location, and size of mains, trunk sewers, pumping stations, and force mains. Several management models are available in the literature. Input data to management models generally consist of:

1. Transfer function - quality response due to waste load input. Transfer functions are usually obtained from the water quality models.

2. Water quality criteria - Maximum acceptable concentrations of critical water quality constituents in the water system must be defined.

3. Lower bound on treatment levels - the minimum acceptable degree of treatment as specified by the pollution control agency in the region.

4. Hydrology of the basin

5. Locations, quantities, and composition of waste effluents generated by the various municipalities and industries in the basin.

6. Cost function - Total cost of treatment as related to the degree of treatment must be defined.

GENERAL MODELING PROCEDURE

In general the modeling effort recommended in conducting a complete water quality planning study consist of:

1. Segmentation of the system - The natural water system is usually segmented according to location of waste inputs, tributaries, and the change in the hydrological characteristics of the water body. Each segment must have its own geometric characteristics and reaction coefficients.

2. Evaluation of all existing hydrologic and water quality data - This procedure will identify any descrepancies which may exist in the available data and, therefore, help define the skeleton of the field survey to collect any additional data that may be needed.

3. Development of the water quality model - All available models must be examined for possible adoption to the basin under investigation.

4. Verification of the model - To determine whether the developed model adequately describes the system, the calculated profiles must be compared to the observed profiles for various combinations of waste loads, temperature and fresh water flows. The model is considered verified if it has successfully predicted the water quality for various conbinations of inputs.

5. Application of the model - Following verification the model may be used to predict future water qualities in the water system for any waste inputs.

6. Optimization of the water quality management. The output from the water quality model is used along with specific constraints to optimize the wastewater management within the basin.

SUMMARY AND CONCLUSIONS

This paper attempted to define the scope and magnitude of the water quality planning problem and describe the general modeling procedure utilized in selecting the least cost plan which satisfies the needs and desires of a river basin. As the reader may have realized, planning for complete water quality management is a very complex problem, the solution of which requires not only a great expenditure but the expertise in several disciplines such as environmental engineering, computer programming, statistics, operation research, hydrology, and economics. Fortunately, however the successful application of mathematical modeling to water quality management problems has been greatly simplified by computer computations.

Mathematical models used in water quality management studies may be classified into water quality models and management models. Water quality models are usually used to predict the response of a water system to a certain waste input. Thus for any waste input, the temporal and spatial distribution of any substance, conservative or nonconservative, may be described, therefore, identifying whether water quality goals can be met. The output from a water quality model referred to as the transfer function usually serves as an input to a management model to determine the most effective plan to the water quality management. Thus it is evident that water quality models serve as the heart for any comprehensive water quality management program. Development of water quality models is usually based upon the principle of conservation of mass around an elemental volume.

Management models utilize the output from the water quality models and linear or nonlinear programming techniques to select the least cost wastewater treatment program that meets the desired water quality goals. Management models may be classified into basin wide models and regional models.

REFERENCES

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2. Shindala, A., Zitta, V. L. and Corey, M. W., "Water Quality Models For The Pascagoula River Basin II. Tidal Estuaries", EIRS-CE-73-2, Mississippi State University, 1973.

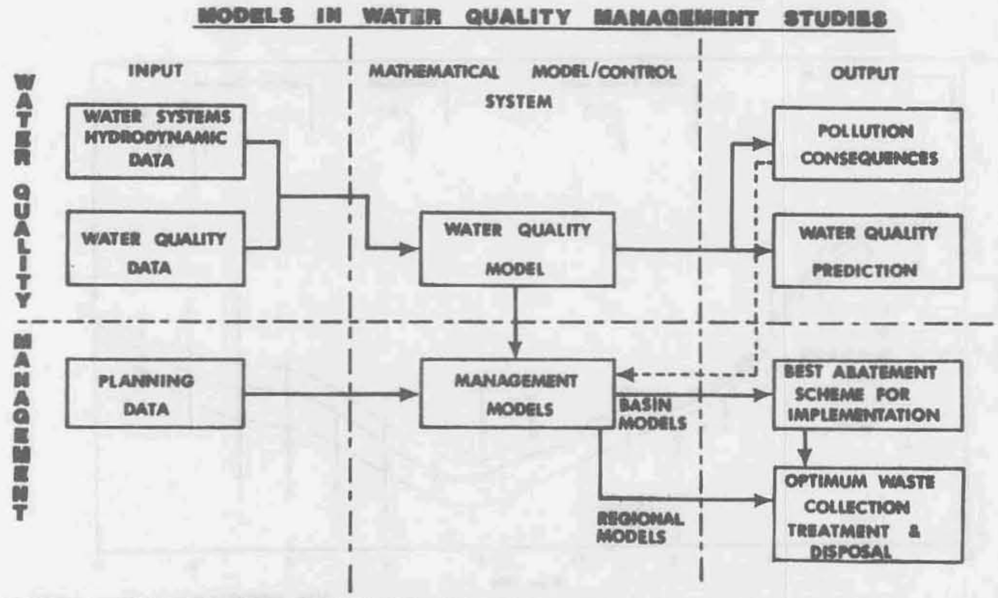

FIGURE I. GENERAL REPRESENTATION OF MODELS USED IN WATER QUALITY MANAGEMENT STUDIES.

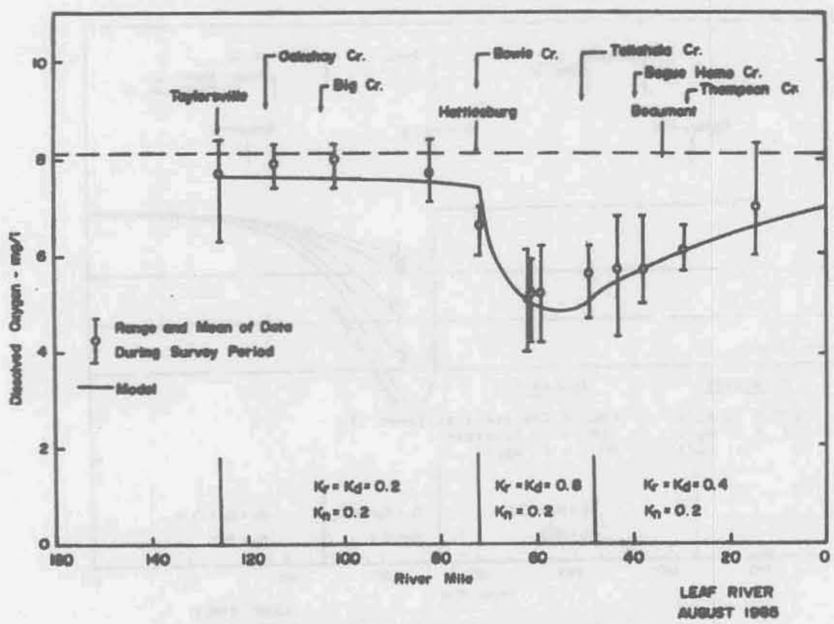

FIGURE 2. FRESH WATER MODEL VERIFICATION

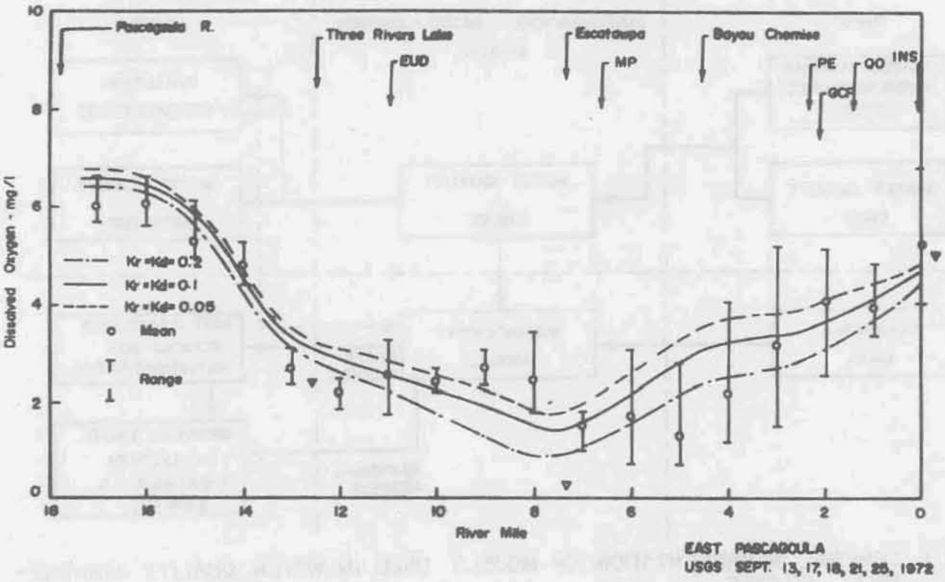

FIGURE 3. ESTUARINE MODEL VERIFICATION

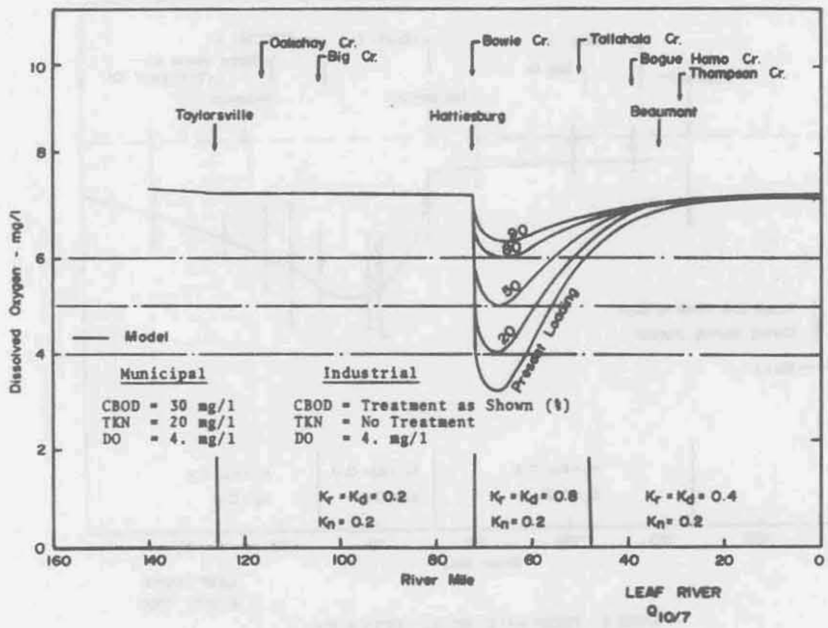

FIGURE 4. FRESH WATER MODEL APPLICATION

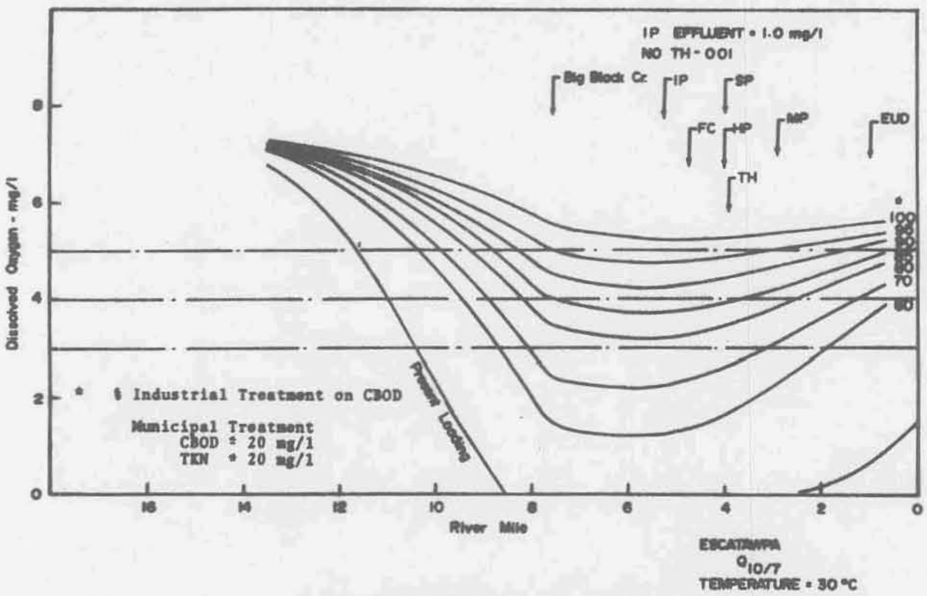

FIGURE 5. ESTUARINE MODEL APPLICATION