DEVELOPMENT OF A WATER QUALITY MODEL FOR THE UPPER TENNESSEE-TOMBIGBEE WATERWAY

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Introduction

The Tennessee-Tombigbee Waterway (Tenn-Tom) is a 233.7 mile river/canal system that connects the north flowing Tennessee River to the south flowing Tombigbee River. It flows in a southeasterly direction from the Tennessee River in northeast Mississippi to Demopolis, Alabama, where it connects to the Black Warrior-Tombigbee River system. The purpose of the Waterway is to provide modern barge traffic with a continuous navigational route suitable for travel from the Tennessee, upper Mississippi, and Ohio River Valleys to the Port of Mobile, Alabama, on the Gulf of Mexico.[1,2]

The Waterway consists of a series of lakes and canals held in place by twelve locks and dams. The modern locks are 600 feet long and 110 feet wide and raise river traffic from an elevation of 73 feet at Demopolis, Alabama, to an elevation of 414 feet at Pickwick Lake which is located at the confluence of the Waterway with the Tennessee River.[1]

In addition to navigation, Tenn-Tom will provide unlimited recreational opportunities and stimulate industrial development within the region. This industrialization, in turn, will tend to promote population growth and economic development within the adjoining communities and counties. Unfortunately, population growth and industrial development are normally accompanied with an increased demand for water and wastewater disposal facilities. It is anticipated that the volume of wastewater generated by industry and the surrounding municipalities will increase in direct proportion to regional development. The Tenn-Tom will receive the vast majority of these wastes. Water quality, and its associated usability for industrial, municipal, and/or recreation purposes, may be adversely impacted by the nature or amount of the contaminants discharged.

Virtually every industry locating along the water way will require wastewater disposal. Each will vie, as will adjacent municipalities, for a share of the waste assimilative capacity provided by the Waterway. In order to preserve the water quality standards of the waterway, it is likely that strict limits will be imposed on all waste discharges. Furthermore, as the Tenn-Tom corridor becomes increasingly developed, restrictions will likely become more stringent. It is essential that all wastes discharged into the waterway be closely and accurately controlled.

Federal and state law mandates that the discharge of pollutants be regulated in a way to minimize or eliminate the impact of this activity on the environment. To achieve this, the Office of Pollution Control (OPC) within the Mississippi Department of Environmental Quality must determine the maximum waste assimilative capacity for this water course. A key element in this determination is the water quality model. A mathematical system used to relate water quality to waste input, the water quality model can be used as a planning tool to permit estimation of assimilative capacity and assessment of the effects of discharging waste to the Tenn-Tom water.

The water quality model previously used by OPC for waste load allocations may not accurately assess the water quality response of the Tenn-Tom. This is due, in part, to the complex hydrologic and geometric characteristics of the waterway and the simplified kinetic formulations incorporated into the existing model. It thereby seems necessary to develop a new water quality model that can accurately describe the waste assimilative capacity, and thus the waste allocation of the Tenn-Tom which constitutes the primary objective of the work reported here. The secondary objective of this work was to define the existing water quality within the waterway.

Mass Transport Equation

The basic equation solved by this model is the one dimensional advection, dispersion mass transport equation, which is numerically integrated over space and time for each water quality constituent.[3] This equation includes the effects of advection, dispersion, dilution, constituent reactions and interactions, and sources and sinks. For any constituent, C, this equation can be written as:

$$\frac{\partial M}{\partial t} = \frac{\partial (A_x D_L \frac{\partial C}{\partial x})}{\partial x} dx - \frac{\partial (A_x \bar{u} C)}{\partial x} dx + (A_x \ dx) \frac{dC}{dt} + S$$

where

M = mass (M)
x = distance (L)
t = time (T)
C = concentration ($M\ L^{-3}$)
A_x = cross-sectional area (L^2)
D_L = dispersion coefficient ($L^2\ T^{-1}$)
u = mean velocity ($L\ T^{-1}$)
s = external source or sinks ($M\ T^{-1}$)

Because M = VC, we can write

$$\frac{\partial M}{\partial t} = \frac{\partial (VC)}{\partial t} = V \frac{\partial C}{\partial t} + C \frac{\partial V}{\partial t}$$

where:

$V = A_x\ dx$ = incremental volume (L^3)

If we assume that the flow in the stream is steady, i.e., $\partial Q/\partial t = 0$, then the term $\partial V/\partial t = 0$ and this equation becomes:

$$\frac{\partial M}{\partial t} = V \frac{\partial C}{\partial t}$$

Combining this equation with the mass transport equation, and rearranging yields:

$$\frac{\partial C}{\partial t} = \frac{\partial (A_x\ D_L \frac{\partial C}{\partial x})}{A_x\ \partial x} - \frac{\partial (A_x \bar{u} C)}{A_x\ \partial x} + \frac{dC}{dt} + \frac{S}{V}$$

The terms on the right-hand side of the equation represent, respectively, dispersion, advection, constituent changes, external sources/sinks, and dilution. The dC/dt term refers only to constituent changes such as growth and decay and should not be confused with the term $\partial C/\partial t$, the local concentration gradient. The latter term includes the effect of constituent changes as well as dispersion, advection, sources/sinks, and dilutions. Under steady-state conditions, the local derivative becomes equal to zero; in other words:

$$\frac{\partial C}{\partial t} = 0$$

Changes that occur to individual constituents or particles independent of advection, dispersion, and waste inputs are defined by the term

$$\frac{dC}{dt} = \text{individual constituents changes.}$$

These changes include the physical, chemical, and biological reactions and interactions that occur in the stream. Examples of these changes are reaeration, algal respiration and photosynthesis, and coliform die-off.

$$\frac{-1}{A_x} \frac{\partial}{\partial x} (A_x\ \bar{u}\ C)$$

equals mass transport due to net advection,

$$\frac{1}{A_x} \frac{\partial}{\partial x} (D_L A_x \frac{\partial C}{\partial x})$$

equals mass transportation to net dispersion,

$$\frac{dC}{dt}$$

equals mass change due to internal constituent physical, chemical, and biological reactions and interactions (e.g., CBOD, NBOD, algal photosynthesis and respiration, sediment oxygen demand). This is sometimes referred to as internal sources and sinks.

$$\frac{S}{V}$$

equals mass change due to external sources and sinks like point waste source, flow withdrawals, etc.

Longitudinal Dispersion

Dispersion is basically a convective transport mechanism. The term "dispersion" is generally used for transport associated with spatially averaged velocity variation, as opposed to "diffusion", which is reserved for transport that is associated primarily with time-averaged velocity fluctuations.

Fischer, et al. (4) suggest the following for an estimate of the dispersion coefficient in real streams:

$$D_L = 1.097 \times 10^{-2} [U^2 B^2 / (H U^*)$$

where:

D_L = longitudinal dispersion coefficient, ft^2/sec,
U = mean river velocity, fps,
B = mean channel width, ft,
H = mean depth, ft,
U^* = average river shear velocity, fps,
$U^* = (g\ H\ S)^{1/2} = (\tau_o/\rho)^{1/2}$,
S = river channel slope, ft/ft,
g = the gravitational constant, 32.2 ft/sec^2,

τ_o = Boundary shear stress, lb/ft^2, and
ρ = Mass fluid density, $lb\text{-}sec^2/ft^4$.

This equation has the distinct advantage of estimating A_x from parameters which are usually known. (French 1985).

Hydraulic Parameters

Every water quality model requires information about hydraulic conditions within the water course being examined. This information often includes such parameters as average velocity, depth, flow, and water surface area and must be defined for the specific conditions being modeled. This can be supplied from field measurements but requires extrapolation and projection based on limited amounts of data. An alternative is to calculate the required values using a mathematical model of the water course's hydraulic characteristics.

The HEC-2 computer program [5] is an example of one hydraulic model that has been found well suited to providing this information. Several water quality models have been used successfully in conjunction with HEC-2. For this study, successful modeling efforts using HEC-2 to provide hydraulic data have transferred this information into this water quality model.

Dissolved Oxygen Model

One of the most important considerations in determining the waste-assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. Dissolved oxygen concentrations in streams are controlled by atmospheric reaeration, photosynthesis, plant and animal respiration, benthal demand, biochemical oxygen demand, nitrification, salinity, and temperature, among other factors. The model includes the major interactions of the nutrient cycles, algae production, benthic oxygen demand, carbonaceous oxygen uptake, atmospheric aeration, and their effect on the behavior of dissolved oxygen. Figure 1 illustrates the conceptualization of these interactions. The arrows on the figure indicate the direction of normal system progression in a moderately polluted environment; the directions may be reversed in some circumstances for some constituents.

Coliforms and the arbitrary nonconservative constituent are modeled as nonconservative decaying constituents and do not interact with other constituents. The conservative constituents, of course, neither decay nor interact in any way with other constituents.

Atmospheric Reaeration

Atmospheric reaeration is the process of oxygen transfer from the atmosphere into the water body. Atmospheric reaeration is the major source of oxygen to a receiving stream.

The model provides for the estimation of K_2 using O'Connor-Dobbins model as published in 1958.[6] This formulation is represented by:

$$K_2 = 12.9\ U^{0.5}/d^{1.5}$$

where:

U = average velocity in the stream, ft/sec.
d = average depth of the stream, ft, and
K_2 = base e reaeration coefficient at 20°C, day^{-1}.

The O'Connor-Dobbins equation was theoretically derived from the surface renewal of the liquid film through internal turbulence. This equation is the most widely used model for predicting the reaeration coefficient of rivers. It has been extensively tested and verified against in-situ measured reaeration coefficients utilizing the radioactive tracer technique. It is recommended for use in rivers having depths ranging from two to thirty feet and velocities of 9.2 to 2.0 fps. It was successfully verified and recommended for use on the lower Ouachita River Basin which, like the Tenn-Tom Waterway, is controlled by lock and dam structures and used exclusively for navigational purposes. Average depth in Ouachita ranged from ten to thirty feet with velocities being observed as low as 0.1 fps.

However it must be noted that during low flow conditions the average velocities in the Tenn-Tom are extremely low (below 0.1 fps). Further, segments of several reaches have average depths in excess of 15 feet. These conditions are outside of the application range for the O'Connor-Dobbins model. When such situations occur, the result is extremely low reaeration coefficients being calculated by the O'Connor-Dobbins equation. To compensate for the influence of wind induced turbulence and surface diffusion, a minimum default value of the reaeration coefficient is incorporated into the model as follows:

$$K_{2,\,min} = K_{L,min}/d$$

In this equation, $K_{2,min}$ equals the minimum value of the reaeration coefficient at 20°C, day^{-1}. According to documentation for the various versions of QUALII and based on research conducted by Hydroscience, Inc.

as published in 1971, the minimum surface diffusion coefficient, $K_{L,min}$, ranges between 2 and 3 feet per day.[3,7,8] Based on data analysis performed as part of this project, $K_{L,min}$ was set equal to 3. Therefore,

$$K_{2,min} = 3/d$$

Carbonaceous Oxygen Demand (CBOD)

Carbonaceous biochemical oxygen demand (CBOD) is the amount of oxygen utilized by the heterotrophic organisms for the oxidation of organic matter. For the Tenn-Tom model, CBOD decay and CBOD removal through sedimentation are assumed to follow first order kinetics represented by:

$$dL/dt = -K_1 L - K_3 L$$

or

$$dL/dt = -(K_1 + K_3)L$$

where:

L = the concentration of ultimate CBOD, mg/L

K_1 = effective deoxygenation rate, day^{-1}, and

K_3 = rate of CBOD loss due to settling, day^{-1}.

It is important to note that the water quality model is based upon ultimate CBOD rather than 5-day CBOD. However, if the user desires to input or output 5-day CBOD instead of ultimate, the model will make the necessary conversions utilizing the following equation:

$$BOD_5 = BOD_u [1 - e^{-(5)(KBOD)}]$$

where:

BOD_5 = 5-day CBOD, mg/L,

BOD_u = ultimate CBOD, mg/L, and

KBOD = laboratory-derived CBOD decay rate, day^{-1}.

It must be noted that KBOD is user specified (i.e., no default values are coded into the model) and is assumed the same for all forcing functions (i.e., headwaters, incremental flows, point loads, and the downstream boundary condition) when applied to the model.

Nitrogenous Oxygen Demand (NBOD)

Two modeling options are provided in the Tenn-Tom model to account for oxygen demand of the nitrification process in the dissolved oxygen model. The first option is to model the individual components of the nitrification process - the organic nitrogen, ammonia, nitrite, and nitrate. The loss of oxygen due to conversion of ammonia to nitrite and nitrite is then incorporated into the DO model. The second approach simply combines the organic and ammonia nitrogen (the TKN) and assumes that all of the TKN will be oxidized to nitrate. Kinetic formulations of each option are presented below.

Photosynthesis and Respiration

In the Tenn-Tom model, two options are available to account for the average gross photosynthetic oxygen production and average respiration:

Option 1 - Direct Input. The values for direct input can be derived from classic light-dark bottle measurements of average gross production and respiration. Using this option, the net rate of change in oxygen concentration, dO/dt, is calculated as:

$$dO/dt = P_g - R$$

where:

P_g = Average Gross Photosynthetic Oxygen Production, mg/L-day, and

R = Average Respiration, mg/L-day.

Option 4 - Phytoplankton-Based Model. Photosynthetic oxygen production and respiration are simulated in terms of algal growth and respiration as follows:

$$dO/dt = (\alpha_3\mu - \alpha_4 \rho)A$$

where:

α_3 = the rate of oxygen production per unit of algal photosynthesis, mg-o/mg-A,

α_4 = the rate of oxygen uptake per unit of algae respired, mg-0/mg-A,

μ = algal specific growth rate, day^{-1},

ρ = algal respiration rate, day^{-1}, and

A = algal biomass concentration, mg-A/L.

Phytoplankton (Algae) Model

The approach used is to simulate algae as an aggregate of all algae (total phytoplankton) into a single constituent, total algae. Processes assumed to impact phytoplankton dynamics in the river included growth, respiration, and settling. Respiration rate incorporates the endogenous respiration and excretion where nutrients (organic nitrogen and organic phosphorus) are recycled back into the water column. The resulting equation is as follows:

$$dA/dt = (\mu - \rho - \sigma_1/d)A$$

where:

A = algal biomass concentration, mg-A/L,

μ = specific growth rate of algae, day^{-1},
ρ = respiration rate of algae, day^{-1},
σ_1 = settling rate for algae, ft/day, and
d = average depth, ft.

The algal biomass concentration is assumed to be directly proportional to chlorophyll a concentration as follows:

$$\text{chl a} = \alpha_0 A$$

where:

chl a = chlorophyll a concentration, µg-chl a/L, and
α_0 = proportionality coefficient, µg-chl a/mg-A.

Algal specific growth rate is principally affected by temperature, light, and nutrients. The major growth limiting nutrients are assumed to be nitrogen and phosphorus. The classical approach that is generally followed in all phytoplankton models is to adjust the maximum growth rate at a reference temperature and optimal conditions of saturated light intensity and excess nutrients for the combined effects of temperature and the growth limiting functions of light and nutrients. In a functional form:

$$\mu = \mu_{max}[FL\ FN\ FP\ FT]$$

where:

u = algal specific growth rate, day^{-1},
u_{max} = maximum algal growth rate at a particular reference temperature and under optimal conditions of saturated light intensity and excess nutrients, day^{-1},
FL = algal growth limiting function for light,
FN = algal growth limiting function for nitrogen
FP = algal growth limiting function for phosphorus, and
FT = temperature function for growth.

Adjustment for light limitation is accomplished using the Steele[9] formulation which is considered to be the most commonly used photo inhabitation relationship.

$$FL = \frac{2.718}{\lambda d}\,[e^{-(I/K_L)}e^{-\lambda d} - e^{-(I/K_L)}]$$

where:

FL = depth-averaged algal growth attenuation factor for light,
K_L = light intensity at which growth rate is maximized, Btu/ft^2-hr,
λ = light extinction coefficient, ft^{-1},
d = depth of flow, ft, and
I = surface light intensity, Btu/ft^2-hr.

For steady state algal simulation, an adjustment in FL must be made to account for the fact that light also varies with time. This adjustment produces a daily averaged light limitation function. For the Tenn-Tom model, this function is approximated by multiplying the depth averaged light limitation function by the photoperiod expressed as fraction of day, f, and by replacing the surface light intensity, I, with an average light intensity during the daylight hours, I_{alg}. The resulting equation is:

$$FL = \frac{2.718\,f}{\lambda d}\,[e^{-(I_{alg}/K_L)e^{-\lambda d}} - e^{-(I_{alg}/K_L)}]$$

and

$$I_{alg} = I_{tot} / N,$$

where:

I_{alg} = daylight average, photosynthetically active, surface light intensity, Btu/ft^2-hr,
I_{tot} = total daily photosynthetically active solar radiation, Btu/ft^2, and
N = duration of daylight during a day, hr.

Both I_{tot} and N are supplied by the user as input information.

Nutrient limitation factors for nitrogen and phosphorus (FN, FP) can be based on the concepts of biokinetics.

Phosphorus Cycle

Outside of constituent tracking, the phosphorus cycle is incorporated in the model because of the interaction between phosphorus and phytoplankton growth and respiration functions. Two forms of phosphorus are incorporated into the Tenn-Tom model, organic and soluble inorganic. Organic phosphorus resulting from waste loads and phytoplanktic respiration is modeled with respect to biochemical hydrolysis and removal through sedimentation mechanisms. Dissolved inorganic phosphorous is present in the water column as a result of organic phosphorus hydrolysis, waste inputs, and sediment feedback. It is a key nutrient in algal growth as previously discussed.

Conversion to inorganic phosphorus and net sedimentation decrease organic phosphorus while recycle from phytoplankton death and respiration causes increases. The equation used in the Tenn-Tom model which simulates these processes is:

$$dp_1/dt = \alpha_2 \rho A - \beta_4 P_1 - \sigma_5 P_1$$

where:

P_1 = the concentration of organic phosphorus, mg-P/L,
α_2 = phosphorus content of algae, mg P/MG-A,
ρ = algal respiration rate, day^{-1},
A = algal biomass concentration, mg-A/L,
β_4 = organic phosphorus decay rate, temperature dependent, day^{-1}, and
σ_5 = organic phosphorus settling rate, temperature dependent, day^{-1}

As discussed above, the dissolved inorganic phosphorus level present is assumed to naturally increase as a result of the hydrolysis reaction on organic phosphorus. Another, though potentially minor, natural input would be the return of dissolved phosphorus to solution from the sediment. The sink for this species is its uptake by phytoplankton as a nutrient,
where:

$$dP_2/dt = \beta_4 P_1 - \alpha_2 \mu A + \sigma_2/d$$

where:
P_2 = concentration of inorganic or dissolved phosphorus, mg-P/L, and
σ_2 = benthos source rate for dissolved phosphorus, mg-P/ft^2-day.

Sediment Oxygen Demand (SOD)

Sediment oxygen demand represents the oxygen consumed by benthic sediments and organisms. Generally, SOD is measured either in-situ or by collecting sediment samples and evaluating oxygen uptake in the laboratory.[10] The results are usually expressed as a rate term and have the units of mass of oxygen consumed per area per day (gm O_2/m^2-d or gm O_2/ft^2-d). This aerial demand is incorporated into the DO model as follows:

$$dO/dt = -K_4 / d$$

where K_4 the sediment oxygen demand, g-O_2/ft^2-day. For the Tenn-Tom model, SOD was measured both in-situ, following EPA chamber method, and in the laboratory.

Model Summary

As a result of the modeling parameters outlined above, the Tenn-Tom model contains two formulations, or options. These are:

Option 1. Common sources of dissolved oxygen are those doe to atmospheric reaeration, the photosynthetic contribution of algae and incoming flow, while the sinks are the respiration of bacteria which is composed of the carbonaceous and nitrogenous components (CBOD AND NBOD), the respiration of algae, and the sediment oxygen demand. Formulations describing the rate of oxygen production or utilization by each source or sink were presented in the preceding sections. Combining all the sources and sinks result in the following dissolved oxygen model:

$$dO/dt = K_2(O^* - O) + (\alpha_3\mu - \alpha_4 \rho)A$$
$$- K_1 L - K_4/d - \alpha_5\beta_1 N_1 - \alpha_6\beta_2 N_2$$

Option 4. Given the modeling options as outlined above, two substitutions can be made to this equation. Once again, these changes concern the modeling of oxygen concentration as affected by phytoplanktic activity and nitrogen reactions. If the direct input of data from light-dark field studies is to be used, the second term of this equation must be modified as follows:

$$(\alpha_3 \rho - \alpha_4 \rho) A = P_g - R$$

Further, if the one step NBOD method is used to evaluate the impact of nitrogenous reactions on oxygen concentration, the following relationship must be used for the fifth and sixth terms:

$$\alpha_5 \beta_1 N_1 + \alpha_6 \beta_2 N_2 = 4.5 K_{NBOD}(N_1 + N_4)$$

It should be noted that programming constraints dictate that if the modeler chooses either of these options, both will have to be used; hence, the use of the term Option 4 rather than Option 2. This was done because of an interdependence of the algal and nitrogen components of the model. In short, data generated from each of these segments of the model is needed by the other segment. Further, it was felt that a modeler who wished to make one of these substitutions, for whatever reason, would most likely prefer to make both.

Given this, the alternative model formulation provided as part of the Tenn-Tom water quality model is:

$$dO/dt = K_2 (O^* - O) + [P_g - R] - K_1 L - K_4/d - [4.57 K_{NBOD} (N_1 + N_4)]$$

To apply the model for the simulation of dissolved oxygen and subsequently for waste load allocations will require the evaluation of a number of specific rate constants and kinetic coefficients. The work presented by Bowie et al.[8] provides initial values for the various reaction variables. In defining each of the rate constants and coefficients ultimately used for solution of this water quality model, some of these values were adjusted based on data collected during this project while others were modified after an extensive search of the literature. It is ideal to be able to field evaluate every rate constant, however, constraints on budget, time, and personnel limited field evaluation to the parameters having the most significant impact on the model results. It should be reemphasized that the literature estimated parameters were based on a very vigorous and extensive search conducted by the investigators.

If a reaction variable is defined as being affected by changes in water temperature, the modified form of the van't Hoff equation is used during modeling to compensate for temperature. This modification takes the form of:

$$X_T = X_{20}\,\Theta^{(T-20)}$$

where:

X_T = the value of the coefficient at the temperature defined as part of initial modeling conditions, oC,

X_{20} = the value of the coefficient at standard temperature (20oC), and

Θ = an empirical constant for the specific reaction coefficient.

Model Formulation

The primary objectives of this effort were: (a) to formulate a comprehensive but simple water quality model to be used for the sole purpose of waste load allocations in the upper Tennessee-Tombigbee Waterway located within Mississippi, and (b) to evaluate the necessary model parameters (hydrologic, geometric, and rate constants) that are specific to the Tenn-Tom Waterway. With these goals in mind, a detailed review was conducted of water quality models currently in use for waste load allocations by the various regions of the United States Environmental Protection Agency (U.S. EPA) and the various state pollution control regulatory agencies.

This effort was coupled with a comprehensive literature search of water quality modeling techniques and personal communications with the U.S. EPA Region IV Water Quality Section and the U.S. EPA Environmental Research Laboratory in Athens, Georgia. Emphasis centered around: (a) gaining an insight of the pros and cons of the various water quality models currently in use; (b) isolating the most efficient and accurate field and lab procedures for evaluating the various model parameters; and (c) ascertaining answers to the following concerns raised by the research team:

a. whether to use a steady-state or a time varied modeling procedure,
b. whether a single model is needed or whether coupling separate models for the channel, the lock pool, and the lock tail water areas will be applicable,
c. whether a one-dimensional modeling system will provide reasonable accuracy or whether two-and/or three dimensional systems will be required,
d. whether mass transport can be modeled by advection only or whether advection and dispersion must be coupled, and
e. whether locking procedure and frequency constitute a significant parameter to be modeled separately.

Based on these efforts, coupled with field investigations of the hydrology and operation of the Waterway, led to the selection of QUAL2E-UNCAS as the base water quality model that satisfies the criteria established for the Tenn-Tom Waterway. The QUAL2E-UNCAS is a comprehensive and versatile one-dimensional water quality model that is used extensively by state pollution control regulatory agencies, U.S. EPA regional offices, and consultants for waste load allocations. This model, used as a developmental basis, offered numerous advantages. The water quality model was further enhanced through interrelationship with the HEC-2 hydraulic model.

Solution Technique

The Tenn-Tom version of QUAL2E, like the foundation program itself, is a comprehensive and versatile water quality model. It can simulate up to 15 water quality constituents in almost any combination desired by the user. Constituents which can be simulated are: a) Dissolved Oxygen, b) Biochemical Oxygen Demand, c) Algae as Chlorophyll a, d) Organic Nitrogen, e) Ammonia, f) Nitrite, g) Nitrate, h) Organic Phosphorus, and i) Dissolved Phosphorus. If either the phosphorus cycle or the nitrogen cycle are not being simulated, the model presumes they will not limit algal growth. It assumes that the major transport mechanisms, advection and dispersion, are significant only along the main direction of flow (longitudinal axis of the stream or canal). It allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow.

Hydraulically, the model is limited to the simulation of time periods during which both the stream flow in river basins and input waste loads are essentially constant. As modified and calibrated, the developer intended for the programs to be operated as a steady-state model. As such, it can be used to study the impact of waste loads magnitude, quality, and location on the waterway's water quality. With some effort on the part of the programmer, it also can be used in conjunction with a field sampling program to identify the magnitude and quality characteristics of non-point source waste loads.

The model has been developed to provide simulation of a one-dimensional waterway system. The first step in model development was to subdivide the Tenn-Tom into segments. Each segment was established by either a state boundary or a waterway lock structure. Each segment is computationally divided into reaches as defined by modeling constraints or programming limitations. Modeling contraints require reaches to begin and end at points of input and to have a uniform set of hydraulic characteristics.

Forcing functions are the user specified inputs that drive the system being modeled. As applied to the Tenn-Tom, only two of these are used: a) Headwater inputs are typically the upstream boundary conditions at the beginning of the system. They are the conditions required to generate the solution of the mass balance equations for the first computational element in each headwater reach. Headwaters are also the source of water for flow augmentation; and b) Point sources inputs and withdrawals are used to represent discharges into the system (e.g., sewage and industrial waste, storm water runoff) and losses from the system resulting from diversions.

The numerical solution technique used evaluates the ordinary differential equation for each of the time-based computational elements in the reach and for each constituent. Because it is not possible to obtain analytical solutions to these equations under most prototype situations, a finite difference method has been used. More specifically, the classical implicit backward difference method is employed.[11] The foundation for this numerical solution is to find the value of a variable (e.g., constituent concentration) as a function of space at a time step n+1 when its spatial distribution at the n^{th} time step is known. Time step zero corresponds to the initial condition. Backward difference, or implicit, schemes are characterized by the fact that all spatial derivatives ($\partial/\partial x$) are approximated in difference for at time step n+1. Because of this numerical solution technique programmed to solve the differential equations involved, all reaches must consist of an integer number of computational elements of equal length. Further, each reach can contain no more than 20 elements. For these reasons, the Tenn-Tom water quality model utilizes computational elements that are 0.1 mile in length yielding a maximum reach length of 2.0 miles as a programing constraint. Further programming limitations set were for the maximum number of reaches (50) and the maximum total number of computational elements (500).

Model Calibration/Verification

The collection and preservation of samples in the field was carried out in accordance with procedures generally used by personnel at U.S. EPA Region IV's Environmental Research Laboratory when performing similar modeling programs. Laboratory analyses were performed in accordance with Standard Methods.[12]

Model Calibration

The dissolved oxygen water quality model was tested (calibrated) against two sets of field data collected on August 25 and November 11, 1989. Two model options were tested. Option 1 incorporated the algae and nitrogen cycle models while option 4 utilized the field data from the light/dark bottle technique to account for algal photosynthesis and respiration and substitutes one step nitrification for the nitrogen cycle. A set of model parameters (rate constants/coefficients) were selected following an extensive and vigorous fine tuning along with sensitivity analysis. Subsequent testing of the calibrated model, utilizing the selected parameters, was then accomplished against several additional field data collected in 1990 under different river flows and temperatures.

Headwater (background) and other chemical inputs for the two calibration runs for each reach were based on samples collected just downstream from the lock structures. Hydraulic data was based on information obtained from the lock operators with regard to number of lockages and spillway discharges, as appropriate. The results of initial modeling were depicted by comparing observed and calculated dissolved oxygen profiles. The results of both visual and numeric data comparison illustrated that it was safe to assume at this stage that the model is calibrated. It is also important to note that even at this level of model development, that Options 1 and 4 provide very similar results.

It should be reemphasized here again that the reaeration coefficient, K_2, for all calibration and the subsequent verification runs were calculated utilizing the O'Connor-Dobbins equation with a lower limit on K_2 of 3/d (d = average reach depth in feet).

Model Verification

As previously stated, the calibrated model was subsequently verified against a number of field data collected in the summer and fall of 1990 under various river flows and temperatures. Numerous verification dissolved oxygen profiles were developed during this phase of the study. These profiles, which were similar in appearance to those generated during the calibration phase, illustrated that the dissolved oxygen model successfully predicted the DO in the waterway under a variety of river flows and temperatures. Furthermore, predicted profiles were almost identical under both options.

One observation that was discovered from the calibration-verification runs which was further stressed through sensitivity analysis is the extreme sensitivity of the algae model (Option 1) to the concentrations in the waterway of the nutrients inorganic nitrogen and phosphorus.

Recalling that the algae model is equationally depicted as:

$$dA/dt = \mu A - \rho A - (\underline{\sigma}/d) A$$

or

$$dA/dt = [\mu - \rho (\underline{\sigma}/d)] A$$

it must be remembered that the maximum specific growth rate of the algae, μ_{max}, is corrected for light and nutrients, utilizing the minimum formulation as follows, to estimate the specific growth rate, μ, for the model:

$$\mu = \mu_{max} (FL) \{Min [(FN) \text{ or } (FP)]\}$$

When the concentration of either nutrient in the waterway or as predicted by the model is very low, FN or FP become correspondingly very small. The affect of this is an extremely small μ as compared to ρ.

From a modeling perspective, this results in algal death, which is driven by respiration and is accompanied with the release of the nutrients. The released nutrients enter the respective N or P system and cycle back, thus increasing the levels of FN or FP. This increase will in turn result in higher algal growth rate, μ, which is accompanied with nutrient uptake. A cycle is thus created where the values of the growth limiting factors (FN or FP) will cycle back and forth from an extremely high to an extremely low value. This fluctuation creates a condition where the solution of the algae model will not converge. This modeling problem is most pronounced at a relatively high algal concentration.

To correct this condition, one or both of the following modeling approaches are recommended:

1. the level of either the dissolved phosphorus or the sum of the ammonia plus nitrate nitrogen should be set, at minimum, to the detection level ($\leq$ 0.05 mg/L) and/or
2. increase algae respiration rate, ρ, beyond the recommended value of 0.05 d^{-1} at an increment of 0.02 d^{-1} until the model converges. The recommended range for ρ is 0.05-0.25 d^{-1}.

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