MATHEMATICAL MODELING OF WATER QUALITY

by

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INTRODUCTION

Concern with the environment has made it necessary to attempt to assess the "Environmental impact" of proposed water resource projects. Whether the project is a waste discharge into a waterway or a large impoundment, the engineer must try to determine the effect of the project on the physical, chemical, and biological characteristics of the existing water resource system. Generally this determination can best be made through the use of a "model" to represent the existing system. The model can then be modified by the proposed project and the effect observed over space and time.

One type of model is a physical model, usually to a smaller scale than the prototype. Assuming all the pertinent parameters can be appropriately scaled for the model, this type of modeling allows three-dimensional spatial representation of the system, and the effect of the proposed project can be observed and evaluated. Some limitations to this type of modeling are the cost, the amount of time required, and the somewhat limited flexibility if a large number of system variations must be studied.

A second type of model is an analog model. The analog model represents the physical system by an electronic network. An advantage of this type of model is that it produces a continuous solution. Analog models have not been generally applied to water quality problems and their potential in this area has yet to be developed.

A third type of model is the mathematical model. This type of model is developed by representing the physical system processes by mathematical relationships. These relationships can then be evaluated for various values of the input parameters. The mathematical model is generally inexpensive, requires little operation time, and has great flexibility. The biggest limitations to this type of modeling are first formulating the mathematical relationships to represent the physical processes and second being able to evaluate those relationships.

Any one type of model or any combination of models might be applied to a particular situation depending on the situation's requirements.

MATHEMATICAL MODELS

Mathematical modeling of water quality parameters involves mathematically describing the function of each quality parameter in relation to the physical environment as well as the interrelationships between individual parameters. Mathematically, these relationships soon become formidable. Present application of mathematical models to water quality parameters has involved the introduction of certain simplifying assumptions so as to allow solution to the mathematical relationships. One of the most common of these simplifying assumptions is that of uniformity in two spatial directions. This reduces the problem to a one-dimensional spatial variation problem, which can generally be solved with the aid of a digital computer.

River Modeling

Mathematical models have been developed to represent the temperature, conservative chemical content, and biochemical oxygen demand - dissolved oxygen content of a river system. To reduce the model to a one dimensional spatial model the assumption is made that the river is fully mixed in the vertical and lateral directions and that variation occurs only in the longitudinal direction. The river can then be discretized into longitudinal sections or reaches. A typical reach with a schematic representation of material balance[1] is shown in Figure 1.

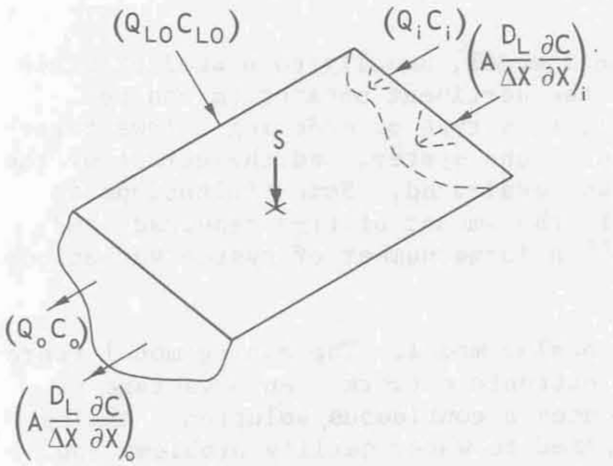

Fig. 1. Schematic of Material Balance in a Typical Reach[1]

where Q_i = Rate of flow into the reach
C_i = concentration of the constituent in Q_i
Q_o = Rate of flow out of the reach
C_o = Concentration of the constituent in Q_o
Q_{Lo} = Local inflows or withdrawals
C_{Lo} = Concentration of the constituent in Q_{Lo}
S = Sources or sinks of a non-conservative constituent

$(A \frac{DL}{\Delta x} \frac{\partial C}{\partial x})_i$ = Total longitudinal dispersion of the constituent on the inflow side of the reach

$(A \frac{DL}{\Delta x} \frac{\partial C}{\partial x})_o$ = Total longitudinal dispersion of the constituent on the outflow side of the reach

From this schematic representation, the basic equation describing the mass transport of conservative and non-conservative constituents with time can be written[1],

$$A \frac{\partial c}{\partial t} = \frac{\partial (ADL \frac{\partial C}{\partial X})}{\partial x} - \frac{\partial (AVC)}{\partial x} \pm AS \qquad (1)$$

where A = Cross sectional area
C = Concentration of the constituent

V = Mean velocity of the river
D_L = Longitudinal dispersion coefficient
t = Time
X = Longitudinal distance
S = Sources or sinks of non-conservative constituents

For each of the various water quality constituents, the sources and sinks are evaluated and the model yields the distribution of the constituent in space and time. For example, the sources and sinks for temperature (net heat exchange at the air water interface) can be computed from meteorological data, and for dissolved oxygen can be approximated with first-order rate equations.[1]

Variations to the river model include consideration of variation in the lateral as well as longitudinal directions (two-dimensional model), consideration of unsteady flow conditions, and consideration of other water quality parameters.

Reservoir Modeling

In a reservoir, most water quality parameters can be in some way related to density stratification. Temperature is considered to be the dominant factor controlling density stratification and hence considerable work has been done in mathematical modeling of reservoir thermal stratification. Modeling of water quality parameters in a reservoir is similar to the approach used for the river model except, one-dimensional spatial variation is assumed in the vertical direction only. The reservoir is discretized into vertical layers, and within each layer the quality constituents are assumed to be uniform in the lateral and longitudinal directions. A schematic representation of the thermal balance for a typical layer[2] is shown in Figure 2.

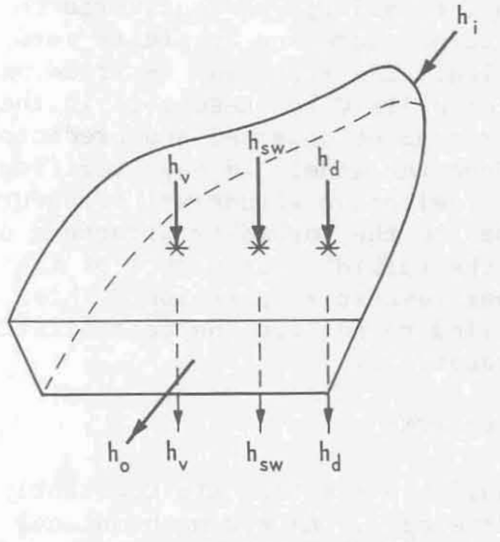

Fig. 2. Schematic of the Thermal Balance in a Typical Layer

where h_i = Rate of heat inflow to the layer
h_o = Rate of heat outflow from the layer
h_v = Net vertical advection of heat into the layer
hsw = Net short wave radiation into the layer
hd = Net vertical diffusion of heat into the layer

From this schematic, the equation for the conservation of heat in the layer can be described as[3],

$$\frac{\partial T}{\partial t} + \frac{1}{A}\frac{\partial (Qvt)}{\partial Z} = \frac{1}{A}\frac{\partial}{\partial Z} KA\frac{\partial T}{\partial Z} + \frac{TLQL}{A\Delta Z} - \frac{ToQo}{A\Delta Z} + \frac{1}{pcpA}\frac{\partial H}{\partial Z} \quad (2)$$

where T = Temperature
t = Time
A = Horizontal cross sectional area
Qv = Vertical flow
Z = Elevation
K = Vertical diffusion coefficient
TL = Temperature of inflow
QL = Inflow
To - Temperature of outflow
Qo = Outflow
p = Density of water
Cp = Specific heat of water
$\frac{\partial H}{\partial Z}$ = External heat source

By describing appropriate boundary conditions and the sources and sinks of heat, the model yields the vertical distribution of temperature in the reservoir as a function of time. Like the river models, reservoir models have been used to represent the conservative chemical content and biochemical oxygen demand - dissolved oxygen content of reservoirs, and again numerous variations of reservoir models exist.

USE OF THE MATHEMATICAL MODEL - AN EXAMPLE STUDY

Engineers at the Waterways Experiment Station, U. S. Army Corps of Engineers, recently completed a study[4] in which a mathematical model was used to simulate the thermal and turbidity structure of an impoundment. Turbidity is an optical property of water related to the concentration of suspended sediment. For this study, turbidity was considered to act as a conservative constituent. Both temperature and turbidity were assumed to effect density stratification. The model was verified with observed thermal and turbidity data for Hills Creek Reservoir in the Willamette Basin, Oregon. Some comparisons of observed and predicted profiles[4] are shown in Appendix A. Once the model had been verified, it was used to evaluate the effects of selective withdrawal procedures and various reservoir operation schemes on the turbidity structure of the reservoir. The study indicated that the turbidity structure of the reservoir could be controlled by proper reservoir operation. This mathematical model has since been applied to analyze the possibilities for turbidity control at a proposed reservoir.

FUTURE APPLICATIONS

Mathematical models for water quality parameters are constantly being improved and new models being developed. As new mathematical techniques become available, more complex relationships can be analyzed and the need for "simplifying assumptions" reduced. Two dimensional reservoir models are currently under development. Also, greater quantities of quality parameters must now be considered. "Ecosystem models" have been applied to several Corps of Engineers projects. In addition to temperature, conservative chemicals, and dissolved oxygen, these models simulate such parameters as algal and fish populations and acidity or alkalinity (PH). Entire river basin water quality models consisting of coupled river and reservoir models are being developed.

Mathematical models provide a powerful tool for the analysis of water quality parameters. The engineer should, by using mathematical, physical, and analog models, have the ability to make reasonable assessments of the "environmental impact" of proposed projects. As modeling techniques continue to improve, so will these assessments.

LITERATURE CITED

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3. Eiker, E. E., "Heat Budget Analysis of Reservoirs," paper presented to the Development of Data for Design of Selective Withdrawal Outlets Training Course, 13-17 November 1972, U. S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, Mississippi.

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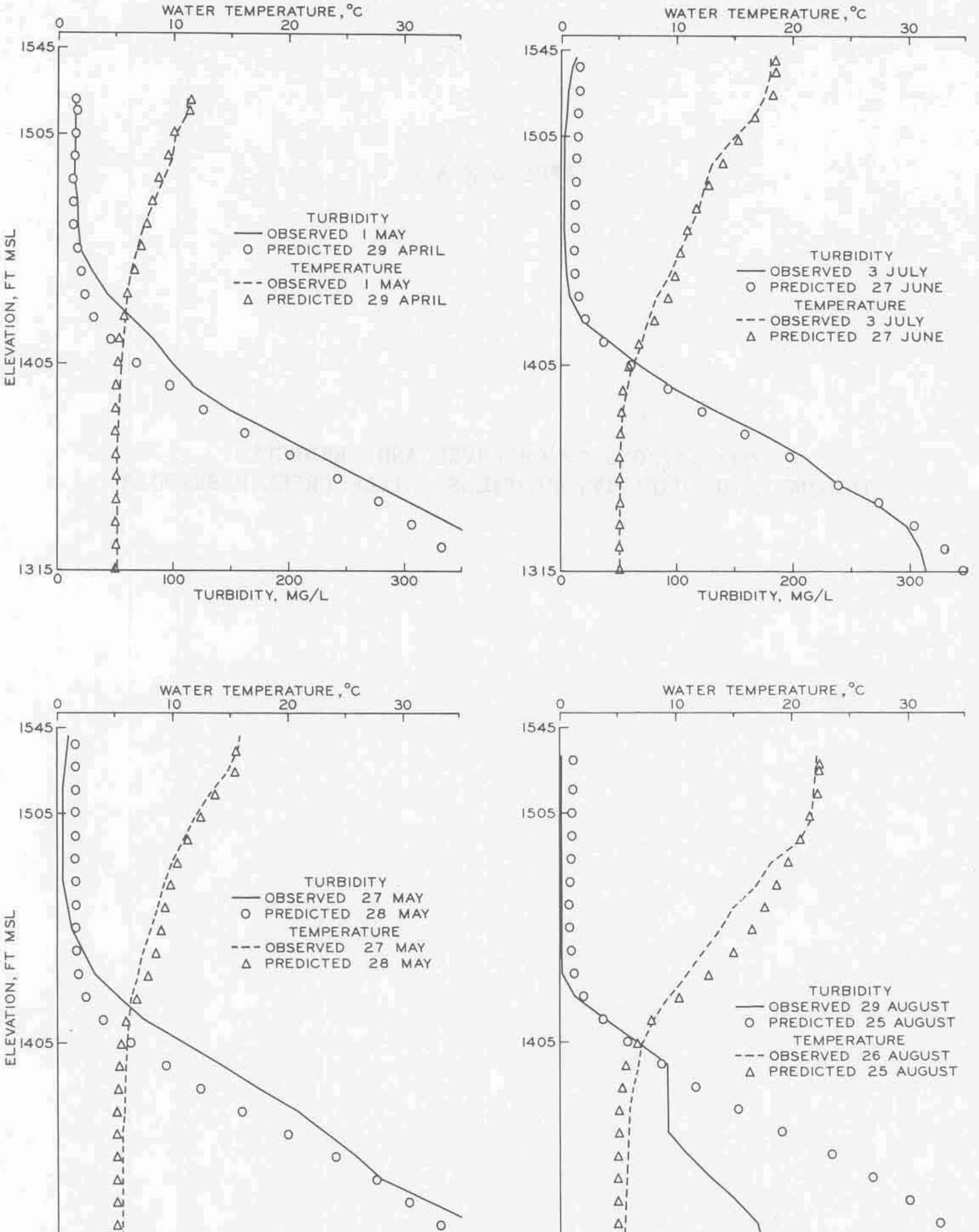
APPENDIX A

COMPARISONS OF OBSERVED AND PREDICTED THERMAL AND TURBIDITY PROFILES, HILLS CREEK RESERVOIR



HILLS CREEK RESERVOIR, 1971

OBSERVED AND PREDICTED TEMPERATURE AND TURBIDITY PROFILES

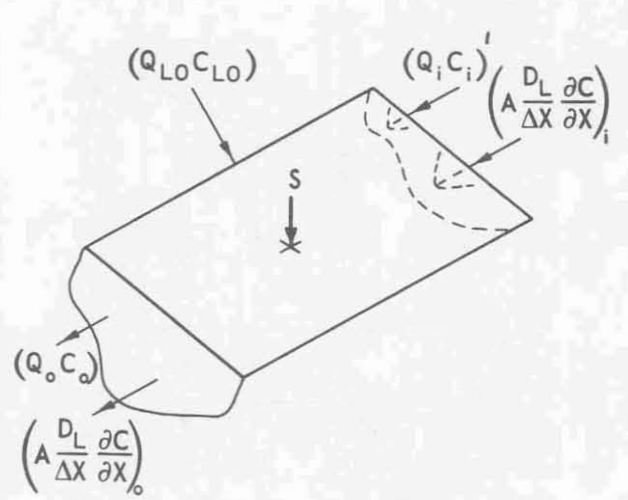


Fig. 1. Schematic of Material Balance in a Typical Reach[1]

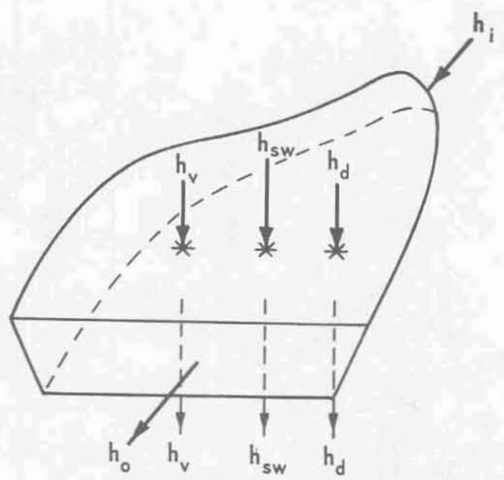


Fig. 2. Schematic of the Thermal Balance in a Typical Layer