Simulating Unsteady Transport of Nitrogen, Biochemical Oxygen Demand, and Dissolved Oxygen in the Chattahoochee River Downstream from Atlanta, Georgia

By HARVEY E. JOBSON

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SYMBOLS

Symbol	*Definition*
A	cross-sectional area of the river
C_p	specific heat capacity of water
c	concentration (or temperature)
c_1	concentration of constituent 1
c_i^n	concentration of parcel i at the end of a time step
c_i^o	concentration of parcel i at the beginning of a time step
cR	concentration at which internal production ceases
$cR_{1,n}$	concentration of constituent n at which the production of constituent 1 due to n ceases.
D	longitudinal dispersion coefficient
D_f	dispersion factor $D/u^2\Delta t$
e_o	saturation vapor pressure of air at a temperature equal to that of the water
K	rate coefficient of production of a constituent due to internal reactions
K_{BO}	extraction-rate coefficient for BOD at 20°C
K_{NH}	extraction-rate coefficient for ammonia at 20°C
K_{NO}	decay-rate coefficient for nitrite at 20°C
K_{ON}	decay-rate coefficient for organic nitrogen at 20°C
L	latent heat of vaporization
S	rate of production of concentration which is independent of the concentration
T_E	equilibrium temperature
T_R	average of water and equilibrium temperature expressed on the absolute scale
TT	traveltime
t	time
u	cross-sectional mean stream velocity
t_o	time that a parcel was located at x_o
V	wind speed
W	channel width
$XK_{1,n}$	rate coefficient for production of constituent 1 due to the presence of constituent n.
x	Eulerian distance coordinate along the river
x_o	the location of a parcel at time t_o
γ	psychrometric constant
Δh	fall in water-surface elevation
Δt	time-step size
ε	emissivity of water
ξ	Lagrangian distance coordinate
σ	Stefan-Boltzmann constant for black body radiation
Φ	change in concentration due to tributary inflow
Ψ	wind function
e'_o	slope of the saturation vapor-pressure curve

Simulating Unsteady Transport of Nitrogen, Biochemical Oxygen Demand, and Dissolved Oxygen in the Chattahoochee River Downstream from Atlanta, Georgia

By Harvey E. Jobson

Abstract

As part of an intensive water-quality assessment of the Chattahoochee River, repetitive water-quality measurements were made at 12 sites along a 69-kilometer reach of the river downstream of Atlanta, Georgia. Concentrations of seven constituents (temperature, dissolved oxygen, ultimate carbonaceous biochemical oxygen demand (BOD), organic nitrogen, ammonia, nitrite, and nitrate) were obtained during two periods of 36 hours, one starting on August 30, 1976, and the other starting on May 31, 1977. The study reach contains one large and several small sewage outfalls and receives the cooling water from two large powerplants.

An unsteady water-quality model of the Lagrangian type was calibrated using the 1977 data and verified using the 1976 data. The model provided a good means of interpreting these data even though both the flow and the pollution loading rates were highly unsteady. A kinetic model of the cascade type accurately described the physical and biochemical processes occurring in the river. All rate coefficients, except reaeration coefficients and those describing the resuspension of BOD, were fitted to the 1977 data and verified using the 1976 data.

The study showed that, at steady low flow, about 38 percent of the BOD settled without exerting an oxygen demand. At high flow, this settled BOD was resuspended and exerted an immediate oxygen demand. About 70 percent of the ammonia extracted from the water column was converted to nitrite, but the fate of the remaining 30 percent is unknown. Photosynthetic production was not an important factor in the oxygen balance during either run.

INTRODUCTION

During the period April 1975 to June 1978, the U.S. Geological Survey conducted an intensive assessment of water quality in the Chattahoochee River basin near Atlanta, Ga. (Stamer and others, 1979). One objective of this project was to assess the magnitude, nature, and effect of point and nonpoint discharges on river quality. Three intensive data-collection efforts were conducted on a 69 kilometer reach of the river downstream of Atlanta. During two of three data-collection efforts, all of the nitrogen species, as well as the water temperature and concentrations of dissolved oxygen and carbonaceous biochemical oxygen demand (BOD), were determined. Although the studies were planned to be performed under steady-state conditions, the waste-loading conditions were quite unsteady during the 1977 run and the flow was unsteady during the 1976 run.

The purposes of this report are to interpret these water-quality and flow data by use of an unsteady water-quality model of the Lagrangian type and to verify that a cascade-type kinetic model adequately describes the physical and biochemical processes occurring in the river.

The river reach (fig. 1) extends from the Atlanta gage to the Whitesburg gage. Although 26 inflow or diversion points exist in the reach, the Atkinson and McDonough powerplants (located together) dominated the stream temperature and the Clayton wastewater treatment facility (WTF) dominated other water-quality constituents.

A complete presentation of the data and study procedures has been published by Stamer and others (1979). In summary, during each data-collection period, the flow and concentration data were obtained at 21 point sources and at 12 instream sites periodically during a 36-hour period. In this report, a model of the stream temperature and of the dissolved oxygen, BOD, organic nitrogen, ammonia, nitrite, and nitrate concentrations is calibrated using data obtained beginning on May 31, 1977, and is verified using data obtained beginning on August 30, 1976.

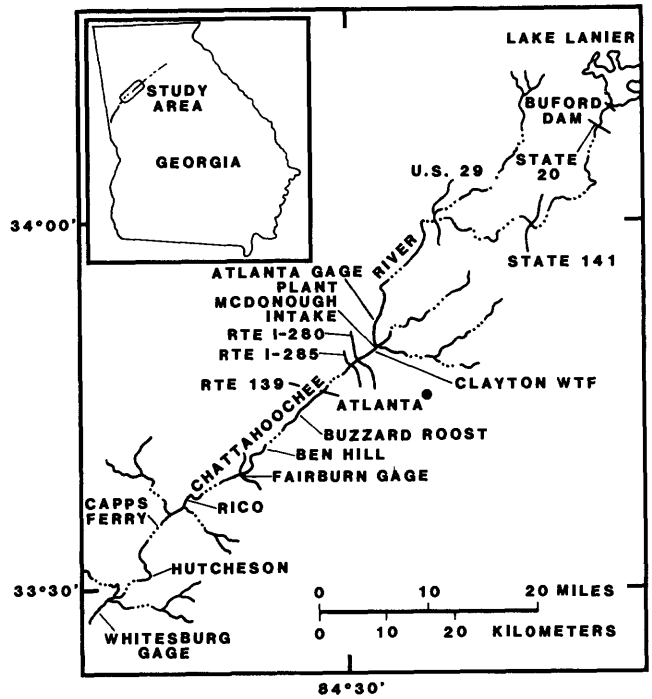

Figure 1. Data-collection points.

Following a brief description of the model and model kinetics, the results of the model calibration are discussed in detail. The results of the model verification are then presented and the overall results are discussed.

THE MODEL

Flow.—The river flow was modeled dynamically using a linear implicit finite-difference model documented by Land (1978). The 69-kilometer reach was discretized using 43 grid points spaced unequally along the channel. Points of inflow or diversion accounted for by the flow model are listed in table 1. The discharge of all tributaries or diversions (except the Clayton WTF) were assumed constant because of the lack of data and because their impact on the river was small.

In addition to tributary inflow, the model requires a discharge at the upstream end and a stage at the downstream end as boundary conditions. The flow model produces a data file containing the velocity, cross-sectional area, top width, and tributary flow rate at each grid point and time step. This file is then used as input to the water-quality model.

Transport.—The transport model used here has been documented by Jobson (1980a). It is applicable to one-dimensional, unsteady, nonuniform flow and allows for tributary inflow at any or all grid points. The model uses a Lagrangian reference frame which follows individual fluid parcels and allows for the transport of any number of interacting constituents.

In the Lagrangian reference frame, the continuity of mass equation for a specific fluid parcel is

$$\frac{\partial c}{\partial t}-\frac{\partial}{\partial \xi}\left(D\frac{\partial c}{\partial \xi}\right)=K(c-cR)-\Phi+S, \qquad (1)$$

in which c is concentration, t is time, D is the longitudinal dispersion coefficient, K is the rate coefficient for production of the constituent due to internal reactions, cR is the concentration at which the internal production ceases, Φ is the change in concentration due to tributary inflow, S is the rate of production of concentration which is independent of the concentration and ξ is the distance from the parcel. The Lagrangian distance coordinate, ξ, is given by

$$\xi=x-x_o-\int_{t_o}^{t}u\,dt', \qquad (2)$$

in which ξ is 0 at the parcel for any time, x is the Eulerian distance coordinate along the river, u is the cross-sectional mean stream velocity, and x_o is the location of the parcel at time t_o.

The finite-difference solution is constructed by adding a new parcel at the upstream boundary at each time step and tracking each parcel as it traverses the system. As parcels pass each tributary, their volumes and concentrations are adjusted from mass-balance considerations in order to evaluate Φ.

Approximating the distance between parcels, $d\xi$, as the velocity times the time-step size Δt, the explicit finite-difference form of equation 1 becomes

$$c_i^n=c_i^o+\frac{Di}{U_i^2\Delta t}(c_{i+1}^o-c_i^o)-\frac{D_{i-1}}{U_{i-1}^2\Delta t}(c_i^o-c_{i-1}^o) \qquad (3)$$
$$+\int_0^{\Delta t}(K(c-cR)-\Phi+S)\,dt',$$

in which c^o_i and c^n_i are concentrations of the parcel i at the beginning and end of the time step, respectively. The parcels are numbered consecutively in the downstream direction and the value of the dispersion coefficient, Di, is evaluated at the downstream boundary of parcel i. The solution of equations 2 and 3 for a series of fluid parcels is straightforward and gives very accurate results.

Table 1. Sampling points and range in flow rates for the Chattahoochee River and tributaries during calibration and verification of model

Site name	Actual river mile	Model grid: River mile	Model grid: Grid number	Flow, in cubic meters per second: Calibration	Flow, in cubic meters per second: Verification
Atlanta gage	302.97	302.97	1	34.0[1] 32.1	123.9 33.7
Atlanta water-supply facility	300.62	300.62	6	-3.96	-3.34
Cobb County wastewater treatment facility.	300.56	300.44	7	.37	.34
Nancy and Peachtree Creek	300.52	300.44	7	.79	1.10
Clayton wastewater treatment facility.	300.24	300.29	8	4.05 2.27	 2.18
Atkinson powerplant intake	299.46	299.20	11	-1.42	-1.42
McDonough powerplant intake	299.23	299.20	11	-1.41	-1.41
Atkinson powerplant outfall	299.19	299.10	13	1.42	1.42
McDonough powerplant outfall	299.15	299.10	13	1.41	1.41
Chattahoochee River at Route I-280.	298.77	298.77	15	36.6 35.0	113.0 34.0
Route I-285.	297.75	297.73	18	36.6 35.0	112.2 34.0
Proctor Creek	297.50	297.06	19	.21	.17
Nickajack Creek	295.13	295.30	21	.59	.37
Chattahoochee River at Route 139.	294.65	294.70	22	37.3 35.8	110.6 34.8
South Cobb County wastewater treatment facility.	294.28	293.92	23	.42	.17
Utoy wastewater treatment facility.	291.60	290.54	26	.51	.46
Utoy Creek	291.57	290.54	26	.37	.26
Chattahoochee River at Buzzard Roost.	290.57	290.54	26	38.5 37.2	104.2 35.8
Sweetwater Creek	288.58	287.86	27	6.06	3.82
Chattahoochee River at Ben Hill.	286.07	286.07	29	44.56 43.2	105.1 40.6
Camp Creek wastewater treatment facility.	283.78	281.79	31	.25	.15
Camp Creek	283.54	281.79	31	.54	1.14
Deep Creek	283.27	281.79	31	.54	.98
Chattahoochee River at Fairburn.	281.79	281.79	31	45.8 44.6	102.9 42.8
Annewakee Creek	281.48	281.07	32	.74	0.38

Table 1. Sampling points and range in flow rates for the Chattahoochee River and tributaries during calibration and verification of model—Continued

Site name	Actual river mile	Model grid River mile	Model grid Grid number	Flow, in cubic meters per second Calibration	Flow, in cubic meters per second Verification
Pea Creek	277.70	281.07	32	.14	0.10
Bear Creek (right bank)	275.95	274.12	35	.99	0.21
Chattahoochee River at Rico.	275.81	274.12	35	48.3 47.3	95.2 43.7
Bear Creek (left bank)	274.49	274.12	35	.79	.16
Dog River	273.46	272.20	36	3.28	.85
Chattahoochee River at Capps Ferry.	271.19	271.22	37	51.6 50.5	95.2 44.5
Wolf Creek	267.34	266.02	41	.54	.59
Chattahoochee River at Hutcheson.	265.66	266.02	41	52.1 51.1	93.5 45.1
Snake Creek	261.72	263.62	42	1.16	2.48
Cedar Creek	261.25	263. 62	42	.85	.66
Chattahoochee River at Whitesburg.	259.85	259.85	43	54.1 53.1	89.6 48.3

[1] Where two numbers are shown they indicate the range of values observed.

A dimensionless ratio, called the dispersion factor, D_f is defined as

$$D_f = \frac{D}{u^2 \Delta t} = \left(\frac{\sqrt{D \Delta t}}{u \Delta t} \right)^2 \qquad (4)$$

It can be shown that the accuracy of the numerical solution is totally controlled by the value of the dispersion factor (Jobson, 1980b). The characteristic distance scale for a diffusion process is $\sqrt{D\Delta t}$ (Carslaw and Jaeger, 1959). The length scale $\sqrt{D\Delta t}$ is a measure of how far the diffusion front advances in time Δt, and $u\Delta t$ is, of course, the distance traveled by a parcel during the same time. The dispersion factor is, therefore, the square of the ratio of the distance the diffusion front advances to the distance moved by the parcel during a time step in the model. It has been shown empirically (Jobson, 1980b) that the accuracy of equation 3 is optimal at a D_f value of 0.2 but that the accuracy remains very good as long as $0.05 \leq D_f \leq 0.4$. As the value of D_f departs from 0.2 in either direction, the numerical solution tends to underestimate the actual dispersion.

The advantages of a Lagrangian approach, as outlined above, are as follows: (1) the scheme is very accurate in modeling the convection and dispersion terms compared with the usual Eulerian approach (Jobson 1980b, 1980c), (2) the Lagrangian model is totally stable for any time-step size, (3) the coding is relatively simple and straightforward, (4) the conceptual model is easy to visualize in the physical sense, (5) the model is economical to run, and (6) the model output naturally includes information that is not easily determined from a Eulerian approach but is very helpful in model calibration and data interpretation.

The concentrations of many water-quality constituents are interdependent. To simulate interdependent constituents, equation 1 is solved for each constituent in each parcel. It is convenient to number the constituents, and then all equations can be represented by a single expression of the form

$$\frac{\partial c_1}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_1}{\partial \xi}\right)=S_1+\Phi_1+\sum_{n=1}^{m} XK_{1,n}(c_n-cR_{1,n}), \quad (5)$$

in which c_l is the concentration of the constituent numbered 1, S_l and Φ_l are source terms for constituent 1, $XK_{l,n}$ is the rate coefficient for production of constituent 1 due to the presence of constituent n, and $cR_{l,n}$ is the concentration of constituent n at which the production of constituent 1 due to n ceases.

The Lagrangian model solves equation 5 (using the approximation shown in eq. 3) for each parcel and each constituent. The kinetics of the interaction between the constituents is determined by the values of the coefficients S, XK, and cR. For each parcel, these coefficients are updated whenever any of the following occur: a new time step is started, a parcel passes a grid point, or any concentration changes by a specified amount. The coefficients can be functions of time, position in the river, meteorologic variables, local flow variables, or concentrations of any constituent. The equation is solved by subdividing the time step such that no concentration changes by more than 10 percent of the departure from equilibrium $(c-cR)$ or 0.3 units, whichever is larger, during a partial time step. For each partial time step, the integration implied in equation 3 is performed using a first order Runge-Kutta approximation. The procedure of subdividing the time step allows highly nonlinear reactions to be accurately simulated without adjusting the model time-step size even though equation 5 is linear in form.

Kinetics.—Seven constituents were of interest in the Chattahoochee: temperature, T; dissolved oxygen, DO; ultimate carbonaceous biochemical oxygen demand, BOD; organic nitrogen, ON; ammonia, NH; nitrite, NO2; and nitrate, NO3. The general conceptual model of the interaction among the constituents is shown in figure 2. The kinetic model illustrated in figure 2 is of the cascade type presented by Thomann and others (1971). The term "cascade" is derived from the assumption that the nitrification process proceeds through a series of reactions which convert organic nitrogen to nitrate as the final form.

Letting temperature be constituent 1, the equation for temperature, from equation 5, becomes

$$\frac{\partial c_1}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_1}{\partial \xi}\right)=\Phi_1+XK_{1,1}(c_1-cR_{1,1}), \quad (6)$$

in which c_l is temperature, $XK_{1,1}$ is the kinetic surface exchange coefficient, $cR_{1,1}=T_e$ is the equilibrium temperature, and all other XK values are zero because the temperature is assumed not to be a function of the concentration of any other constituent.

The kinetic surface exchange coefficient is determined as

$$XK_{1,1}=\frac{-W}{AC_p}\left(4\sigma\varepsilon T_R^3+L\Psi(e'_o+\gamma)\right), \quad (7)$$

in which W is channel width, A is the cross-sectional area of the river, C_p is the specific heat capacity of water, σ is the Stefan-Boltzman constant for black body radiation, ε is the emissivity of water (0.97), T_R is the average of water and equilibrium temperature expressed on the absolute scale, L is the latent heat of vaporization, Ψ is the wind function, e'_o is the slope of the saturation vapor pressure curve, and γ is the psychrometric constant. The slope of the saturation vapor pressure curve was evaluated from an empirical expression at a temperature of T_R

The wind function was assumed to be proportional to the value determined by an expression developed for use on the San Diego Aqueduct (Jobson, 1980d),

$$\Psi=3.02+1.13V, \quad (8)$$

in which Ψ is wind function in millimeters per day per kilopascal when the windspeed, V, is expressed in meters per second.

The ultimate carbonaceous biochemical oxygen demand (BOD) is also assumed to be independent of the concentrations of other constituents and was numbered constituent 3. The dissolved oxygen concentration, numbered constituent 2, will be discussed last. Writing equation 5 for BOD,

$$\frac{\partial c_3}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_3}{\partial \xi}\right)=S_3+\Phi_3+XK_{3,3}(c_3-0), \quad (9)$$

in which c_3 is BOD concentration, S_3 represents the rate of entrainment of BOD from the bed, $XK_{3,3}$ is the negative of the extraction rate for BOD, and $CR_{3,3}=0$. The value of $XK_{3,3}$ was adjusted for temperature using the expression (Velz, 1970, p. 146)

$$XK_{3,3}=-K_{BO}(1.047)^{(c_1-20)}, \quad (10)$$

in which K_{BO} is the extraction-rate coefficient at a reference temperature of 20°C. The reaction was stopped by setting $XK_{3,3}=0$ when the DO concentration fell below 0.1 mg/L. This condition was never encountered, however.

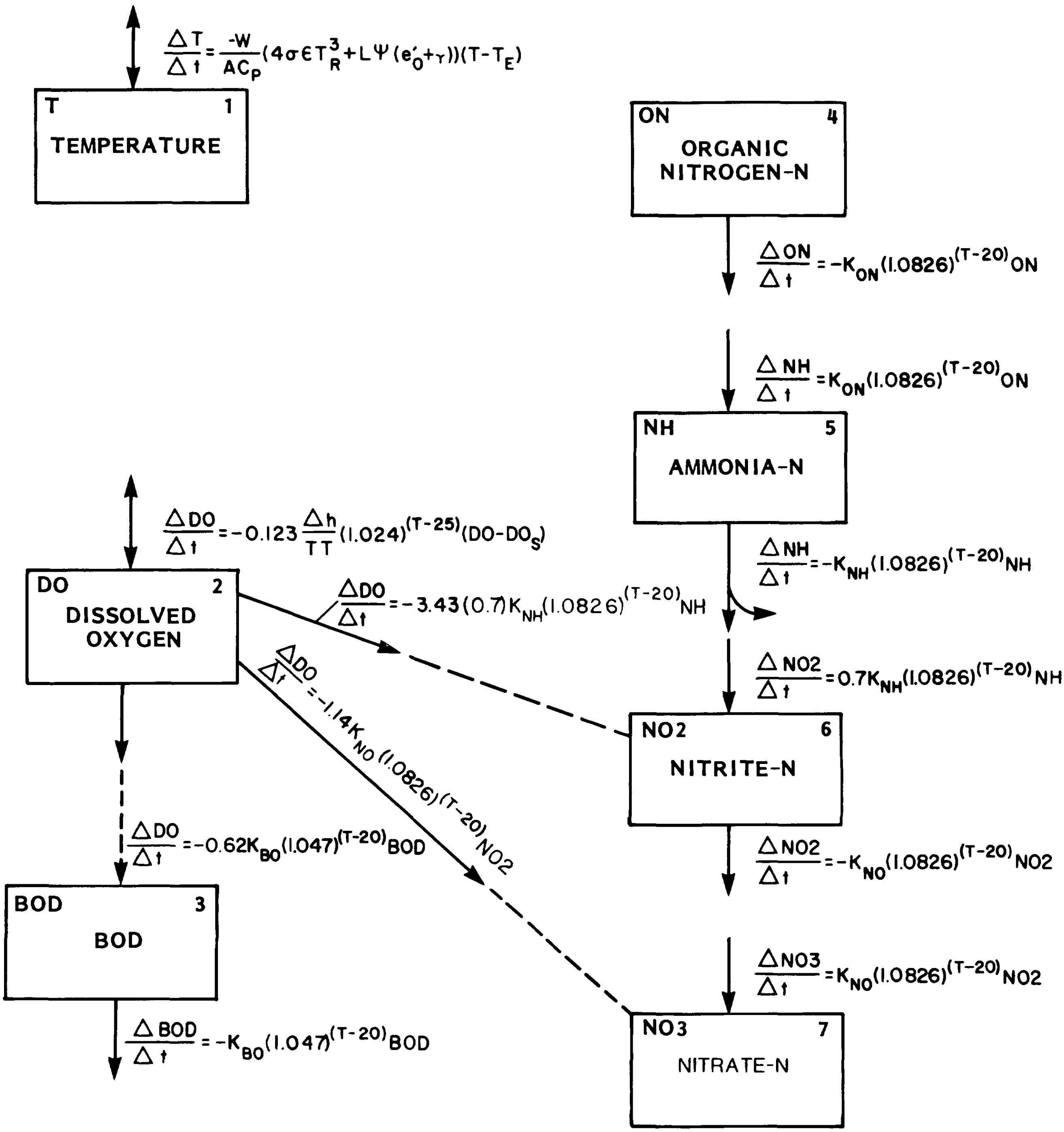

Figure 2. Schematic diagram of kinetic model for the Chattahoochee River downstream of Atlanta, Ga.

The extraction-rate coefficient for BOD, K_{BO}, represents the total loss of BOD from the water column. If no settling of oxygen demanding particulate matter occurs, the value of K_{BO} is numerically equal to the biochemical deoxygenation rate. If settling occurs, K_{BO} represents the sum of the deoxygenation rate and the settling rate. Insofar as the concentration of BOD is concerned, it is immaterial whether the loss occurred as a result of settling or of deoxygenation.

The dominant reactions assumed to be involved with the nitrogen species are illustrated in figure 2. The first order differential equations for this representation of the nitrification process have been presented by Thomann and others (1971). It is assumed that the nitrification process can be represented by a set of coupled sequential reactions involving the decay of organic nitrogen and ammonia nitrogen through nitrite-nitrogen to nitrate-nitrogen. In these reactions, one form of nitrogen is converted to another form of nitrogen. The model formulation allows the reactions to go either way, and not all of the nitrogen lost from one form needs to be converted to the next form. This allows for various unknown sinks of any form, such as volatilization, settling, or uptake. Writing equation 5 for total organic nitrogen (ON), which is designated constituent 4 one obtains

$$\frac{\partial c_4}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_4}{\partial \xi}\right)=\Phi_4+XK_{4,4}(c_4-0) \qquad (11)$$

in which c_4 is the concentration of total organic nitrogen as nitrogen, $XK_{4,4}$ is the rate coefficient for production of organic nitrogen (since decay is actually occurring, the value of $XK_{4,4}$ will be negative), and $cR_{4,4}=0$. The value of $XK_{4,4}$ was computed as a function of water temperature from

$$XK_{4,4}=-K_{ON}1.0826^{(c_1-20)}, \qquad (12)$$

in which $K_{ON}=$ the decay-rate coefficient for organic nitrogen at 20°C. The coefficient 1.0826 represents the average of the suggested values reported by Zison and others (1978, p. 190).

Equation 11 expresses the principle of conservation of elemental nitrogen, as will all other equations for the various nitrogen species. Expressing the equations in terms of elemental nitrogen eliminates the problem of biomass stoichiometry. Nitrification is assumed to follow first order kinetics, and the variation in bacterial biomass is ignored.

Ammonia is assumed to be produced biochemically by the decay of organic nitrogen and to decay itself according to a first order reaction. Writing equation 5 for total ammonia (NH), which is designated constituent 5, one obtains

$$\frac{\partial c_5}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_5}{\partial \xi}\right)=\Phi_5+XK_{5,4}c_4+XK_{5,5}c_5, \qquad (13)$$

in which c_5 is concentration of total ammonia nitrogen as nitrogen, $XK_{5,4}$ is the rate coefficient for production of ammonia from organic nitrogen, and $XK_{5,5}$ is the rate coefficient for production (decay) of ammonia. The values of $XK_{4,4}$ and $XK_{5,4}$ are numerically equal but opposite in sign (fig. 2) because no loss or gain of ammonia is assumed to occur in the transformation from organic nitrogen to ammonia. The value of $XK_{5,5}$ was computed from

$$XK_{5,5}=-K_{NH}1.0826^{(c_1-20)}, \qquad (14)$$

in which K_{NH} is the extraction-rate coefficient for ammonia at 20°C. The transformation from ammonia to nitrite was stopped by setting $XK_{5,5}=0$ if the dissolved oxygen level had dropped below 0.1 mg/L.

Ammonia is converted to nitrite through the actions of nitrosomona bacteria. In addition, other losses of ammonia such as volatilization, sediment uptake, or the synthesis of new organisms (Huang and Wozniak, 1981; White and others, 1977; Tuffey and others, 1974) can occur. Also, nitrite is rapidly converted to nitrate through the action of nitrobacter bacteria. Writing equation 5 for total nitrite (NO2), which is designated constituent 6, one obtains

$$\frac{\partial c_6}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_6}{\partial \xi}\right)=\Phi_6+XK_{6,5}c_5+XK_{6,6}c_6, \qquad (15)$$

in which c_6 is the concentration of total nitrite as nitrogen, $XK_{6,5}$ is the rate of production of nitrite from ammonia, and $XK_{6,6}$ is the rate of production (decay) of nitrite to nitrate. The value of $XK_{6,5}$ is assumed to be numerically smaller than, but proportional to and opposite in sign from, $XK_{5,5}$. This allows a fixed percentage of the ammonia nitrogen that is decayed to be lost from the system owing to unspecified causes. The transformation of nitrite to nitrate was stopped if the dissolved-oxygen concentration fell below 0.1 mg/L, and the value of $XK_{6,6}$ was determined from the expression

$$XK_{6,6}=-K_{NO}1.0826^{(c_1-20)}, \qquad (16)$$

in which $K_{NO}=$ decay-rate coefficient for nitrite at 20°C.

Nitrate is produced from the nitrification of nitrite, and the major source of nitrate decay is through uptake by living plants or algae. Writing equation 5 for total nitrate (NO3), which is designated constituent 7, one obtains

$$\frac{\partial c_7}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_7}{\partial \xi}\right)=\Phi_7+XK_{7,6}c_6+XK_{7,7}c_7, \qquad (17)$$

in which c_7 is the concentration of total nitrate as nitrogen, $XK_{7,6}$ is the production-rate coefficient of nitrate from nitrite, and $XK_{7,7}$ is the production- (decay-) rate coefficient of nitrate. Since no losses were assumed to occur in the conversion of nitrite to nitrate, the values of $XK_{6,6}$ and $XK_{7,6}$ were numerically equal but opposite in sign.

Little algae was observed in the river, and the observed ammonia concentration was always above 0.2 mg/L. Najarian and Taft (1981, p. 1145) state that uptake of nitrate by phytoplankton is inhibited for ammonia concentrations above 0.2 mg/L. For these reasons, no decay of nitrate was allowed and the value of $XK_{7,7}$ was set at zero.

Oxygen is the most complex of any of the constituents modeled because it is affected by the concentrations of most of the other constituents. Writing equation 5 for dissolved oxygen (DO), which is designated constituent 2, one obtains

$$\frac{\partial c_2}{\partial t}-\frac{\partial}{\partial \xi}\left(D\,\frac{\partial c_2}{\partial \xi}\right)=\Phi_2+XK_{2,2}(c_2-cR_{2,2}) \quad (18)$$

$$+XK_{2,3}c_3+XK_{2,5}c_5+XK_{2,6}c_6,$$

in which c_2 is the concentration of dissolved oxygen, $XK_{2,2}$ is the negative of the reaeration coefficient, $cR_{2,2}$ is the saturation value of dissolved oxygen, $XK_{2,3}$ is the negative of the biochemical deoxygenation rate coefficient, $XK_{2,5}$ is the production- (consumption-) rate coefficient of oxygen in the production of nitrite from ammonia, and $XK_{2,6}$ is the production- (consumption-) rate coefficient of oxygen in the production of nitrate from nitrite.

The per hour reaeration coefficient was computed from the equation

$$XK_{2,2}=(-0.123\Delta h/TT)(1.024^{(c_1-25)}), \quad (19)$$

in which Δh is the fall in water-surface elevation through a reach, in meters, and TT is traveltime of a water parcel as it traverses the reach, in hours. Equation 19 was derived for use on the Chattahoochee River between Atlanta and Fairburn using a gas-tracer technique (Tsivoglou and Wallace, 1972).

The saturation value for dissolved oxygen, $cR_{2,2}$, was computed using the empirical expression (Committee on Sanitary Engineering Research, 1960)

$$cR_{2,2}=14.652-0.41022\ c_1$$
$$+0.007991\ c_1^2-0.000077774\ c_1^3, \quad (20)$$

in which $cR_{2,2}$ is the saturation value for dissolved oxygen in mg/L and c_1 is temperature in degrees Celsius.

The deoxygenation coefficient for nitrite production $XK_{(2,5)}$, was assumed equal to 3.43 times the rate of nitrite production ($XK_{6,5}$) based on the standard stoichiometric relation of oxygen to ammonia nitrogen in conversion to nitrate (Velz, 1970, p. 155). By computing the deoxygenation coefficient from the production of nitrite rather than from the decay of ammonia, it is inferred that the ammonia lost in the transition to nitrite does not exert an oxygen demand. This is a reasonable assumption, especially if the loss is caused by volatilization or uptake by bacteria. The deoxygenation rate for nitrate production ($XK_{2,6}$) was assumed equal to 1.14 times the rate of nitrate production ($XK_{7,6}$), after Velz (1970, p. 155).

Equation 18 has no provision for photosynthetic production or for benthic demand. These terms normally would be included in the source (S) term. Stamer and others (1979, p. 37) indicate that photosynthesis is not significant in this reach of the Chattahoochee River.

MODEL CALIBRATION

Flow.—The Chattahoochee River from Atlanta to Whitesburg has been studied many times. The flow model used here has been calibrated and verified for highly unsteady flow through the reach (Faye and others, 1979). Because the flow model had been well verified previously, its accuracy was not questioned or re-verified in this study.

The flow model was run with a 1-hour time step starting at 1800 hours on May 31, 1977, and ending at 0600 hours on June 2, 1977. The discharge at the upstream boundary, the Atlanta gage, was obtained from U.S. Geological Survey records of stage, which were converted to discharge by means of a rating curve. The flow at the Atlanta gage was nearly steady during the calibration run, varying only from 32 to 34 m^3/s. The stage at the downstream boundary, the Whitesburg gage, was also obtained from U.S. Geological Survey records.

All tributary inflows except the discharge from the Clayton WTF were assumed to be constant during the run. Data for tributary inflows were obtained from the U.S. Geological Survey WATSTORE files. During the calibration period, the flow in most tributaries was measured only once and in many was not measured at all, but data were available for May 30, 1977.

Seven observations of discharge from the Clayton WTF were available during the run. These data were plotted as a function of time, and the hourly discharge values for the Clayton WTF outfall were obtained from a smooth curve drawn through the points. The minimum reported discharge of the Clayton WTF of 2.27 m^3/S occurred at 0600 hours on June 1, 1977, and the maximum discharge of 4.05 m^3/S occurred at 1300 hours on June 1, 1977.

The cooling-water flow rate through the Atkinson and McDonough powerplants was not measured. The two powerplants were treated as a single heat source and an arbitrary cooling flow rate of 2.83 m^3/S was assumed.

The discharge in all tributaries as well as in the river is listed in table 1. Where discharges were not constant, the range in discharge is shown. The minimum flow in the river occurred at the beginning of the study for all river stations. In several places (listed in table 1), inflow from two or more tributaries was input to the model at a single grid point.

Transport.—A major difficulty in applying any unsteady water-quality model is determining the initial and boundary conditions. The boundary conditions were especially difficult in this study because of the many tributaries involved. Table 2 lists the mean input concentration for each constituent at each tributary. Also shown is the number of observations from which the average was computed. Where the number of observations was different for different constitutents, a range is shown. All data were obtained from the U.S. Geological Survey WATSTORE files. In general, no data were available for natural tributaries during the 36-hour study period. If zero observations are indicated in table 2, the listed concentration represents the average of one or more observations obtained on May 30, 1977.

If no observations were available during the run, the input concentration was assumed constant and equal to the value shown in table 2. The wastewater quality of Pea Creek was assumed to be the same as that of Annewakee Creek. Wastewater treatment facility outfalls were sampled six to nine times during the study. These data and the data for the Atlanta gage were plotted as a function of time, and smooth curves were drawn through the data points. The input concentrations for the model were read from these curves. In cases in which more than one input occurred at a single grid, the hourly concentrations were weighted in proportion to discharge and were averaged to determine the input concentration. The input temperature of all tributaries was assumed equal to the equilibrium temperature in order to obtain a reasonable diel variation.

A comparison of the observed concentrations with the predicted concentrations of BOD, organic nitrogen, and ammonia at the McDonough powerplant intake and Route I-280 indicated that the reported data for these constituents at the Clayton WTF were not representative of the actual constituent discharges. For flow conditions during the calibration run, the traveltime from the Clayton WTF outfall to the McDonough intake is only about 1.6 hours and the traveltime from the intake to Route I-280 is only about 0.4 hours. Since little time for decay occurs before the water arrives at these two observation points, the model results essentially represent a mass balance of the input loads. Furthermore, the diffuser system for the Clayton WTF outfall appeared to be very efficient, so complete mixing should also occur before the water reaches the observation sites. The concentrations of these constituents in the Clayton WTF outfall were, therefore, adjusted until the predicted and observed concentrations at the McDonough intake or Route I-280 were in reasonable agreement.

The reported and synthesized values of the concentrations of these three constituents in the Clayton WTF outfall are shown in figure 3. The means of the synthesized data are shown in table 2.

No data relative to the heat loads released by the Atkinson and McDonough powerplants were available. The thermal loads of the powerplants were synthesized by increasing the temperature of their return flow until the computed and observed temperatures at Route I-280 were in reasonable agreement. The traveltime from the powerplant outfalls to Route I-280 was only about 0.3 hours. The thermal loading was then computed from the temperature increase between the intake and outfall and the assumed flow rate through the plants. The inferred thermal loading varied from a low of about 440 megawatts (MW) at 0200 hours on June 2 to a high of about 840 MW at 1900 hours on June 1. The plant capacity is stated to be 730 MW, so, assuming an efficiency of 40 percent, the load factor varied from 24 to 46 percent. The inferred loading pattern varied smoothly throughout the day, with periods of nearly constant loading extending for 2 to 4 hours separated by short periods of increasing or decreasing loading.

The initial conditions were inferred from the first available instream observation.

The task of calibrating the unsteady water-quality model began by selecting a dispersion coefficient. The model was first run with a set of rate coefficients, which had been estimated from a steady-state analysis, using dispersion factors that ranged from 0 to 0.4. For each model run, the predicted and observed concentrations at each of the nine instream sites for which data were available during the calibration period were compared and a root-mean-square (RMS)

Table 2. Mean input concentrations for all tributaries during the May 31–June 2, 1977, calibration

Name of tributary	Number of observations	Concentration, in milligrams per liter					
		DO	BOD	ON	NH3	NO2	NO3
Cobb County wastewater treatment facility.	7 to 9[1]	0.7	64	6.9	10.3	0.03	0.28
Nancy and Peachtree Creeks	0[2]	6.7	7.0	.3	.1	.02	.47
Clayton wastewater treatment facility.	6 to 8	1.1	79.3	5.2	14.6	.01	.00
Proctor Creek	0	4.0	2.9	5.1	3.4	.04	.28
Nickajack Creek	0	8.7	4.6	.4	.0	.01	.67
South Cobb County wastewater treatment facility.	6 to 7	.6	86.3	8.3	13.5	.08	.04
Utoy wastewater treatment facility.	6 to 7	3.0	30.6	2.3	14.1	.01	.01
Utoy Creek	0	7.5	5.7	.4	.2	.02	.40
Sweetwater Creek	1	7.7	5.1	.5	.1	.01	.28
Camp Creek wastewater treatment facility.	6 to 7	3.7	10.5	1.0	6.4	.08	1.80
Camp Creek	0	8.0	4.4	.4	.1	.03	.67
Deep Creek	0	8.4	4.4	.4	.0	.01	.45
Annewakee Creek	0	8.8	4.0	.2	.0	.01	.44
Pea Creek	0	-	-	-	-	-	-
Bear Creek (right bank)	0	10	4.3	0.1	0.0	0.01	0.18
Bear Creek (left bank)	0 to 1	8.6	3.6	.2	.0	.01	.36
Dog River	0 to 1	9.0	4.1	.2	.0	.01	.23
Wolf Creek	0	8.6	3.7	.2	.0	.00	.18
Snake Creek	0	8.8	3.8	.2	.0	.01	.19
Cedar Creek	0 to 1	8.2	3.7	.1	.1	.01	.21

1 Seven observations were available for some of the constituents and nine were available for others.

2 For zero observations, the listed concentration represents the average of one or more observations obtained on May 30, 1977.

error was determined for each of the seven constituents based on all available data. Between 78 and 91 observations were available for individual constituents at various times and locations. The RMS errors in the computed organic nitrogen and ammonia concentrations were fairly sensitive to the assumed dispersion factor. As will be seen later, a fairly well defined pulse of these materials was released from the Clayton WTF and downstream data were taken at times and locations suitable for defining the dispersion of this material. The RMS error in organic nitrogen concentration was a minimum for a dispersion factor of 0.16 and the RMS error for ammonia concentration was a minimum for a dispersion factor of

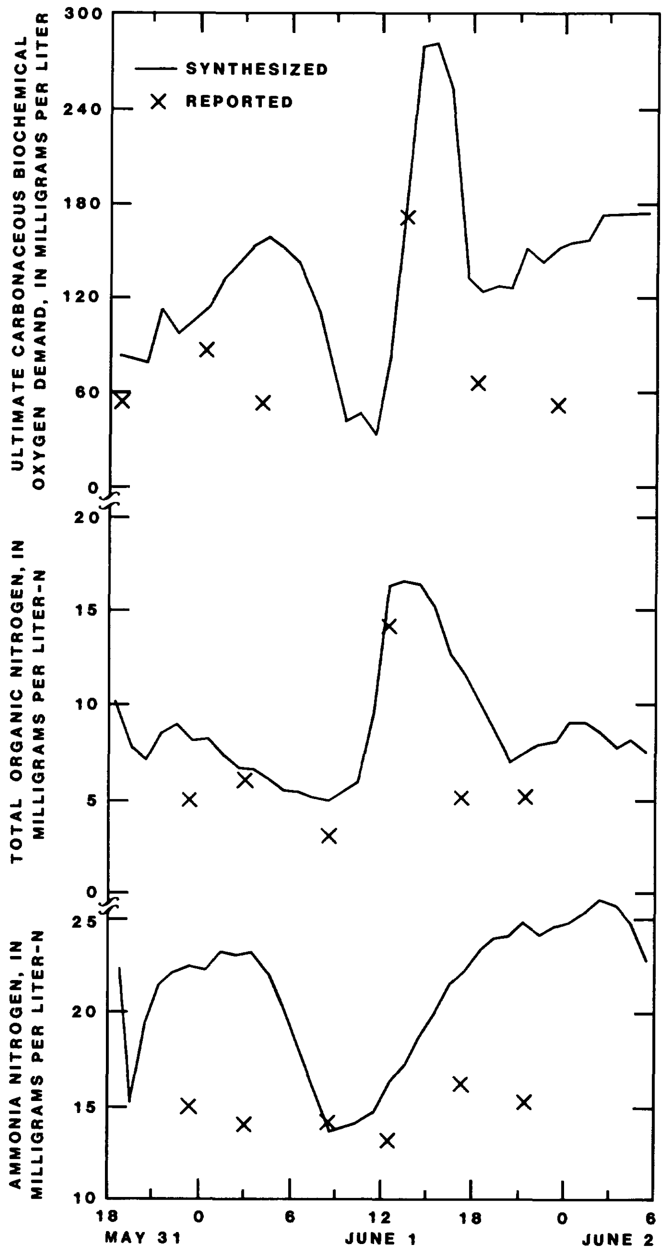

Figure 3. Comparison of synthesized and reported concentrations for the Clayton wastewater treatment facility outfall for May 31 to June 2, 1977.

0.27. Considering the rather crude nature of these estimates, it was decided to use a dispersion factor of 0.2.

The dispersion factor can be converted to a dispersion coefficient by use of equation 4. The mean velocity in the river during the calibration run was about 0.48 m/s, so the optimum dispersion coefficient was 170 m^2/S. The average slope was 0.000297 and the average depth was about 1.4 m. Fischer (1973) reports observed dispersion coefficients in rivers that vary from 74 to 7,500 times the product of the depth and the shear velocity. The selected dispersion coefficient for the Chattahoochee is equal to 1,900 times the product, which is a reasonable value relative to observed dispersion coefficients in other rivers.

Temperature.—The temperature model requires a windspeed and equilibrium water temperature as input data. The only meteorologic data available were those recorded by the National Weather Service at Hartsfield-Atlanta International Airport. Windspeed as well as air and dewpoint temperatures are available at 3-hour intervals.

Initial attempts to use the air temperature as an estimate of equilibrium temperature resulted in fair agreement between the computed and observed river temperatures, yielding a RMS error of 0.69°C and a mean error of 0.12°C based on the 81 observations of river temperature. The diel swings in the downstream reaches were underpredicted, however, and the computed river temperatures peaked about midnight rather than around 1800 hours as would be expected.

The equilibrium temperature was then computed and used as model input. The National Weather Service does not record solar radiation in Georgia, but indicated that the expected value for Atlanta on June 1 would be 247 w/m^2 (Connie and others, 1980). This value was distributed throughout each day using the formulas and procedure suggested by the Tennessee Valley Authority (1972). The incoming atmospheric radiation was estimated from the air and dewpoint temperatures using the procedure outlined by Koberg (1964). Standard procedures were then used to compute hourly values of equilibrium temperature for use as model input.

Previous modeling efforts (Faye and others, 1979), using meteorological data obtained at the Clayton WTF, indicated that a wind function 70 percent of the value indicated by equation 8 is representative of conditions on the Chattahoochee River. The minimum RMS error in predicted temperatures for this study also occurred when a wind function equal to 70 percent of the value given by equation 8 was used. The agreement in the wind function for these two calibration efforts is considered a verification of the validity of equation 8 as a predictor of the wind function for open channels.

A comparison of the predicted and observed temperatures is provided by figure 4. In this figure, the symbols represent the observed temperatures and the solid curve represents the modeled temperature. Figure 4 shows the time variation of computed and observed temperatures at each of the nine river stations where data were available. The computed and observed temperatures at the Atlanta gage are in perfect agreement because the observed temperatures there were used as the upstream boundary condition. The RMS error is based only on the observations at the stations downstream of the Atlanta gage. The RMS error in the predicted temperatures is 0.66°C with a mean error of 0.03°C based on 81 observations. For purposes of discussion, the times that a few specific water parcels (labeled A, B, C . . . in figures 4 through 18) passed each observation point are indicated in the figure. The interpretation of the data centered around analyzing a large number of specific parcels as they were convected through the system. An analysis of a few of these parcels is presented below because it is believed that this analysis is a good way to assess the adequacy of the model.

Consider parcel A, which passed Fairburn at 1900 hours on May 31 with a temperature of 26.0°C. During the night, it cooled only slightly, to 24.1°C, and arrived at Capps Ferry at 0510 the next morning. During the daylight hours of June 1, 1977, the parcel traversed the reach between Capps Ferry and Whitesburg, arriving there at 1630. The model underpredicted the heat gained by the parcel during this daylight period. The model predicted a temperature rise of 1.8°C while the data indicated a rise of 2.4°C. The model error, quite likely, is the result of a poor estimate of solar radiation in computing the equilibrium temperature.

Parcel C passed the powerplants' outfall at 1730 on May 31, receiving a large thermal load. It arrived at Route I-280 at 1800 hours that day with a temperature near 30°C. During the night it cooled to 25.7°C as it traveled to Fairburn, arriving there at 0730 on June 1. The model results were excellent in predicting this large amount of cooling and were good in predicting the small amount of cooling of parcel A during the same time period. During the daytime, parcel C moved to Capps Ferry, arriving there at 1740. The model predicted it would warm by 1.2°C, while the data indicate it actually warmed by 1.6°C. Thus, the model underestimated the warming of both parcels A and C by 25 percent during the daylight hours of June 1.

Parcel F passed the powerplants' outfall at 0300 on June 1 and received a small thermal load. The parcel cooled during the rest of the night as it moved to Route 139, arriving there at 0715 with a temperature of 24.5°C. During the daylight hours of June 1, it traversed the reach between Route 139 and Fairburn. Although no data were available at Route 139, it would appear that the temperature rise for this parcel was also underestimated during the daylight hours of June 1.

National Weather Service records indicate that on June 1, 1977, Atlanta received 93 percent of the total possible sunshine while on an average day in June 74 percent of the total possible sunshine is received. It seems probable, therefore, that the actual solar radiation on June 1, 1977, was greater than the mean value for June 1 used to compute the equilibrium temperature. Overall, however, the model predictions are very good and the thermal model is accepted as calibrated. It would appear that the observed temperatures at Hutcheson contain a systematic error and that they are about 1°C low.

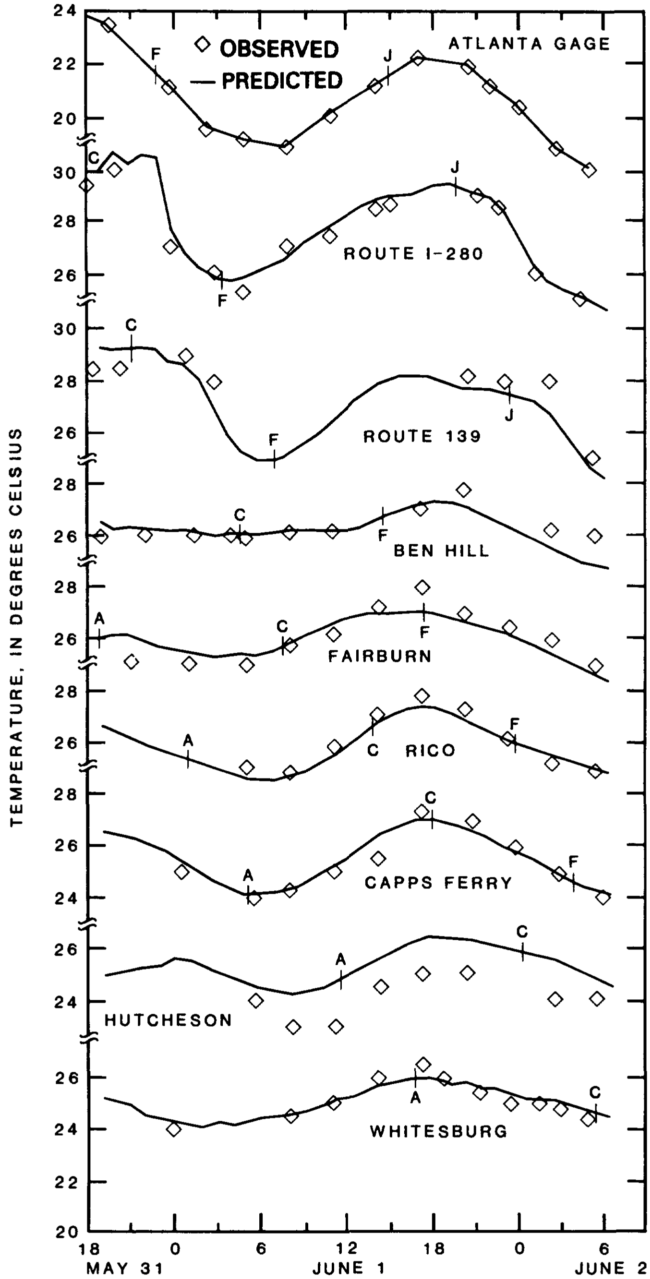

Figure 4. Comparison of predicted and observed water temperatures in the Chattahoochee River, May 31 to June 2, 1977.

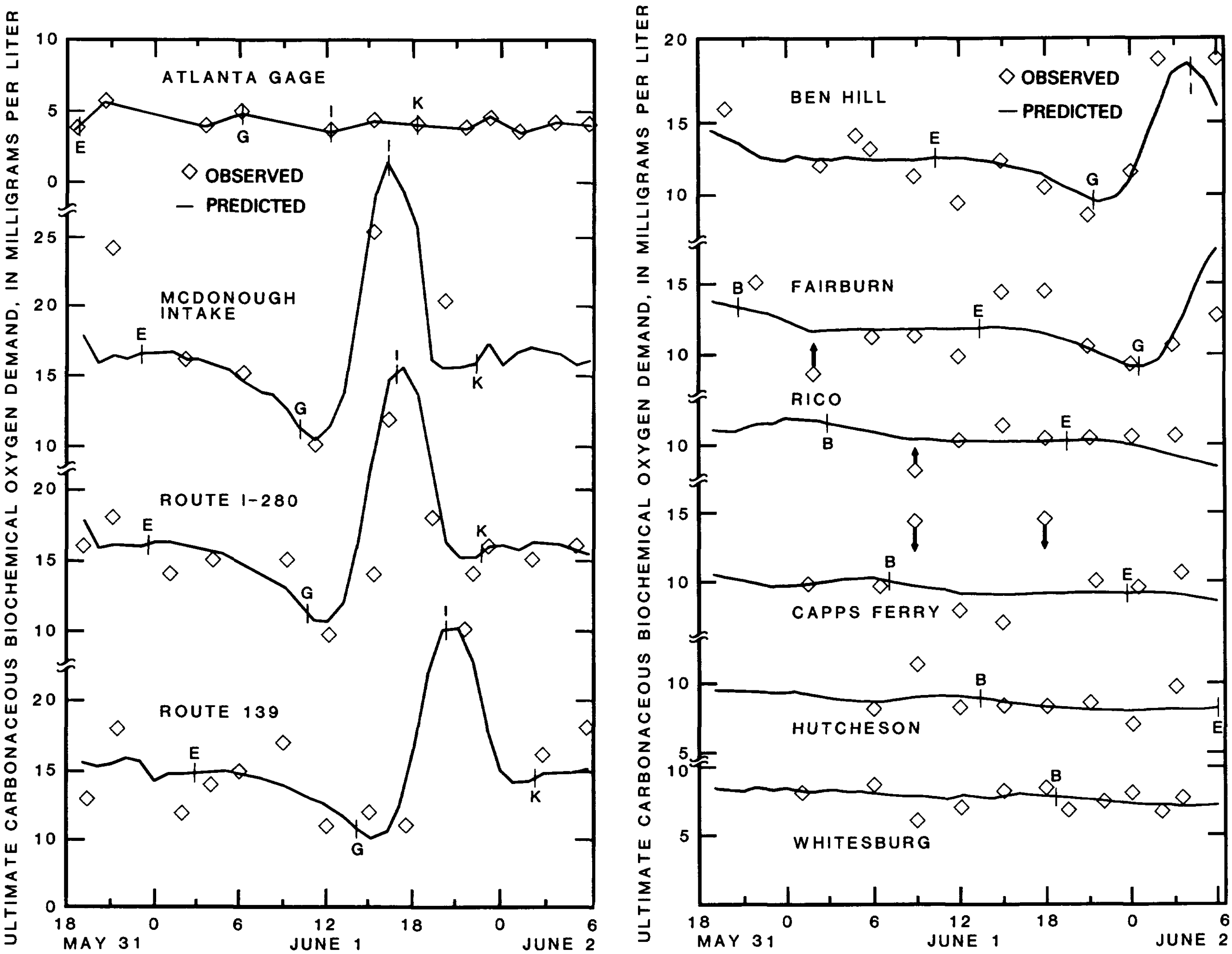

Figure 5. Comparison of predicted and observed ultimate carbonaceous biochemical oxygen demand in the Chattahoochee River, May 31 to June 2, 1977.

Ultimate carbonaceous biochemical oxygen demand (BOD).—The only model coefficient that significantly influences the predicted concentration of BOD in the river is the extraction-rate coefficient K_{BO}. The value of K_{BO} in the model was varied until a minimum RMS error in the predicted BOD's was obtained. The optimum value for K_{BO} was 0.0142 per hour (0.34 per day). Predicted and observed BOD concentrations are shown in figure 5. A few of the BOD observations that appear to be badly in error were ignored in the analysis but are included in figure 5. The RMS error, based on 84 observations, is 0.21 mg/L and the mean error is −0.04 mg/L.

The times that a few parcels pass each observation point are also indicated in figure 5. To illustrate the degree of model calibration achieved and to provide an understanding of the processes controlling the BOD concentrations, three of these parcels will be discussed in some detail.

Parcel B passed Fairburn at 2100 on May 31 with a BOD of about 13.1 mg/L. During its 21.6-hour transit from Fairburn to Whitesburg its BOD was reduced to 7.5 mg/L. According to the model, BOD extraction accounted for most of the change, decreasing BOD concentration by 3.9 mg/L while tributary inflow reduced BOD concentration by 1.1 mg/L and dispersion decreased it by 0.6 mg/L. The model appears to do a good job of simulating these changes.

Parcel G passed the Atlanta gage at 0600 on June 1 with a low BOD concentration of 5.0 mg/L. It passed the Clayton WTF outfall 2.5 hours later, receiving a relatively small BOD load, and arrived at the McDonough intake at 1000 with a BOD concentration of 11.0 mg/L. During the next 14.4 hours, the parcel was convected to Fairburn while its BOD concentration fell to 8.4 mg/L. Because parcel G received a minimal BOD load from the Clayton WTF, dispersion from high-concentration parcels both upstream and downstream increased its BOD by 0.1 mg/L during the transit from the McDonough intake to Fairburn, while tributary inflow increased its BOD by another 0.1 mg/L and decay (or extraction) reduced its BOD by 2.8 mg/L. Looking at the amount of BOD decay that occurred (2.8 mg/L) and the accuracy of the predicted concentrations at Fairburn, one must conclude that the simulation is excellent.

Parcel I, on the other hand, received a large BOD load from the Clayton WTF. During the 11.5 hours required for this parcel to move from the McDonough intake to Ben Hill, its BOD was reduced by 15.9 mg/L. Dispersion, tributary dilutions, and BOD extraction reduced parcel I's concentration by 7.1 mg/L, 2.7 mg/L, and 6.1 mg/L, respectively. Because the data scatter for parcel I is large, the best that can be said is that the model results are reasonable.

Although the scatter in all the data is large, it appears that for the parcels discussed and other parcels, such as E, the model results are good. In addition, the first order decay process used in the model provides a realistic description of the fate of carbonaceous biochemical oxygen demand in the Chattahoochee River under unsteady constituent-loading conditions. The extraction rate of 0.34 per day also appears to be a realistic estimate of the actual extraction rate that was operative in the river.

Total organic nitrogen (ON).—The only model coefficient that significantly influences the predicted concentration of organic nitrogen is the decay rate for organic nitrogen K_{ON}. The decay rate was varied in the model until a minimum RMS error in the predicted concentrations was obtained. The optimum decay-rate coefficient was 0.0077 per hour (0.18 per day). This decay rate resulted in an RMS error of 0.20 mg/L and an average error of 0.01 mg/L for the 78 observations shown in figure 6.

Consider parcel D, which at 1800 hours on May 31 was located just downstream of the Atlanta gage. Its initial organic-nitrogen concentration was only 0.15 mg/L. Four hours later it was located at the McDonough intake and had a concentration of 1.0 mg/L because of the Clayton WTF loading. During the 30.7 hours required for parcel D to move from the McDonough intake to Hutcheson, its organic nitrogen concentration was reduced to 0.62 mg/L. During this time, dispersive effects increased its concentration by 0.08 mg/L while tributary inflow reduced it by 0.12 mg/L. As shown in figure 6, the ammonification loss (0.34 mg/L) is large compared with the probable error of the computed value at Hutcheson.

Parcel G passed the Atlanta gage with an organic nitrogen concentration of 0.07 mg/L. It received a relatively small load from the Clayton WTF outfall and arrived at the McDonough intake at 1000 with a concentration of 0.56 mg/L. The organic nitrogen concentration increased slightly during the next 14.4 hours as the parcel was convected to Fairburn. During the transit, dispersive effects and tributary inflow increased its concentration by 0.14 and 0.11 mg/L, respectively, while ammonification reduced its concentration by only 0.13 mg/L.

Finally, parcel H received a large organic nitrogen load from the Clayton WTF outfall and arrived at the McDonough intake with a concentration of 2.21 mg/L. During the 14.4 hours required for the parcel to be convected to Fairburn, the computed concentration fell to 1.40 mg/L. Dispersion, tributary dilution, and ammonification reduced its concentration by 0.32, 0.15 and 0.34 mg/L, respectively. The scatter in the observed data near this parcel is large.

As shown by the concentrations observed at the McDonough intake (figs. 3, 5, and 6), the loading rate at the Clayton WTF was quite unsteady. The time distribution of the organic nitrogen loading was very similar to the BOD loading (fig. 3).

The ammonification loss was large, relative to the scatter in the data, only for parcel D. For this parcel, however, the model did an excellent job of simulating the observed concentrations. Overall, the model performance is very good and a good calibration of the ammonification process has been achieved. Furthermore, the organic nitrogen decay-rate coefficient of 0.18 per day is a realistic measure of the physical ammonification processes in the river.

Total ammonia nitrogen (NH).—As can be seen from figure 2, the concentration of ammonia is dependent on two rate coefficients. Because no nitrogen loss is assumed to occur in the transformation from organic nitrogen to ammonia, one of these coefficients is already fixed. The value of K_{ON} was fixed at $+0.18$ per day and the value of the extraction rate for ammonia K_{NH} was varied until a minimum RMS error in the predicted concentrations of ammonia was obtained. The optimum value for the extraction rate of ammonia was 0.0167 per hour (0.40 per day). This extraction rate resulted in an RMS error of 0.109 mg/L and a mean error of -0.008 mg/L. Predicted and observed concentrations of ammonia nitrogen are shown in figure 7.

Parcel C was intially located at Route I-280. Its predicted and observed concentrations were in close agreement throughout the 35-hour transit through the system. During its transit from Route I-280 to Whitesburg, the predicted concentration was reduced by 1.77 mg/L as a result of dispersion (-0.37 mg/L), tributary inflow (-0.24 mg/L), production from organic nitrogen ($+0.32$ mg/L), and extraction (-1.48 mg/L). Extraction was the dominant process in determining the parcel's final concentrations. This process must be modeled accurately because the error in the computed concentration of parcel C is always small relative to the magnitude of the change in concentration due to the extraction process.

Parcel G, discussed previously with respect to its concentration of BOD and organic nitrogen, received about the minimum ammonia load to be released from the Clayton WTF. Parcel G arrived at the McDonough intake at 1000 on June 1 with an ammonia concentration of only 1.27 mg/L. During the transit to Fairburn, its concentration was changed by the processes of dispersion (+0.18 mg/L), tributary inflow (+0.13 mg/L), production from organic nitrogen (+0.12 mg/L), and extraction (−0.53 mg/L) such that it arrived there with an ammonia concentration of 1.17 mg/L. Comparing the computed and observed concentrations for parcel G at each measurement site with the magnitude of the change due to extraction indicates a very good calibration of the ammonia phase of the nitrification model.

Finally, parcel J received a large ammonia load from the Clayton WTF and arrived at the McDonough intake at 1900 on June 1 with an ammonia concentration of 2.39 mg/L. During the parcel's 4.2-hour transit to Route 139, its concentration was changed by dispersion to a small extent (>+0.01 mg/L), tributary inflow (+0.02 mg/L), production (+0.04 mg/L), and extraction (−0.29 mg/L). Because of the short traveltime, the changes are fairly small. The extraction term is still fairly large, however, compared with the errors in the computed concentrations.

Large quantities of ammonia, as well as BOD and organic nitrogen, were released from the Clayton WTF. A significant amount of ammonia was also produced through the ammonification process. Parcel G passed the Clayton WTF outfall at about 0830 and received about the minimum load of all three constituents. The peak loading of the three constituents, however, did not occur simultaneously. The maximum BOD load occurred at about 1430, the maximum organic nitrogen load occurred at about 1330, and the maximum ammonia load occurred at about 1730. The ammonia load has a broader peak than the other two and, in contrast to the other loads, appears to have peaked at about the same time on May 31.

In summary, the extraction term appears to be the major process influencing the downstream concentration of ammonia. Considering all the data, the model calibration for the ammonia component appears to be excellent. The extraction rate for ammonia of 0.40 per day seems to be well founded.

Total nitrite-nitrate.—The concentrations of nitrite and nitrate are closely linked and will be discussed together. Because the concentrations of nitrite are typically an order of magnitude smaller than the concentrations of nitrate, results are usually presented as the sum of the two. As stated previously, it was assumed that there would be little uptake of nitrate in the system and that various losses of nitrogen would occur in the transition from ammonia to nitrite. Therefore the production rate and the decay rate of nitrite could not be assumed to be known. However, the production rate was assumed to be a constant percentage of the ammonia extraction rate. Given this conceptualization of the nitrification kinetics, the concentrations of both nitrite and nitrate were dependent on the percentage of ammonia lost in the transformation to nitrite and on the nitrification rate for nitrite. These two coefficients were varied until the combined RMS standard error for nitrite and nitrate was minimized. The combined error was computed as the sum of the standard errors for each constituent, and the standard error for each constituent was determined by dividing the RMS error by the mean value of the observed concentrations.

The optimum results were obtained when it was assumed that 30 percent of the extracted ammonia was lost to unknown sinks and that the nitrification-rate coefficient for nitrate was 0.138 per hour (3.3 per day). Using these coefficients, the RMS error in nitrite concentrations was 0.019 mg/L and the RMS error in nitrate concentrations was 0.06 mg/L. The corresponding mean errors were 0.001 and 0.008 mg/L, respectively. Comparisons of the predicted and observed concentrations are shown in figures 8 and 9.

Because of the expanded scales used on the figures, the results do not appear as good as those obtained for the other constituents. A detailed inspection of the results for specific parcels, however, indicates satisfactory model simulations.

Consider parcel B, which was located about 16 Km upstream of Fairburn when the simulation began and which had concentrations of nitrite and nitrate of 0.08 and 0.69 mg/L, respectively. The parcel arrives at Whitesburg with a predicted nitrite concentration of 0.06 mg/L and a nitrate concentration of 0.93 mg/L. It is obvious from figure 8 that the predicted nitrite concentrations are systematically about 0.02 mg/L lower than the observed values at Hutcheson and Whitesburg. On the other hand, the scale in figure 8 is extremely large, so it is instructive to assess the magnitude of the error in terms of the changes that are occurring. During its 24.6-hour traveltime, dispersion and tributary inflow had little effect on parcel nitrite concentration, increasing it by 0.01 mg/L and decreasing it by 0.01 mg/L, respectively. A

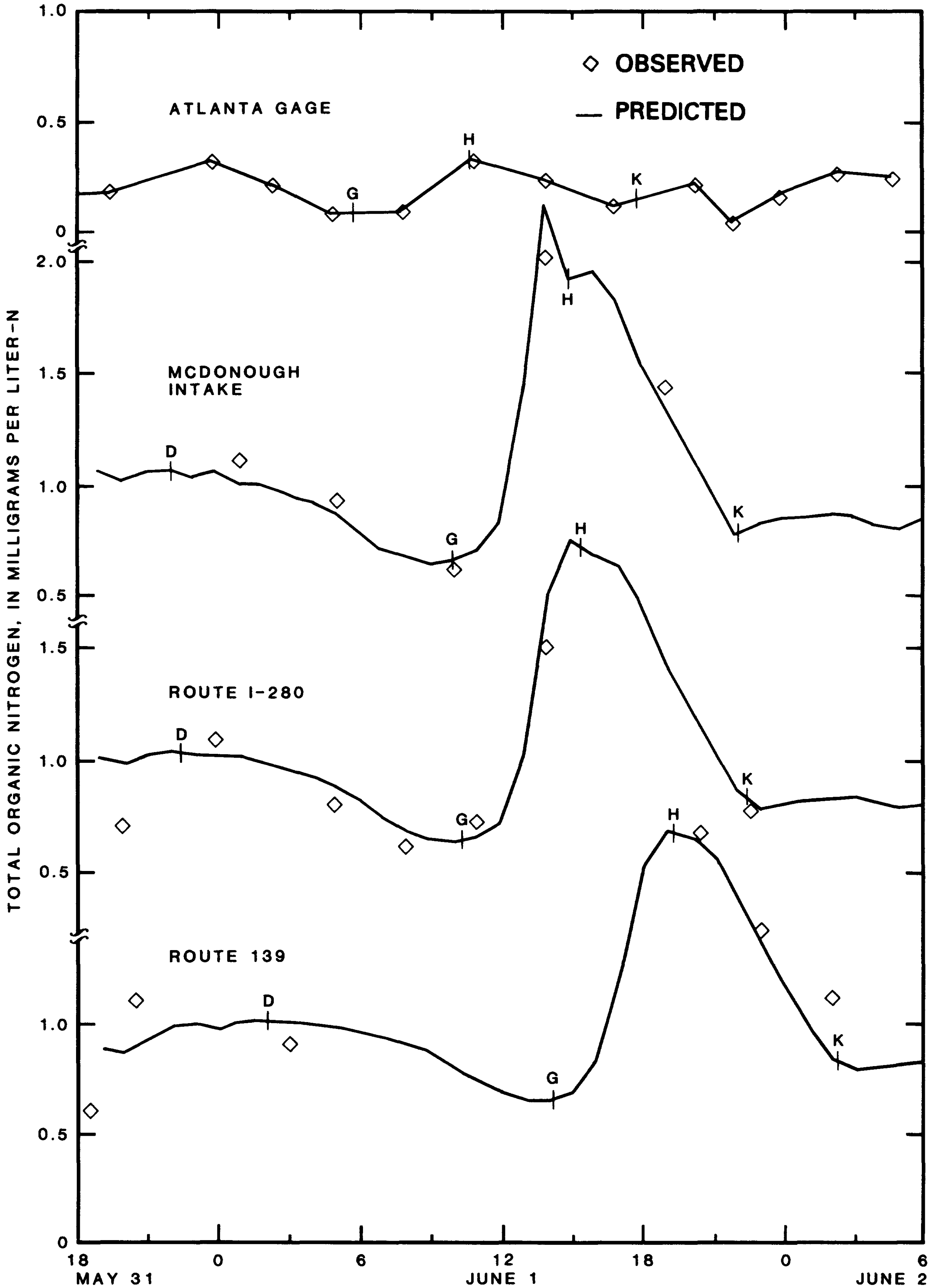

Figure 6. Comparison of predicted and observed concentrations of total organic nitrogen in the Chattahoochee River, May 31 to June 2, 1977.

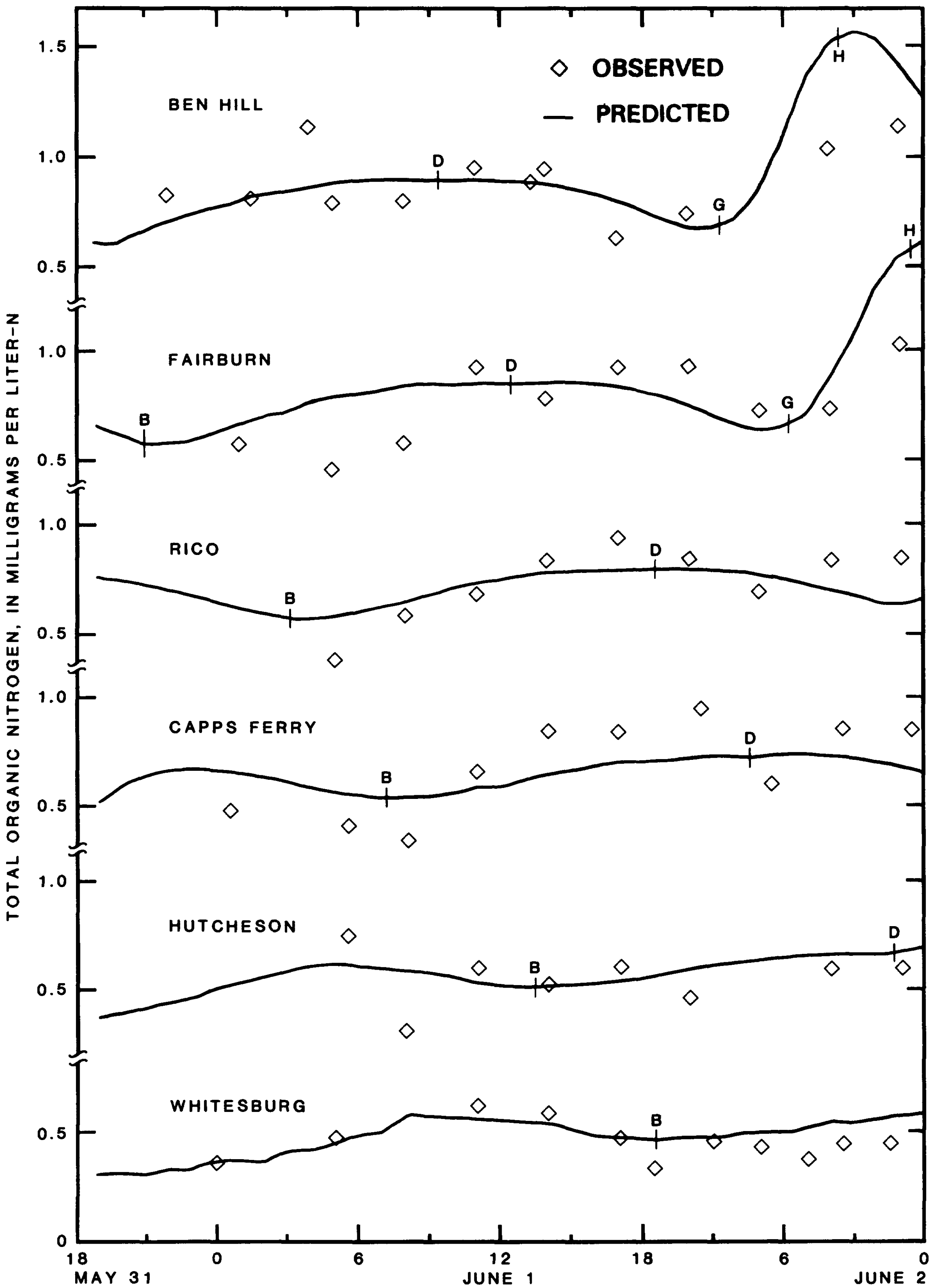

Figure 6. Continued.

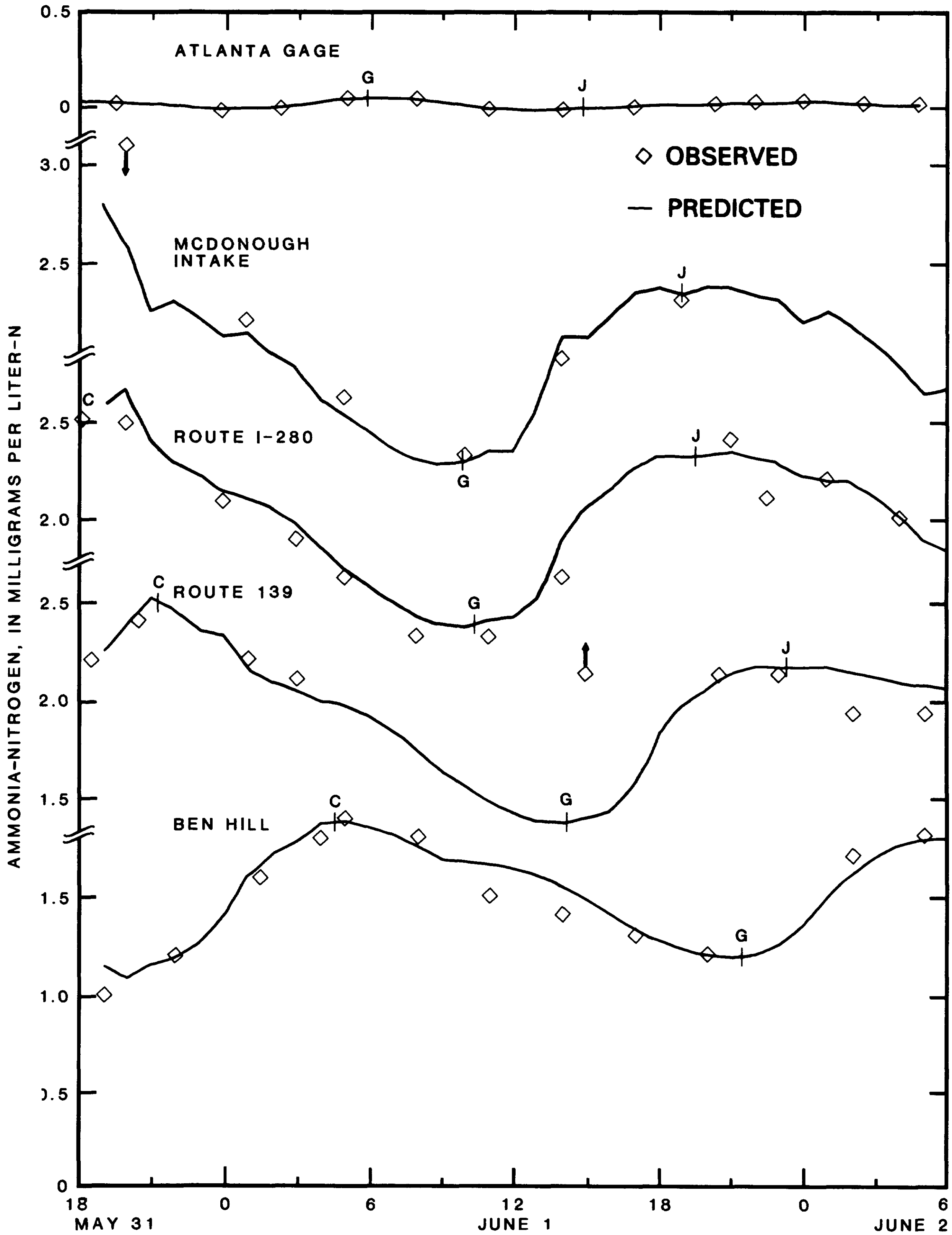

Figure 7. Comparison of predicted and observed concentrations of total ammonia nitrogen in the Chattahoochee River, May 31 to June 2, 1977.

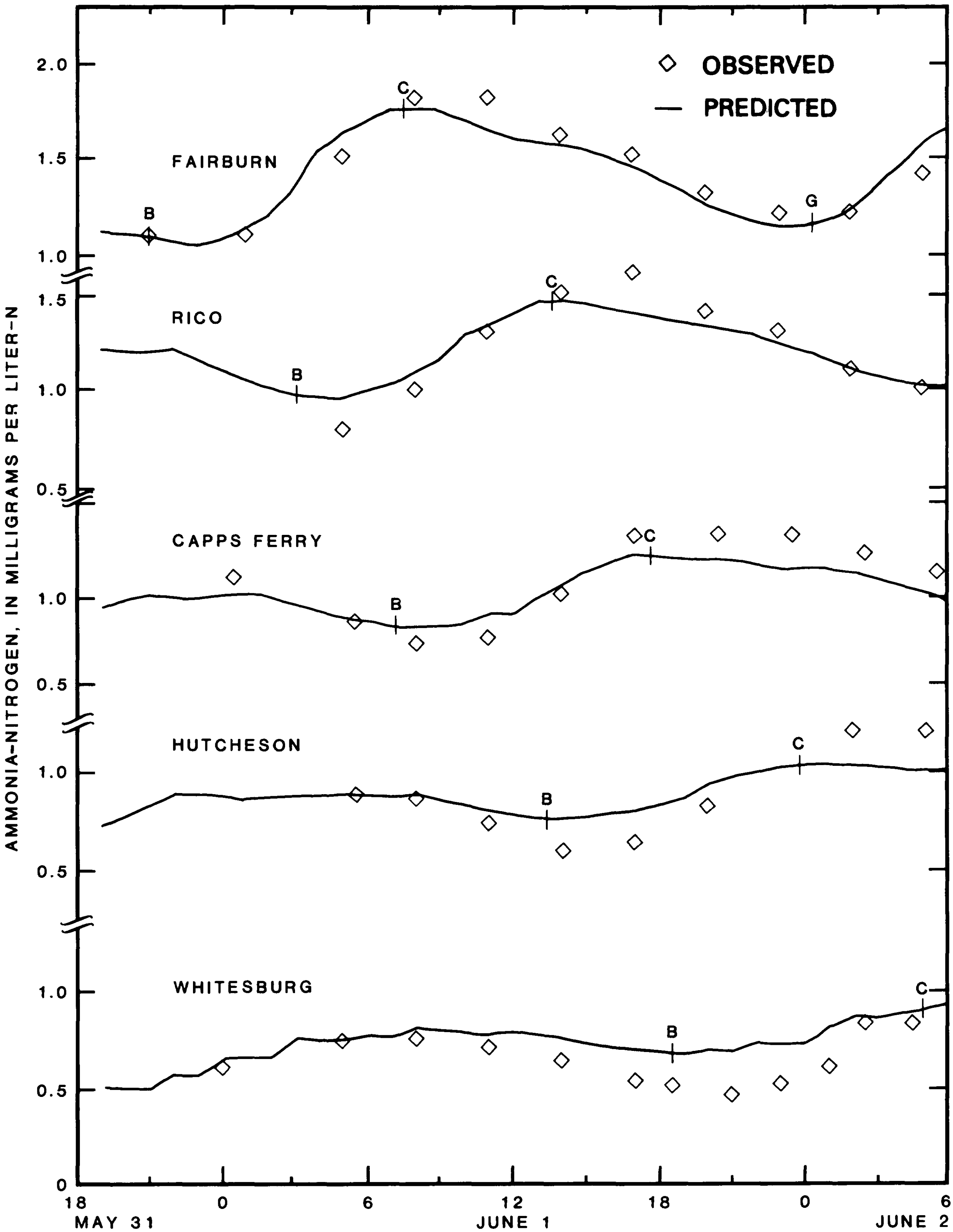

Figure 7. Continued.

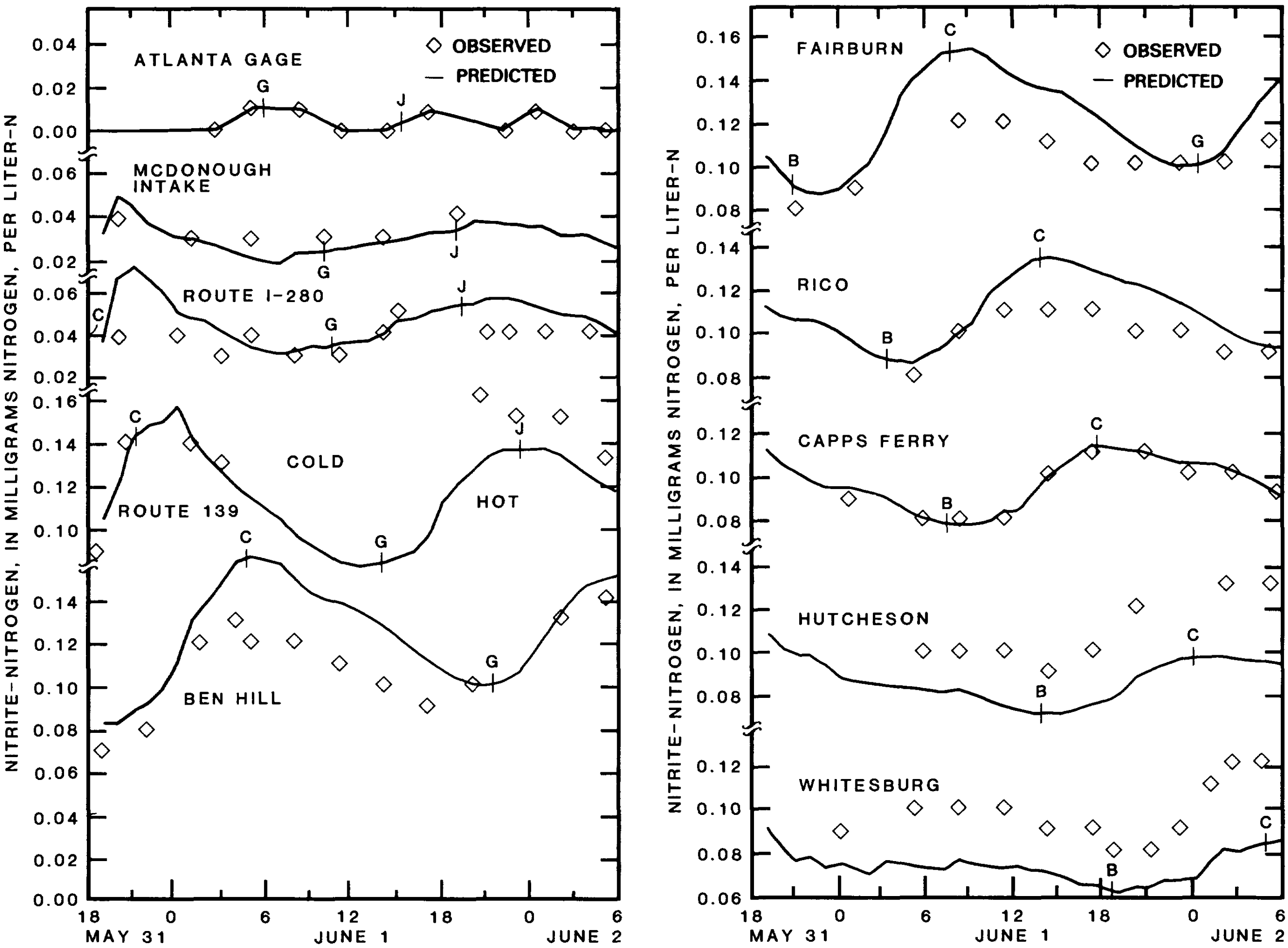

Figure 8. Comparison of predicted and observed concentrations of total nitrite-nitrogen in the Chattahoochee River, May 31 to June 2, 1977.

total of 0.36 mg/L was produced from the nitrification of ammonia, and 0.38 was lost through nitrification to nitrate. The error in the predicted nitrite concentration is small in comparison with the amount that was either produced or decayed. The nitrate concentration of the parcel was modified during its transit as follows: dispersion (−0.01 mg/L), tributary inflow (+0.10 mg/L), and production from nitrite (+0.38 mg/L). The errors in nitrate concentrations for parcel B, shown in figure 9, remain smaller than the amount of nitrate produced during its transit through the system.

The rate coefficients were assumed to be independent of location in the river. Ehlke (1978), however, indicates that nitrobacter at Capps Ferry were more than 40 times as numerous as at Whitesburg during this study. If the rate of nitrification of nitrite to nitrate was reduced because of a shortage of nitrobacter below Capps Ferry, the predicted concentrations at Hutcheson and Whitesburg would be in better agreement with the data.

While parcel B received a small nitrogen load, parcel C received about the maximum nitrogen load from the Clayton WTF. From figures 8 and 9 it would appear that the model did a poorer job of simulating the concentration for parcel C than for any other parcel. Just downstream of the WTF, the model predicts a more rapid buildup in nitrite than is shown by the data, while downstream of Fairburn the model shows a more rapid decline than is indicated by the data. The gradual buildup in the nitrate concentration of parcel C is modeled reasonably well. The concentrations of nitrifying bacteria were not modeled, so the rate coefficients were assumed to be independent of the number of bacteria available. Possibly, there were insufficient nitrifying bacteria to

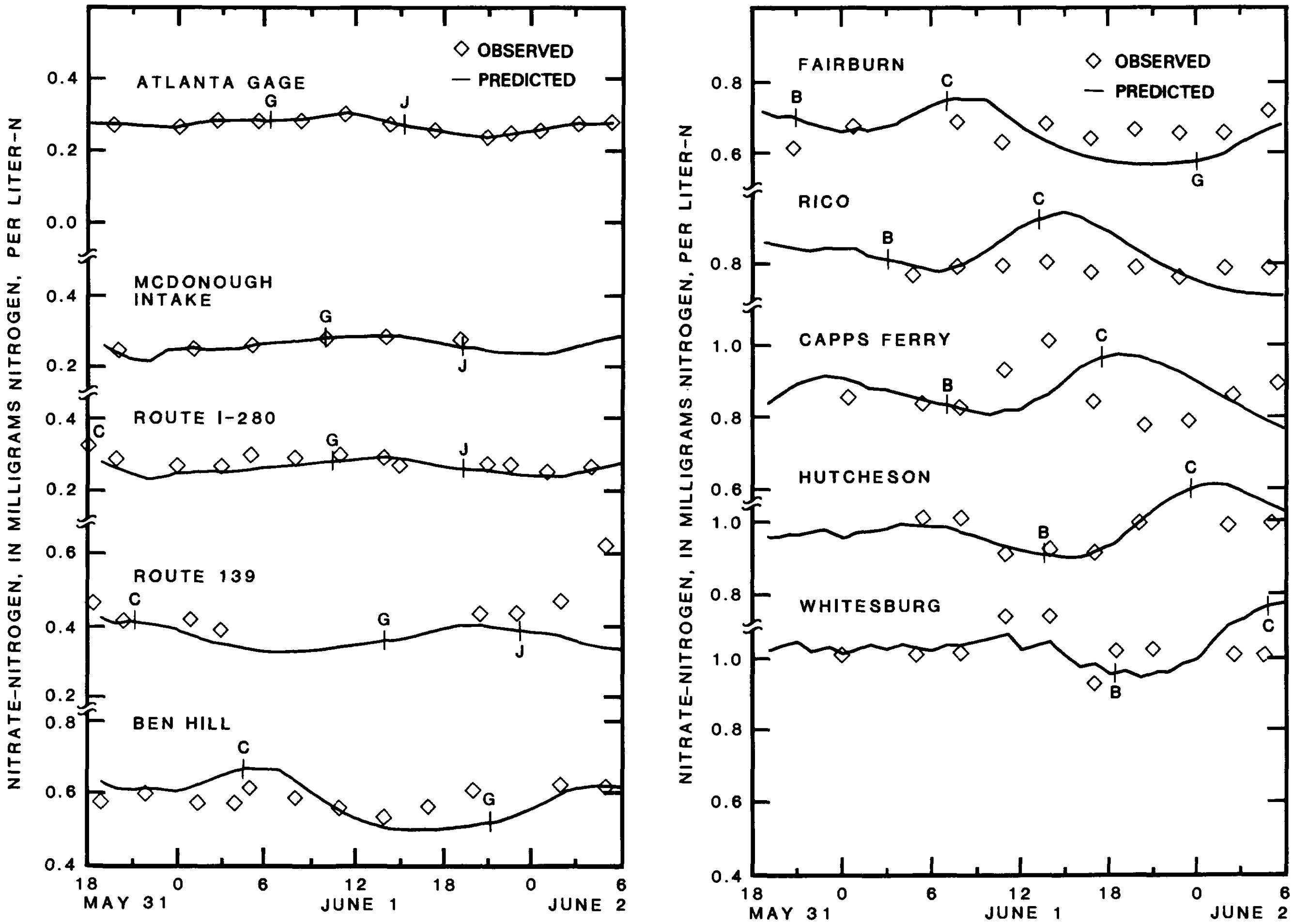

Figure 9. Comparison of predicted and observed concentrations of total nitrate-nitrogen in the Chattahoochee River, May 31 to June 2, 1977.

convert the large pulse of ammonia concentration in parcel C to nitrite in the upstream reaches. While there are systematic errors in the predicted nitrite concentrations, these errors are small compared with the total amount of nitrogen being converted through the species. For example, during the 35-hour traveltime, the nitrite concentration of parcel C was modified by dispersion (−0.02 mg/L), tributary inflow (−0.05 mg/L), production from ammonia (+1.23 mg/L) and decay to nitrate (−1.09 mg/L). The error at any time in figure 8 for parcel C is less than 0.05 mg/L. The nitrate production term (1.09 mg/L) likewise accounted for most of the modeled increase in nitrate concentration between Route I-280 and Whitesburg.

Parcel G received a small load of all constituents at the Clayton WTF outfall and, like the results for parcel B, the simulation results in figures 8 and 9 appear to be good.

In conclusion, the model calibration for the nitrite and nitrate constituents appears to be reasonably good, but perhaps there is some systematic error in the nitrite concentrations for very heavily loaded parcels and for all parcels below Capps Ferry.

Dissolved oxygen (DO).—Dissolved oxygen is the most complex constituent to model because its value depends on the concentrations of several other constituents, but there are few rate coefficients left to determine. Initial simulations assumed that all BOD and ammonia extraction consumed oxygen. Predicted oxygen concentrations using this assumption averaged more than 1 mg/L less than the observed values. Nitrogen lost in the transition from ammonia to nitrite was then assumed not to consume oxygen and the predicted DO concentrations increased by an average of 0.2 mg/L. Finally, a fixed percentage of the BOD extraction was assumed to represent settling and to consume no oxygen. The optimum fit to the observed dissolved oxygen occurred when 38 percent of the BOD extraction represented settling. Velz (1970, p. 163) indicates that untreated waste settleable solids usually constitute about one-third of the total BOD. In contrast Velz's (1970) model, it was assumed that the extracted BOD did not exert a

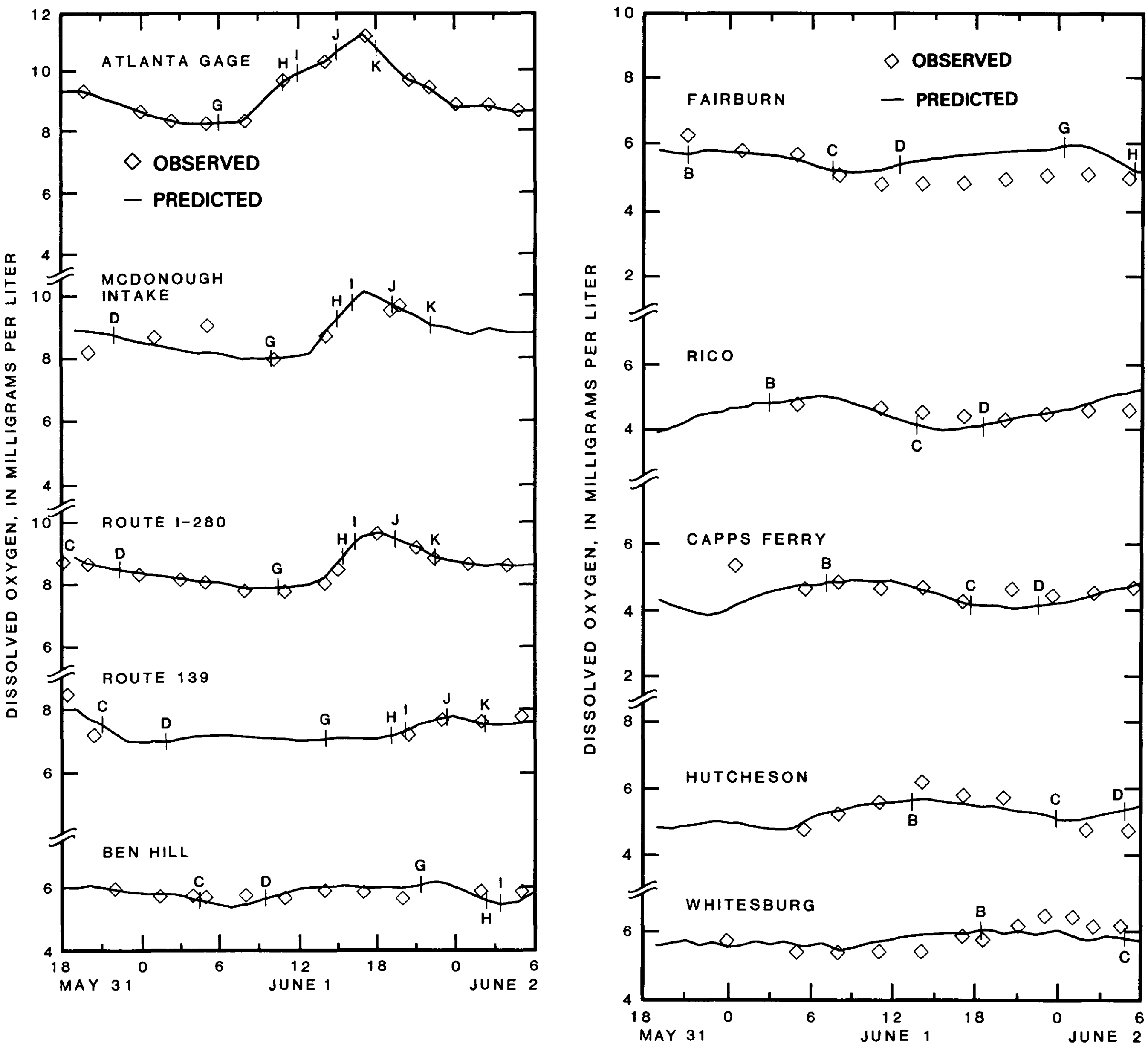

Figure 10. Comparison of predicted and observed concentrations of dissolved oxygen in the Chattahoochee River, May 31 to June 2, 1977.

benthic demand. Predicted and observed oxygen concentrations based on these assumptions are shown in figure 10. The RMS error in figure 10 is 0.38 mg/L and the mean error is 0.002 mg/L.

The model was then run assuming that all BOD and ammonia extraction consumed oxygen, but the reaeration coefficient, computed by equation 17, was increased to match the observed concentrations of oxygen. The optimum fit yielded an RMS error of 0.63 mg/L when the reaerationcoefficient was increased by a factor of 2.2.

The reaeration coefficient computed from equation 17 varies significantly from reach to reach. The minium value, at 25°C, of 0.36 per day occurred in the reach from Fairburn to Rico and the maximum value of 2.9 per day occurred in the reach from Atlanta to the Clayton WTF. A reaeration coefficient computed from the expression presented by Bennett and Rathbun (1972) does not vary much from reach to reach. The optimal results using the Bennett-Rathbun equation occurred with a BOD settling of only 5 percent and yielded an RMS error of 0.54 mg/L.

All things considered, it was concluded that 38-percent settling with the Tsivoglou reaeration equation (eq. 17) provided the best description of the observed data. The plotted results for all the alternatives looked very similar to the data, however, and a clearcut case cannot be made for any of the various options.

The locations of all parcels tracked in figures 4–8 are also noted in figure 10. Consider parcel B, which was previously discussed in relation to its BOD, nitrite, and nitrate concentrations. Upstream of Fairburn parcel B started with a DO concentration of 5.97 mg/L. According to the model, its minimum concentration of 4.61 mg/L occurred at 0500 hours on June 1 when it was located about 5 km downstream of Rico. At this low point, the parcel had gained oxygen owing to dispersion (0.06 mg/L), tributary inflow (0.20 mg/L), and reaeration (0.79 mg/L) and had lost oxygen owing to BOD deoxygenation (1.55 mg/L), nitrite production (0.64 mg/L), and nitrate production (0.22 mg/L). As shown in figure 10, the predicted concentration at the sag point seems to agree well with the observed results. After 0500 hours, the recovery begins, and by the time parcel B reaches Whitesburg, its DO has recovered to 5.93 mg/L, almost exactly where it started. In the recovery phase, the parcel gained oxygen owing to dispersion (0.03 mg/L), tributary inflow (0.53 mg/L), and reaeration (2.92 mg/L) and lost oxygen to BOD deoxygenation (1.33 mg/L), nitrite production (0.61 mg/L), and nitrate production (0.22 mg/L). Simulation of the recovery phase is modeled very well. The underprediction of the DO level at Hutcheson may result from some local photosynthetic production as the parcel traveled through this reach during the daylight hours.

Parcel C remained in the system longer than any other parcel. It received a large load of ammonia but small loads of BOD and organic nitrogen at the Clayton WTF. Because the parcel also received a large heat load (fig. 4), it arrived at Route I-280 slightly supersaturated with dissolved oxygen. Its minimum DO level of 3.65 mg/L occurred at 1600 hours on June 1 when it was located between Rico and Capps Ferry. The reduction in dissolved oxygen was the result of BOD deoxygenation (3.9 mg/L), nitrite production (3.3 mg/L), and nitrate production (0.9 mg/L). Oxygen additions were due to dispersion (0.1 mg/L), reaeration (1.6 mg/L), and tributary inflow (0.6 mg/L). For parcel C, nitrification consumed 1.07 times as much oxygen as BOD, while, for parcel B, nitrification consumed only 0.55 times as much. Nevertheless, the DO concentrations of both parcels seem to be modeled accurately. The recovery of 1.99 mg/L during parcel B's 13-hour transit to Whitesburg is also well modeled. During recovery, both BOD deoxygenation and nitrification consumed 1.25 mg/L.

Parcel G received small BOD and nitrogen loads at the Clayton WTF. The parcel also had a small DO concentration (92 percent of saturation) as it passed the Atlanta gage at 0600 hours on June 1. At Route I-280, the predicted and observed results are in excellent agreement. Downstream of Route I-280, the predicted results for parcel G are higher than observations, and this parcel represents about the poorest fit for any parcel modeled. By the time the parcel arrives at Fairburn, the model error seems to be about 0.9 mg/L. Modifications to the parcel concentration downstream of Atlanta were due to dispersion (−0.06 mg/L), tributary inflow (−07 mg/L), reaeration (+1.29 mg/L), BOD deoxygenation (−1.96 mg/L), nitrite production (−1.34 mg/L), and nitrate production (−0.34 mg/L). The cause of the poor agreement is not known, but perhaps BOD settling is less than 38 percent of the total extraction for the small BOD load in this parcel.

Parcels H, I, and J received the peakloads of organic nitrogen, BOD, and ammonia, respectively, from the Clayton WTF. Only parcel I will be discussed, but the behavior of all three is similar. Parcel I passed the Atlanta gage with a DO concentration of 9.87 mg/L, which was 1.12 times the saturation value. The supersaturation is presumably the result of photosynthetic production in the clear water upstream of the Clayton WTF outfall. Upon arriving at Route I-280, the DO concentration had fallen to 9.27 mg/L, but because of the heat load contributed at the McDonough outfall, it was then 1.18 times the saturation value. The effect of photosynthesis is still apparent at Route I-280. By the time the water arrived at Route 139, the oxygen concentration had been reduced to 7.14 mg/L, which is 92 percent of saturation there. Almost all evidence of the photosynthetic production had been eliminated by the large demands of BOD and nitrification. At Ben Hill and Fairburn, the modeled results show a definite sag in DO due to the large BOD load, which is not necessarily confirmed by observations. Perhaps more than 38 percent of the peak BOD load settled without consuming oxygen. Whether by design or by chance, the heavy loading of the Clayton WTF could not have been timed better to take advantage of the photosynthetically produced oxygen. At Ben Hill the predicted concentration of parcel I has fallen to 5.22 mg/L. The processes of dispersion, tributary inflow, and reaeration have added 0.20, 1.07, and 0.45 mg/L, respectively, to the parcel since it passed the Atlanta gage and the processes of BOD deoxygenation, nitrite production and nitrate production have consumed 4.22, 1.76, and 0.39 mg/L, respectively.

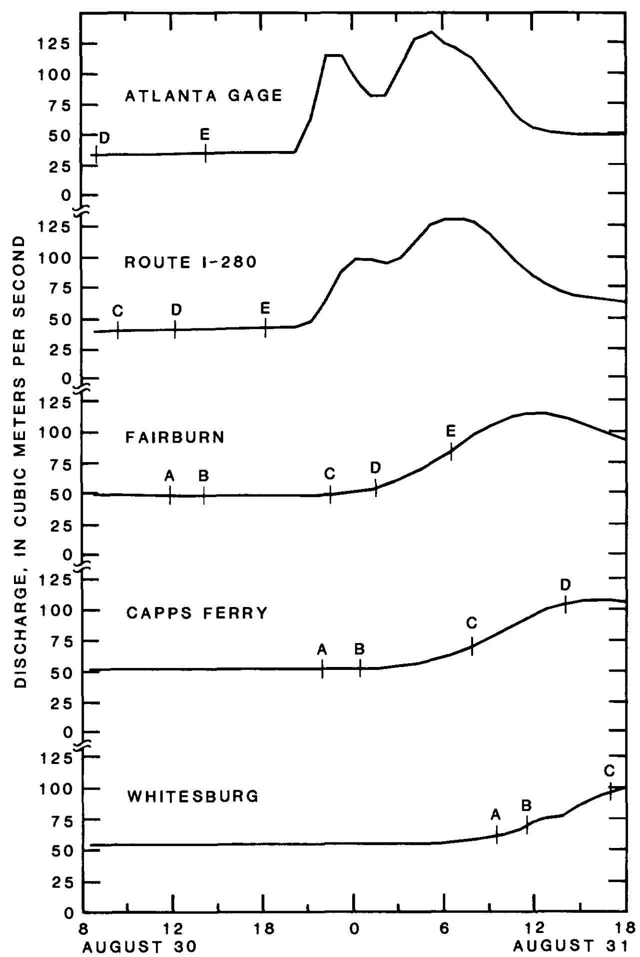

Figure 11. Variations of discharge in the Chattahoochee River during the 1976 verification of the Lagrangian transport model.

A comparison of parcels I and K provides support for the assumption that the settled BOD did not exert a significant oxygen demand. Parcel I had a large BOD concentration and parcel K had a small concentration (fig. 5). In both cases, reaeration contributed little to the DO balance (−.07 mg/L for parcel I and −0.03 mg/L for parcel K), since both were supersaturated for most of the time while in the reach from the McDonnough intake to Route 139. The BOD loss for parcel I was large (2.34 mg/L) while that for parcel K was much smaller (1.13 mg/L). Had all BOD losses consumed oxygen, a reaeration in this reach (with a negative gradient) of 0.89 mg/L to parcel I and 0.70 mg/L to parcel K would be required to match the observed oxygen concentrations. Photosynthetic production is also highly unlikely since parcel K traversed the reach at night and parcel I experienced only a small amount of daylight. Nitrification consumed 0.70 mg/L of DO from parcel I and 0.69 mg/L from parcel K. Allowing 38 percent of the BOD to settle provided an accurate prediction of the dissolved oxygen concentrations in both parcels.

Overall, the calibration for dissolved oxygen is considered excellent. The model provides a realistic simulation of all the major kinetic processes operating in the river during the calibration period of May 31 to June 2, 1977.

MODEL VERIFICATION

Flow.—Data obtained during 1976 were used to verify the water-quality model. A period beginning at 0600 hours on August 30, 1976, and ending at 1800 hours on August 31, 1976, was modeled. The data were obtained in the same manner as previously discussed for the calibration. Because only one observation was available, the flows in all tributaries (shown in table 1), including the Clayton WTF outfall, were assumed to be constant.

Unlike the calibration run, the river flow during the verification period was quite unsteady, varying from a minimum of 33.7 m^3/s to a maximum of 123.9 m^3s at the Atlanta gage. The modeled variation of discharge with time at five locations on the river is shown in figure 11. The verification results will be discussed in detail for five fluid parcels. The times these parcels pass each reference point are indicated in figure 11 for later comparison. It is easy to see that the flood wave travels faster than a fluid parcel by observing the movement of parcel D through the system. Parcel D passed the Atlanta gage at 0800 on August 30 when the discharge was steady and low. The discharge remained nearly constant for about 14 hours after parcel D passed the Atlanta gage. The peak discharge and parcel D arrived at Capps Ferry at nearly the same time, however.

Transport.—As with the calibration run, data for the verification run were incomplete. A single observation of the concentration of water-quality constituents was available for all tributaries during the modeling period. Table 3 contains the constant input concentrations used for each constituent in each tributary. The dispersion coefficient and all rate coefficients were assumed to be the same as those used in the model calibration.

Only 5-day BOD's were available for the verification period. The ratio of the ultimate (20 day) to the 5-day BOD was computed for each observation during the calibration period. The ratios computed from instream data and tributary data appeared to define separate populations. The average ratio for the tributary data was 2.65 and the average ratio for the instream data was 3.28. These two ratios were applied to the verification data to obtain the ultimate values shown in table 3 and in later figures. The hourly constitutent loads at Clayton WTF were synthe-

Table 3. Input concentrations for all tributaries during the August 30–31, 1976, verification

Name of tributary	Concentration, in milligrams per liter					
	DO	BOD	ON	NH3	NO2	NO3
Cobb County wastewater treatment facility.	7.3	7.4	8.0	12.0	0.30	0.44
Nancy and Peachtree Creeks	6.7	2.4	8.0*	.1	.01	.30
Clayton wastewater treatment facility.	6.8	4.8	11.0	12.0	.01	.02
Proctor Creek	5.6	20.7	8.0	.01*	.0*	3.00*
Nickajack Creek	8.4	3.5	.3	.01	.01	2.90
South Cobb County wastewater treatment facility.	3.3*	5.3	5.0	5.0	.16	3.10
Utoy Wastewater	2.4	20.4	6.0	13.0	.01	.03
Utoy Creek	5.0	9.3	.5	.4	.05	.40
Sweetwater Creek	6.4	1.6	.5*	.02	.05*	.40*
Camp Creek wastewater treatment facility.	3.1	4.5	1.5	.02	.0	8.20
Camp Creek	6.6	2.4	.3	.01	.01	.30
Deep Creek	6.8	1.3	.3	.1	.01	.40
Annewakee Creek	6.9	2.1	.1	.02	.01	.30
Pea Creek	1.9	1.1	.3	.01	.01	.12
Bear Creek (right bank)	8.2	1.1	.2	.0	.01	.22
Bear Creek (left bank)	6.6	2.4	.3	.01	.01	.38
Dog River	8.2	0.3	0.2*	0.02	0.01*	0.28*
Wolf Creek	8.9	1.3	.2	.01	.0	.14
Snake Creek	9.1	2.1	.3	.0	.01	.16
Cedar Creek	4.6	1.9	.2	.02	.0	.17

*Inferred value.

sized during the first 12 hours of the verification period in order to best match the observed instream values downstream. The synthesized BOD's varied from a minimum of 1.0 mg/L at 1000 hours on August 30 to a maximum of 76.4 mg/L at 1400 hours of the same day. On August 31, the input BOD concentrations were assumed constant at the value given in table 3. The synthesized BOD concentrations used during the verification period were much lower than the values used during the calibration, but the diel variations appear to be similar both in timing and in amplitude.

Total organic nitrogen and ammonia concentrations at the Clayton WTF outfall were also synthesized for August 30. The synthesized concentrations of organic nitrogen and ammonia indicated a local minimum of 2.1 and 13.1 mg/L, respectively, within 1 hour of the minimum in BOD loading. Similarly the synthesized maximums of 7.1 and 43.3 mg/L, respectively, occurred within 2 hours of the peak BOD load. As observed during the calibration period, the peak ammonia load occurred after the peak BOD load. On August 31, the loads were assumed constant and equal to the values shown in table 3. On

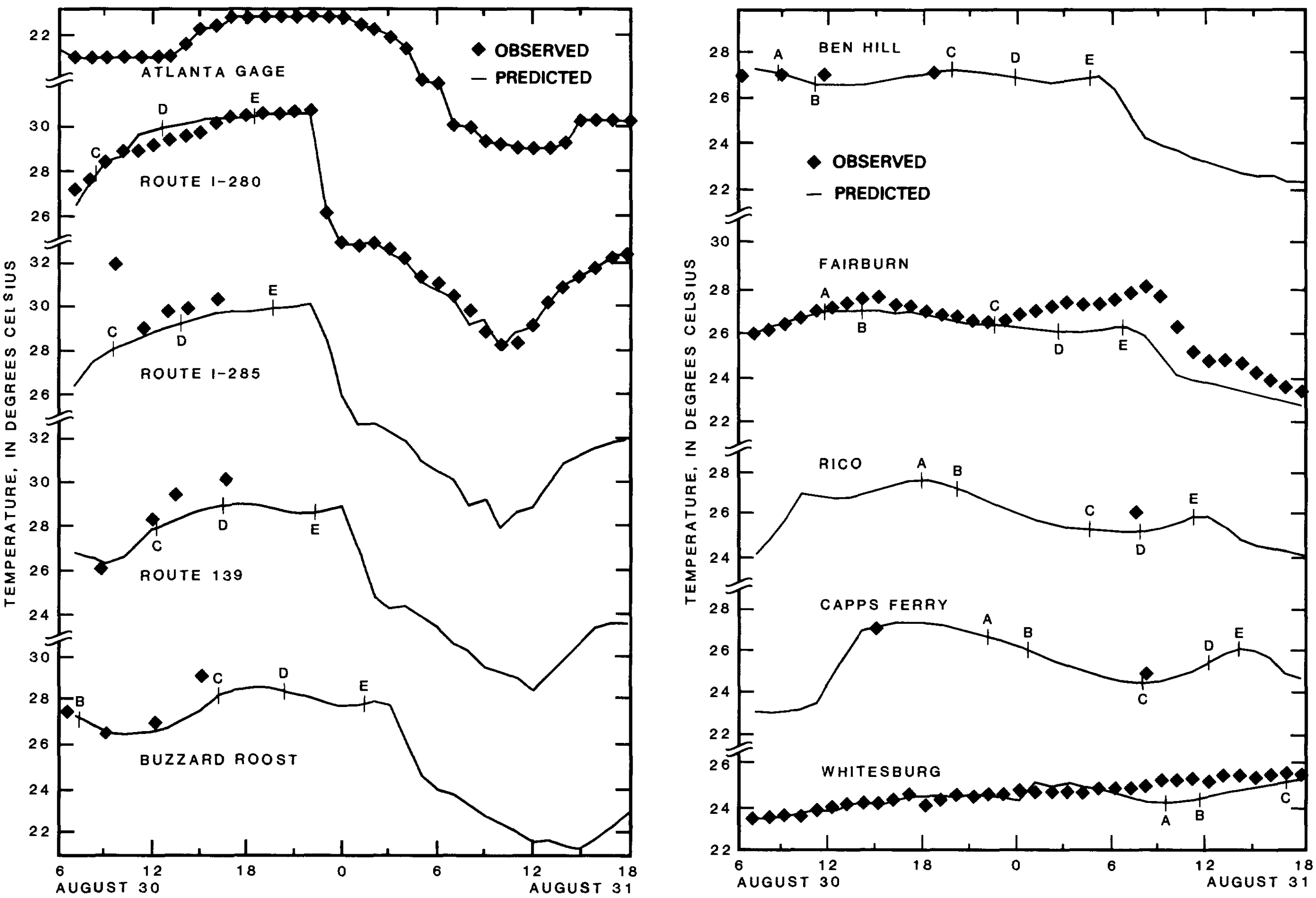

Figure 12. Comparison of predicted and observed water temperatures in the Chattahoochee River, August 30 to August 31, 1976.

August 31, the flow in the river was large so the Clayton WTF loading had little impact on the river quality.

The synthesized thermal loads from the Atkinson and McDonough powerplants gradually increased from 0600 hours to 0900 hours on August 30 and remained nearly constant from 0900 hours to midnight at 950 MW (load factor = 0.87). After midnight the load decreased to about 480 MW (load factor = 0.44) and remained constant until about 0700 hours on August 31. The load then increased to about 1100 MW (load factor = 1.0) for the rest of the study. The equilibrium temperature data were obtained using a procedure identical to that used during the calibration.

Temperature.—A comparison of the predicted and observed temperatures during the verification period is provided by figure 12. The continuous data at Route I-280 and Whitesburg were obtained from unpublished water-quality records of the U.S. Geological Survey. These records were of rather poor quality but have been adjusted to match the few published data available in WATSTORE. The record at Fairburn also has been adjusted, but only slightly, to be in agreement with the WATSTORE data. The RMS error for all data is 0.7°C.

Following single parcels is perhaps the best way to evaluate the accuracy of the verification. Consider parcel C which was located about 3 km downstream of the Atlanta gage at 0600 hours on August 30 and which remained within the study reach for the next 35 hours. As the parcel passed the power plants, outfall, it was warmed by more than 7.5°C and arrived at Route I-280 with a temperature of 27.5°C at 0900 hours on August 30. Figure 12 shows that the parcel's temperature remained nearly constant for the rest of the day as it traveled to Buzzard Roost Island, arriving there at 1600 hours. During the night, it cooled by about 3.0°C and it arrived at Capps Ferry at 0800 hours August 31. During the day of August 31, the parcel warmed about 0.8°C and arrived at Whitesburg at 1700 hours with a temperature of 25.3°C. Comparing the predicted and observed temperatures

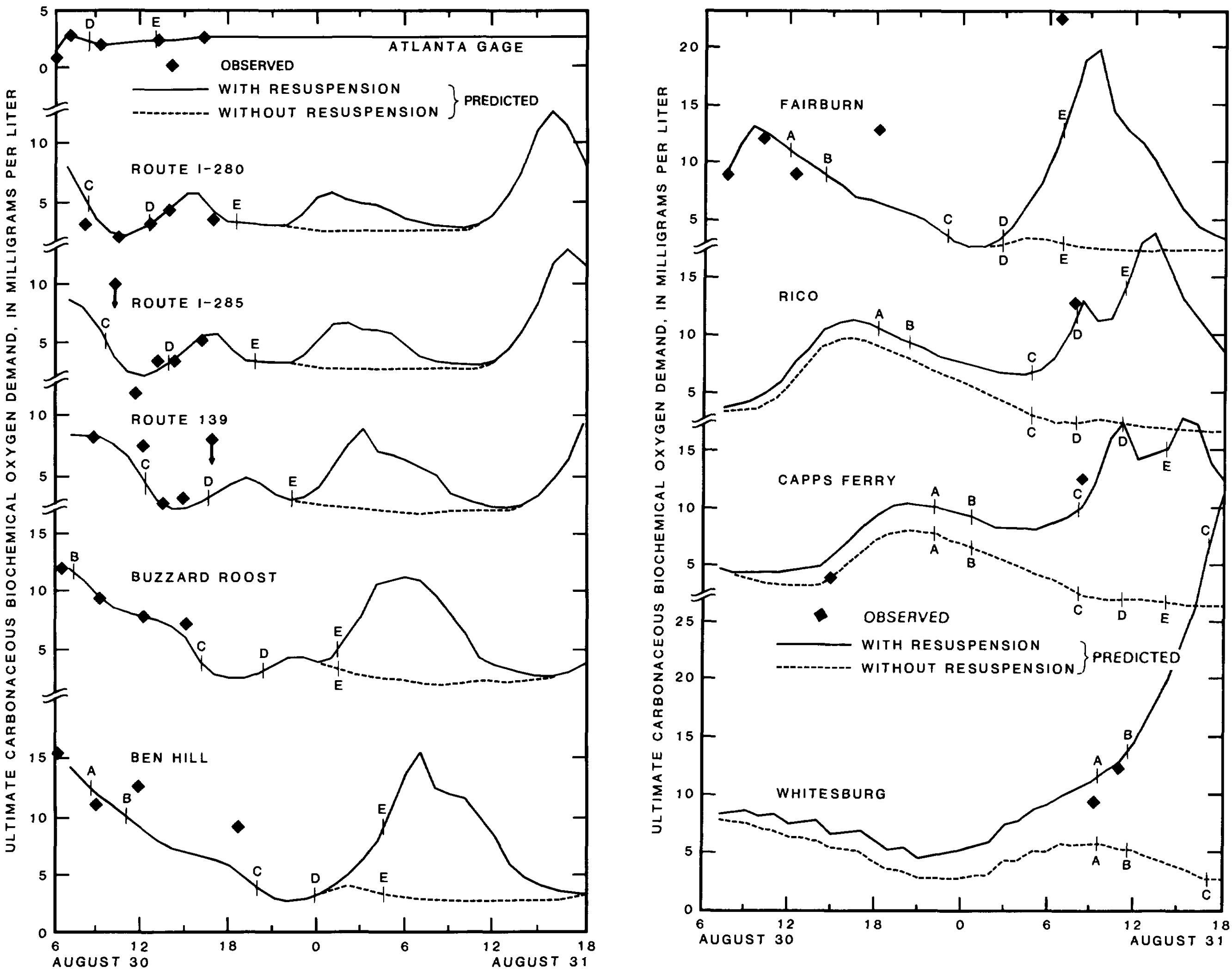

Figure 13. Comparison of predicted and observed ultimate carbonaceous biochemical oxygen demand in the Chattahoochee River, August 30 to August 31, 1976.

for this parcel at all observation points indicates that the model does a reasonably good job of simulating the temperature changes experienced by this and other parcels that traversed the system.

The actual temperature at Route I-280, especially between about 0800 hours and 2300 hours on August 30, is believed to be about 0.5°C higher than the records indicate. There is a consistent underprediction of temperatures for stations downstream when the model is matched to the observed values at Route I-280.

The sudden drop in river temperature at Route I-280 which occurred after 2200 hours on August 30 is the result of the simultaneous arrival of the large riverflow (fig. 11) and the reduction in the load factor at the powerplants.

Although the data are limited, it is believed that the temperature component of the transport model has been verified again.

Ultimate carbonaceous biochemical oxygen demand.—Predicted and observed BOD concentrations during the verification period are shown in figure 13. The dashed curves were predicted using the calibrated model. The RMS error is 5.1 mg/L and the mean error is 2.2 mg/L. Although the results during the first 15 hours, when the flow was low and steady, are good, the model did not predict the large observed concentrations at Fairburn, Rico, Capps Ferry, and Whitesburg that occurred on August 31.

Consider parcel D which passed the Atlanta gage at 0800 hours on August 30 with a concentration of only 2.5 mg/L. After receiving a small load from the Clayton WTF outfall it arrived at Route I-280 at 1232 with a concentration of 3.2 mg/L. Downstream of Route I-280 the modeled concentration slowly decreases because of settling and decay. Since no large point sources exist, the parcel arrived at Rico with a low predicted concentration of 2.6 mg/L. This value is much lower than the observed concentration there. A similar situation occurs for each of the other four parcels tracked in figure 13. Comparison with figure 11 indicates that the large observed concentrations always occur at a time when the parcel is located on the rising limb of the hydrograph.

According to Robert Faye (hydrologist, U.S. Geological Survey, Doraville, Ga., written commun., 1983,) who was actively involved in the data-collection efforts, the bed material for this reach is composed of coarse sand upstream of Capps Ferry and mostly gravel and cobbles downstream of this point. Upstream of Capps Ferry dunes are formed at high flows but the bed is stationary at low flows. Scattered riffles occur throughout the reach but are almost continuous below Capps Ferry. Bencala and Walters (1983) demonstrate that a large amount of water and solute exchange occurs between a flowing stream and the water moving under the bed. Using this information as background, the following processes were conceptualized to explain the apparent temporary storage of BOD during low flows in the river and the release of this BOD with increasing flow.

River water probably entered the bed on the upstream sides of dunes and riffles where the hydrostatic pressure was high and exited the bed in regions of low pressure such as near the crest of dunes or in the lower parts of the riffles. The stationary sand bed at low flow would act as a filter, trapping particulate BOD as the river water enters the bed. The BOD filtered from the water was trapped between sediment particles or in other deadzones and was not effective in exerting an oxygen demand to the water in the river above. Had low flow continued indefinitely, the sand bed and deadzones would eventually become clogged with organic matter. On the Chattahoochee River, however, there are frequent pulses of very high flow because of the use of Buford Dam as a peak power generation facility. These pulses of high flow mobilize the sand bed and resuspend the trapped BOD that has accumulated there during the low-flow period.

To simulate BOD resuspension, the model was modified in the following way. The settling of BOD was terminated by reducing the extraction rate for BOD ($XK_{3,3}$) by 38 percent whenever the local discharge exceeded 45 m^3/s. This, in effect, canceled the settling (or filtering) part of the extraction rate and left only the bio-chemical oxidation. As the flow increased above 45 m^3/s, it was assumed to have an increasing ability to flush the BOD from the bed. The entrainment rate was increased from zero by 0.1 mg/L per hour for each 1 m^3/s of flow in excess of the 45 m^3/s. It was further assumed that the bed sediment had uniformly accumulated a quantity of BOD sufficient to produce 80 mg/L of BOD in the river water above. The model accounted for the amount of BOD entrained from each subreach and terminated further resuspension from a subreach whenever the accumulated BOD had been reentrained.

The model results obtained with the entrainment algorithm are also shown in figure 13, as solid curves. The differences between the solid and dashed curves represent the effect of reduced settling and resuspension when the local flow exceeds 45 m^3/s. The RMS error for the solid curves is 3.0 mg/L and the mean error is 1.0 mg/L.

Upstream of Rico, the BOD resuspension had no effect on the computed results during the first 17 hours when the flow was steady and low. Downstream of Fairburn the flow always exceeded 45 m^3/s because of tributary additions.

The resuspension function certainly improves the fit to the high observed concentrations in the downstream reaches on August 31. Since the high observations are associated with different parcels separated in time by nearly 15 hours, it is unlikely that they result from a large, undetected tributary inflow. It was concluded, therefore, that they resulted from resuspension of BOD trapped in or on the bed. The assumption of a uniform quanity of BOD per unit length of river is probably not realistic, but considering the limited data, further refinement was not warranted.

Except where resuspension is occurring, the data in figure 13 provides a reasonable verification of the BOD component of the model. The loading rates at the Clayton WTF outfall were much smaller than during the calibration period. It seems clear that BOD is resuspended from the bed during the rising hydrograph, but the specific mechanics of this process cannot be accurately defined from the limited data available.

Total organic nitrogen.—The concentrations of organic nitrogen in the river were also much lower in 1976 than in 1977. A comparison of the predicted and observed organic nitrogen concentrations during the 1976 verification is shown in figure 14. The RMS error in the predicted values is 0.12 mg/L and the mean error is -0.02 mg/L.

More observations are available near parcel C than for any of the other parcels, so parcel C will be

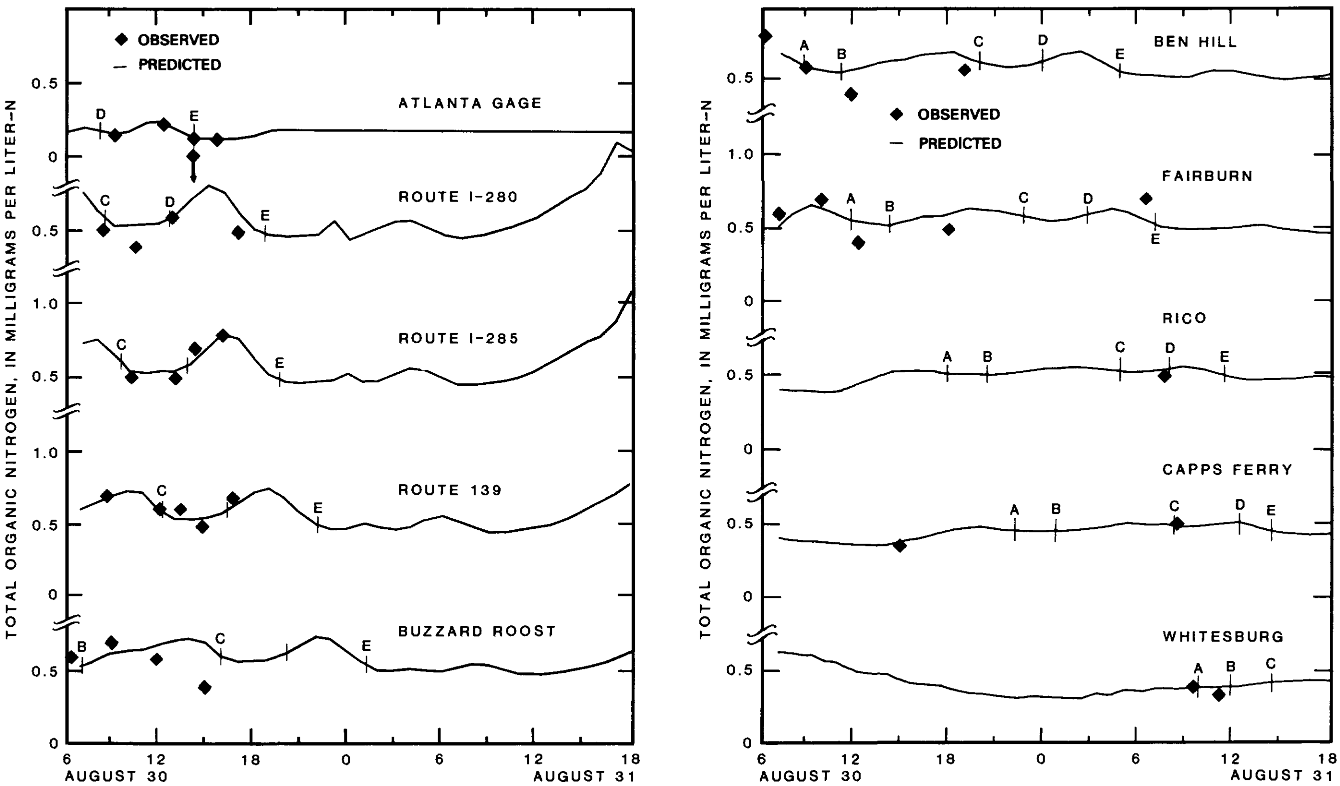

Figure 14. Comparison of predicted and observed concentrations of total organic nitrogen in the Chattahoochee River, August 30 to August 31, 1976.

used to illustrate the accuracy of the verification. The parcel was located upstream of the Clayton WTF outfall at 0600 hours on August 30 and had a concentration of 0.17 mg/L. It arrived at Route I-280 with a computed concentration of 0.59 mg/L—having received 0.47 mg/L from the Clayton WTF. Downstream of Route I-280, its concentration remained nearly constant during its nearly 24-hour traveltime to Capps Ferry. Although the net change in concentration between Route I-280 and Rico was only −0.09 mg/L, individual processes were very important. Through this reach of the river, dispersion increased the parcel's concentration by 0.02 mg/L, tributary inflow increased its concentration by 0.07 mg/L, and ammonification reduced its concentration by 0.18 mg/L. Comparing the error in the predicted concentrations at Capps Ferry and at other sites with the magnitude of the processes being modeled would indicate that the data provides a good verification of the organic nitrogen component of the model. The high flow did not appear to reentrain organic nitrogen as it did BOD. This result is consistent with the model in that the model did not allow for settling of organic nitrogen, and the total extraction was assumed to be converted to ammonia.

Total ammonia nitrogen.—A comparison of predicted and observed ammonia concentrations during the 1976 verification is shown in figure 15. The RMS error in the predicted values is 0.11 mg/L and the mean error is 0.03 mg/L. Unlike the concentrations of BOD and organic nitrogen, which were much lower in 1976 than in 1977, the ammonia concentrations in 1976 are similar to those observed in 1977—even the phasing of the diel pattern is the same.

Parcel C received about the minimum ammonia load from the Clayton WTF and arrived at Route I-280 with a concentration of 1.11 mg/L. The ammonia concentration at the Atlanta gage was assumed to be zero through the verification period. The predicted concentration falls gradually to 0.70 mg/L by the time the parcel arrives at Capps Ferry nearly 24 hours later. During its transit from Route I-280 to Capps Ferry, dispersion increased the parcel's concentration by 0.06 mg/L, tributary inflow decreased it by 0.04 mg/1, 0.18 mg/L was produced from the ammonification of organic nitrogen, and 0.61 mg/L was lost through nitrification to nitrite and other processes. Comparing the accuracy of the simulation in figure 15 with the magnitudes of the processes being

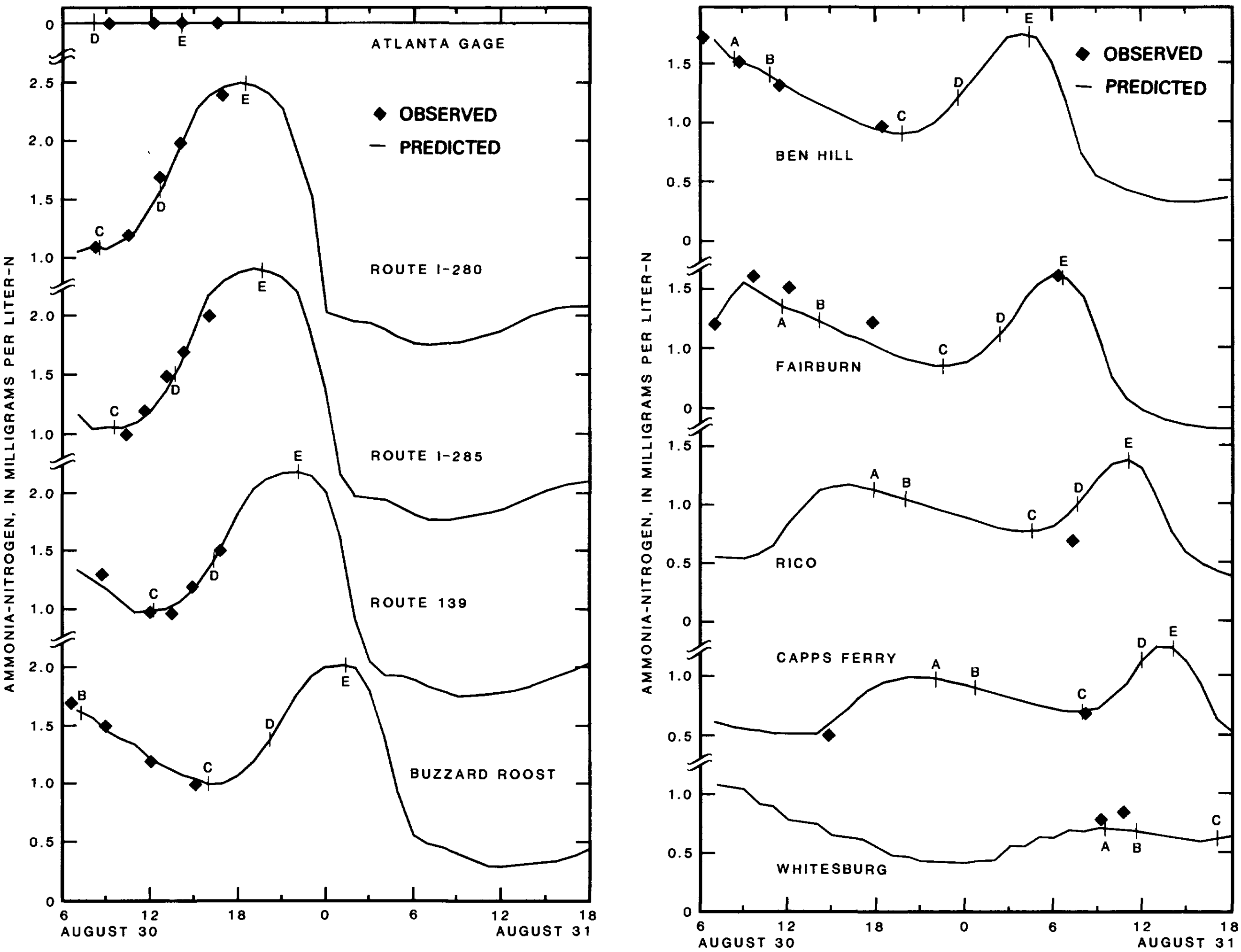

Figure 15. Comparison of predicted and observed concentrations of total ammonia nitrogen in the Chattahoochee River, August 30 to August 31, 1976.

modeled indicates that the model verification for the ammonia component is excellent.

Few data are available for parcel E, but because it appears to have received the maximum load from the Clayton WTF, it will be discussed to some extent. Starting with zero concentration at the Atlanta gage, the parcel received a heavy load from the Clayton WTF and arrived at Route I-280 with a concentration of 2.50 mg/L at 1826 hours on August 30. The increase in discharge shortened its traveltime to Fairburn to 11.1 hours and it arrived there with a concentration of 1.59 mg/L (fig. 15). During its transit from Route I-280, dispersion decreased its concentration by 0.09 mg/L, tributary inflow decreased it by 0.13 mg/L, 0.09 mg/L were produced from organic nitrogen and 0.78 mg/l was lost to decay. Even here where the effect of dispersion should be maximum, the decay term dominated.

Considering all the data, it appears that the verification of the ammonia component of the model is excellent. As with organic nitrogen, no ammonia was resuspended from the bed.

Total nitrite-nitrogen.—A comparison of predicted and observed nitrite concentrations during the 1976 verification is shown in figure 16. The RMS error of the prediction values is 0.03 mg/L and the mean error is −0.02 mg/L. The concentrations of the nitrite during the verification like those of ammonia, are similar to the concentrations observed during the calibration.

Again consider parcel C. Starting with no nitrite and receiving none directly from the Clayton WTF, the parcel arrived at Route I-280 with an observed concentration of 0.02 mg/L. Parcel C received about the minimum ammonia load of any parcel on August 30. As shown in figure 16, the computed concentra-

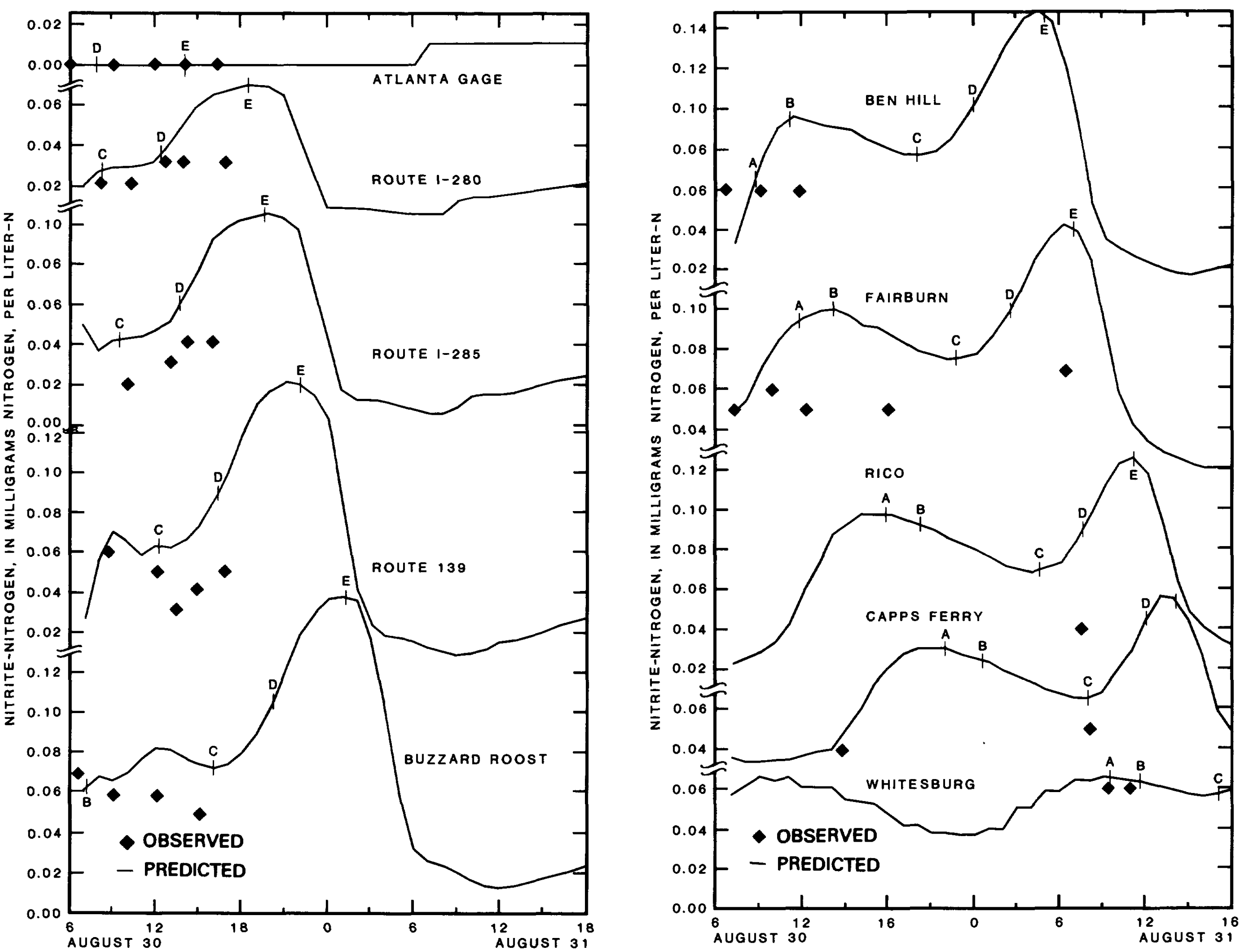

Figure 16. Comparison of predicted and observed concentrations of total nitrite-nitrogen in the Chattahoochee River, August 30 to August 31, 1976.

tion builds up faster than the observed values as the parcel moves downstream to Ben Hill. At Buzzard Roost the observed concentration of 0.05 mg/L is much lower than the computed value of 0.08 mg/L. On the other hand, 0.27 mg/L of nitrite have been produced and 0.19 mg/L have been transferred to nitrate. The error in the predicted value, therefore, could be explained by an error of only 11 percent in the rate of production or an error of 16 percent in the rate of decay. Downstream of Buzzard Roost, the error appears to narrow to about 0.01 mg/L at Capps Ferry.

Parcels A and E received large ammonia loads. Just as in the calibration run, the overprediction of the nitrite concentrations in these heavily loaded parcels just downstream of the outfall appears to be worse than the overprediction for the lightly loaded parcel C.

As with the calibration, the accuracy of the predicted nitrite concentrations was less than had been hoped for. On the other hand, these concentrations are very small and nitrite is a very transient substance. As it did during the calibration run, the model tended to produce nitrite too fast immediately after receiving a load of ammonia, and the error appeared to be worse for heavily loaded parcels. Later, the computed concentrations tended to fall off too rapidly. This rather systematic error could result from assuming that the nitrobacteria population responds instantaneously to changes in ammonia concentrations. It is also possible that the chlorination of the discharge from the Clayton WTF initially inhibited the nitrification rate.

Nevertheless, the errors are small in the absolute sense as well as in comparison with the amount

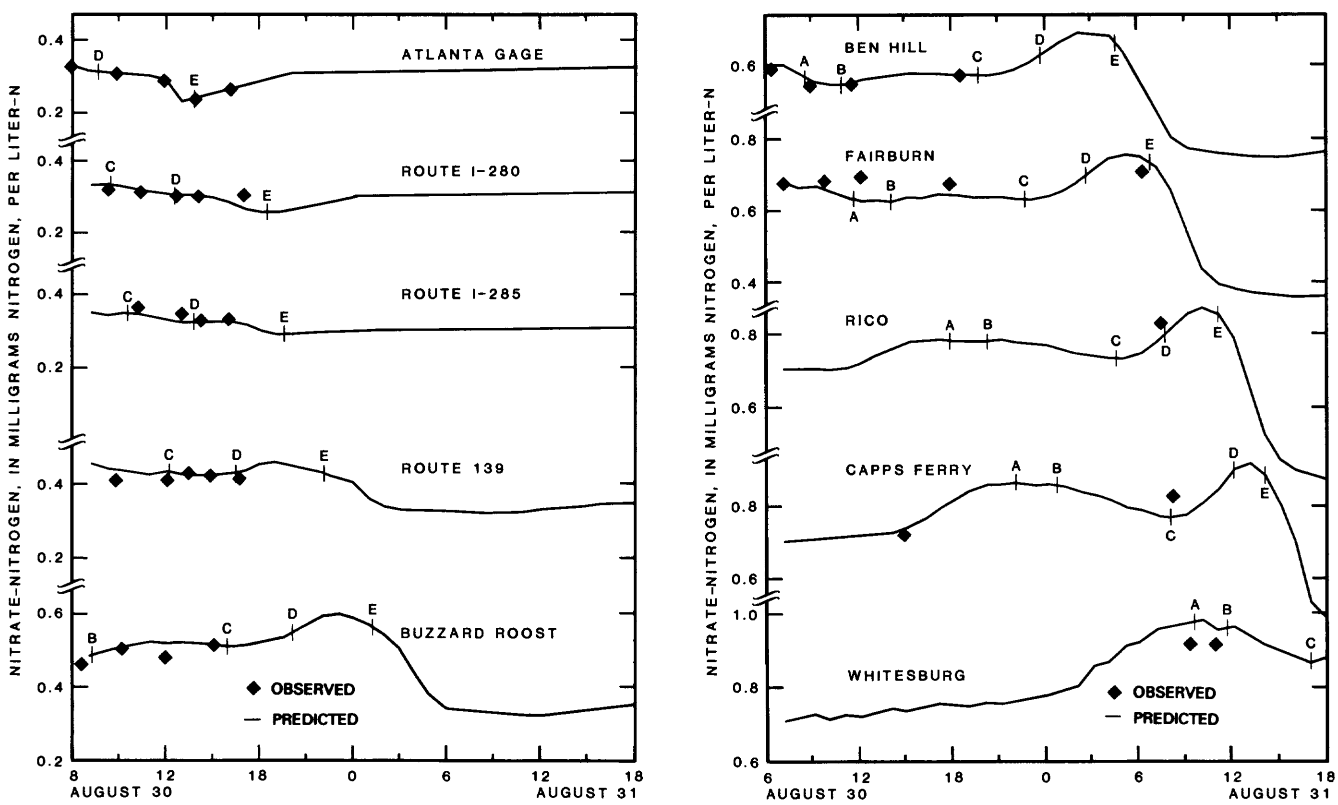

Figure 17. Comparison of predicted and observed concentrations of total nitrate-nitrogen in the Chattahoochee River, August 30 to August 31, 1976.

of nitrogen passing through this phase. It is concluded that the model verification for the nitrite component is adequate.

Total nitrate-nitrogen—A comparison of predicted and observed nitrate concentrations during the 1976 verification is shown in figure 17. The RMS error in the predicted values is 0.03 mg/L and the mean error is −0.01 mg/L. Again, the overall levels are similar to those observed during the model calibration.

Parcel C received a small ammonia load and no nitrate from the Clayton WTF, but it arrived at Route I-280 with a concentration of 0.34 mg/L. Downstream of Route I-280, the nitrate concentration steadily increased because of the nitrification process. The parcel arrived at Capps Ferry with a predicted concentration of 0.77 mg/L which agrees well with the observed value. During its nearly 24 hour transit from Route I-280, dispersion increased its concentration by 0.01 mg/L, tributary inflow increased it by 0.04 mg/L, and nitrification increased it by 0.38 mg/L.

Parcel E received a large load of ammonia at the Clayton WTF but almost no nitrate and arrived at Route I-280 with a predicted concentration of 0.25 mg/L. At Fairburn, about 17 hours later, the computed concentration has increased to 0.73 mg/L in good agreement with the observed value there. During its transit from Route I-280, dispersion decreased parcel E's concentration by 0.01 mg/L, tributary inflow increased it by 0.04 mg/L, and nitrification increased it by 0.45 mg/L.

Overall, the model verification for nitrate is considered excellent.

Dissolved oxygen.—The dissolved oxygen data for the verification run left much to be desired. The data for Routes I-285 and 139 are extremely scattered. Nevertheless, a comparison of predicted and observed oxygen concentrations during model verification is shown in figure 18. The solid curve represents the results obtained with BOD resuspension from the bed and the dashed curve represents the results without resuspension. When BOD resuspension was ignored, the RMS error in the predicted concentrations was 1.05 mg/L and the mean error was 0.13 mg/L. Similarly, when resuspension was modeled, the RMS error was 1.01 mg/L and the mean error was 0.18 mg/L. Because the results with

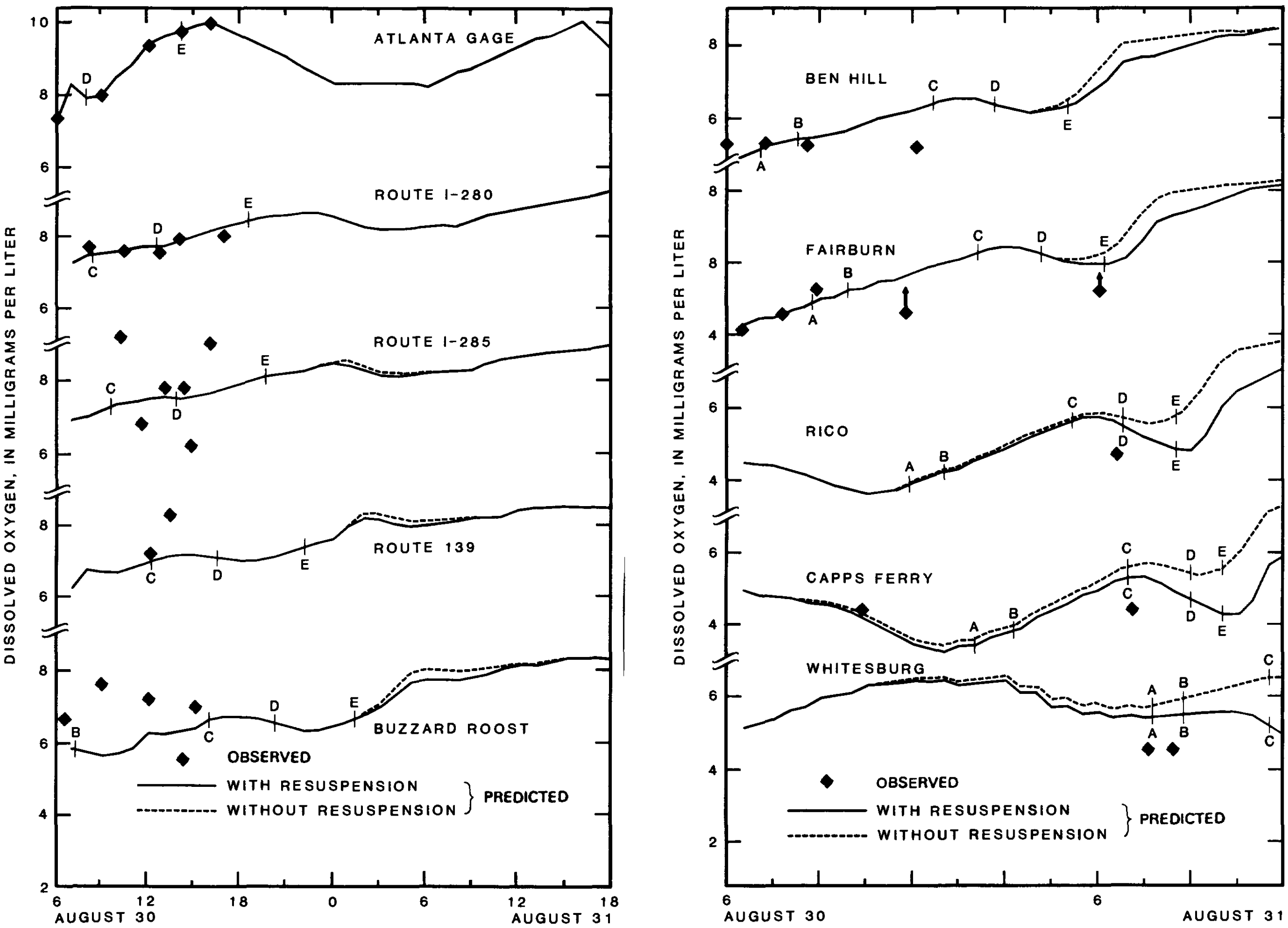

Figure 18. Comparison of predicted and observed concentrations of dissolved oxygen in the Chattahoochee River, August 30 to August 31, 1976.

resuspension are considered more correct, only these results will be discussed in detail.

Consider parcel A, which was initially located just upstream of Buzzard Roost with a dissolved-oxygen concentration of 5.52 mg/L. The predicted and observed concentrations for this parcel agree very well, at least until after the parcel passes Fairburn. At Whitesburg the predicted concentration of 5.43 mg/L for parcel A has changed little from its initial value and is about 1 mg/L higher than the observed value. During its 27.5-hour traveltime, the model predicts the following effects on parcel A's initial concentration: dispersion, + 0.09 mg/L; tributary inflow, + 0.59 mg/L; reaeration, + 5.47 mg/L; BOD decay, − 3.57 mg/L; and nitrification, − 2.76 mg/L. The predicted concentration is 0.50 mg/L lower than was predicted when BOD resuspension was ignored because of the added oxygen use by the resuspended BOD. Studies of the Milwaukee Harbor (Kreutzberger and others, 1980) indicate that resuspended BOD exerts a more rapid oxygen demand than does material that remains in suspension. Since the model does not distinguish between BOD that has or has not been resuspended, it will underestimate the BOD demand rate if the observations on the Milwaukee Harbor are correct. A larger, more rapid dissolved-oxygen demand by the resuspended BOD could explain the error in the predicted concentration at Whitesburg.

Parcel C starts with a concentration of 7.81 mg/L and arrives at Route I-280 with a dissolved-oxygen concentration of 7.56 mg/L which is in good agreement with the observed values there. The scatter in the observed concentrations is large at the next three stations downstream, and nothing definitive about the accuracy of the computed concentration can be said. The last observation of the parcel's concentration is at Capps Ferry. As with parcel A, the computed concentration is about 1.0 mg/L larger than the observed value there. During parcel C's transit from Route I-280, the following processes affected its concentration: dispersion, − 0.19 mg/L;

tributary inflow, +0.01 mg/L; reaeration, +1.25 mg/L; BOD decay, −1.46 mg/L; and nitrification, −1.89 mg/L. The model predicts only a small difference in the DO concentration between the resuspension case and nonresuspension case, because the flow has just started to increase (fig. 11). Again, a very rapid demand of the resuspended BOD could explain the error in the predicted DO values.

Parcel E received a heavy load of ammonia as it passed the Clayton WTF and arrived at Route I-280 with a predicted DO concentration of 8.44 mg/L. The parcel was supersaturated at the Atlanta gage, presumably because of photosynthetic production, and is still supersaturated at Route I-280 because of the temperature rise at the powerplant outfalls (fig. 12). A definite DO sag due to the ammonia load, is apparent in the computed value at Fairburn. During its transit from Route I-280, the following changes occurred: dispersion, +0.04 mg/L; tributary inflow, −0.03 mg/L; reaeration, +0.51 mg/L; BOD decay, −0.83 mg/L; nitrification, −2.38 mg/L. The large influence of the ammonia nitrification is apparent. Similar to the predictions for parcels A and C, the predicted value for parcel E is about 0.8 mg/L too large and the error could be explained by a large, rapid DO demand by the resuspended BOD (fig. 13).

The algorithm to resuspend BOD from the bed improved the predicted oxygen concentrations in all cases (fig. 18). A greater improvement in predicting the oxygen values would have occurred if the deoxygenation rate of the resuspended BOD had been given a large value indicating an almost instantaneous demand. A large, instantaneous DO demand would occur if partial anaerobic decomposition occurred in the stored BOD such that the stored BOD contained reduced products such as hydrogen sulfide. Velz (1970) terms this process the immediate demand, which can occur when some anaerobic decomposition occurs in long sewers. The refinement of including an immediate demand, like allowing the accumulated amount to vary in space, was not considered to be justified because of the small number of data available.

Overall, the verification of the oxygen algorithm for the case of steady low flow was considered verified. The model algorithms describing the resuspension process could not be verified because the process occurred only during the 1976 run. Nevertheless, the data strongly suggest that resuspension of BOD occurs with increasing flow and that the resuspended BOD exerts a large demand.

EVALUATION OF THE LAGRANGIAN APPROACH

A major attempt was made during both the 1976 and 1977 runs to collect data under as nearly steady state conditions as possible. At low flow, the time required for a single water parcel to traverse the entire reach was more than 36 hours. Therefore for a steady-state model to actually represent conditions in the river the flow and the input concentrations would have had to be constant for at least 36 hours preceeding the run as well as during the run. As shown in figures 4 through 18, such was not the case in the studied portion of the Chattahoochee River. Because wastewater-treatment plants and powerplants typically do not operate at constant rates, steady-state water-quality conditions can seldom be expected.

Water-quality studies are sometimes conducted in unsteady conditions by physically tagging a specific slug or parcel of water with dye and collecting data on the single parcel as it passes downstream. Although this approach is more valid than assuming steady-state conditions, it does not allow the dispersive effects to be included. Further at the end of the study, one has data on only a single parcel.

Use of the Langrangian model, however, allows a reasonable interpretation of the unsteady Eulerian data, even though the study period is less than the time required for a single parcel to traverse the system. For example, the parcel labeled C in the calibration run provided a lot of information about the loss of ammonia in a heavily loaded water parcel (fig. 7) even though it was monitored only from Route I-280 downstream. Also, parcel G provided information on the reactions in a lightly loaded parcel even though it was tracked only from the Atlanta gage to Fairburn.

CONCLUSIONS

An unsteady-state water-quality model has been calibrated and verified using data obtained on a 69-kilometer reach of the Chattahoochee River below Atlanta, Ga. The seven constituents of interest were temperature, dissolved oxygen, carbonaceous biochemical oxygen demand, organic nitrogen, ammonia, nitrite, and nitrate. The interactions among the constituents and the rate coefficients, as illustrated in figure 2, were confirmed to be applicable to this reach of the Chattahoochee River. The kinetic model, a cascade type presented by Thomann and others (1971), adequately described the physical and biochemical processes occurring in the river.

At steady low flow, about 38 percent of the BOD settled or was extracted without exerting an oxygen demand. This settled BOD was resuspended at high flow and exerted an immediate oxygen demand.

About 70 percent of the ammonia extracted from the water column was converted to nitrite, but the fate of the remaining 30 percent is unknown.

Photosynthetic production was not an important factor in the oxygen budget for this reach of the river during the June and August periods studied.

Use of a Lagrangian-type transport model allowed a reasonable interpretation of data obtained under highly unsteady conditions in the river.

REFERENCES CITED

Bencala, K. E., and Walters, R. A., 1983, Simulation of solute transport in a pool-and-riffle stream: A transient storage model: Water Resources Research, v. 19, no. 3, p. 718–724.

Bennett, J. P., and Rathbun, R. E., 1972, Reaeration in open-channel flow: U.S. Geological Survey Professional Paper 737, 75 p.

Carslaw, H. S., and Jaeger, J. C., 1959, Conduction of heat in solids (2d ed.): New York, Oxford University Press, p. 101.

Committee on Sanitary Engineering Research, 1960, Solubility of atmospheric oxygen in water: American Society of Civil Engineers, Sanitary Engineering Division Journal, v. SA4, July, p. 41–53.

Connie, L. K., Stoffel, T. L., and Whitaker, T. D., 1980, Insolation data manual: Solar Energy Research Institute, No. SERI–SP–755–789, October, p.64.

Ehlke, T. A., 1978, The effect of nitrification on the oxygen balance of the upper Chattahoochee River, Georgia: U.S. Geological Survey Water-Resources Investigations 79–10, 13 p.

Faye, R. E., Jobson, H. E., and Land, L. F., 1979, Impact of flow regulation and powerplant effluents on the flow and temperature regimes of the Chattahoochee River—Atlanta to Whitesburg, Georgia: U.S. Geological Survey Professional Paper 1108, 56 p.

Fischer, H. B., 1973, Longitudinal dispersion and turbulent mixing in open channel flow: Annual review of Fluid Mechanics, p. 57–98.

Huang, J. Y. C., and Wozniak, D. J., 1981, Nitrogen transformations in streams: Journal of Environmental Sciences, March/April, p. 41–45.

Jobson, H. E., 1980a, Temperature and solute-transport simulation in streamflow using a Lagrangian reference frame: U.S. Geological Survey Water-Resources Investigations 81–2, 165 p.

———1980b, Comment on "A new collocation method for the solution of the convection-dominated transport equation" by George Pinder and Allen Shapiro: Water Resources Research, v. 16, no. 6, p. 1135–1136.

———1980c, A practical Lagrangian transport model: U.S. Geological Survey Open-File Report 80–206, NSTL Station, Mississippi, 31 p.

———1980d, Thermal modeling of flow in the San Diego Aqueduct, California, and its relation to evaporation: U.S. Geological Survey Professional Paper 1122, 24 p.

Koberg, G. E., 1964, Methods to compute long-wave radiation from the atmosphere and reflected solar radiation from a water surface: U.S. Geological Survey Professional Paper 272–F, p. 107–136.

Kreutzberger, W. A., Race, R. A., Meinholz, T. L., Harper, M., and Ibach, J., 1980, Impact of sediments on dissolved oxygen concentrations following combined sewer overflows: Water Pollution Control Federation Journal, v. 52, no. 1, p. 192–201.

Land, L. F., 1978, Unsteady streamflow simulation using a linear implicit finite-difference model: U.S. Geological Survey, Water-Resources Investigations 78–59, May, 57 p.

Najarian, T. O., and Taft, J. L., 1981, Nitrogen-cycle model for aquatic systems: Analysis: American Society of Civil Engineers Environmental Engineering Division Journal, v. 107, no. EE6, December, p. 1141–1156.

Stamer, J. K., Cherry, R. N., Faye, R. E., and Kleckner, R. L., 1979, Magnitudes, nature, and effects of point and nonpoint discharges in the Chattahoochee River basin, Atlanta to West Point Dam, Georgia; U.S. Geological Survey Water-Supply Paper 2059, 65 p.

Tennessee Valley Authority, 1972, Heat and mass transfer between a water surface and the atmosphere: Water Resources Research Laboratory Report 14, Norris, Tenn., April, 127 p.

Thomann, R. V., O'Connor, D. J., and DiToro, D. M., 1971, The effect of nitrification on dissolved oxygen of streams and estuaries: Manhattan College, Bronx, N.Y., Environmental Engineering and Science Program, Tech. Rep., 55 p.

Tsivoglou, E. C., and Wallace, J. C., 1972, Characterization of stream reaeration capacity; U.S. Environmental Protection Agency Report N. EPA–R3–72–012, Washington, D.C., October, 317 p.

Tuffey, T. J., Hunter, J. V., and Matulewich, V. A., 1974, Zones of nitrification: Water Resources Bulletin, v. 10, p. 555–564.

Velz, C. J., 1970, Applied stream sanitation: New York, Wiley and Sons, 619 p.

White, J. P., Schwert, D. P., Ondrako, J. P., and Morgan, L. L., 1977, Factors affecting nitrification in situ in a heated stream: Applied and Environmental Microbiology, v. 33, p. 918–925.

Zison, S. W., Mills, W. B., Deimer, D., and Chen, C. W., 1978, Rates, constants, and kinetics formulations in surface water quality modeling: Athens, Ga., U.S. Environmental Protection Agency, Tech. Rep. EPA–600/3–78–105, 317 p.

METRIC CONVERSION FACTORS

Data listed in this report are defined in metric units. A list of these units and the factors for their conversion to inch-pound units is provided below.

Abbreviations of units are defined in the conversion table below or where they first appear in the text. Symbols are defined where they first appear in the text.

Multiply metric units	By	To obtain inch-pound units
m^3/s (cubic meter per second)	35.31	ft^3/s (cubic foot per second)
m/s (meter per second)	3.28	ft/s (feet per second)
m (meter)	3.28	ft (foot)
m^2 (square meter)	10.76	ft^2 (square foot)
mm (millimeter)	0.03937	in. (inch)
km^2 (square kilometer)	0.3861	mi^2 (square mile)
kilometer	0.6214	mile
MW (megawatts)	3.41×10^6	British thermal unit per hour
square meter per second	10.76	square feet per second
watts per square meter	0.317	British thermal units per hour per square foot
millimeter per day per kilopascal	0.133	inch per day per inch of mercury

Temperature in degrees Celsius (°C) can be converted to degrees Farenheit (°F) as follows:

$$°F = 32 + 9/5\ °C$$