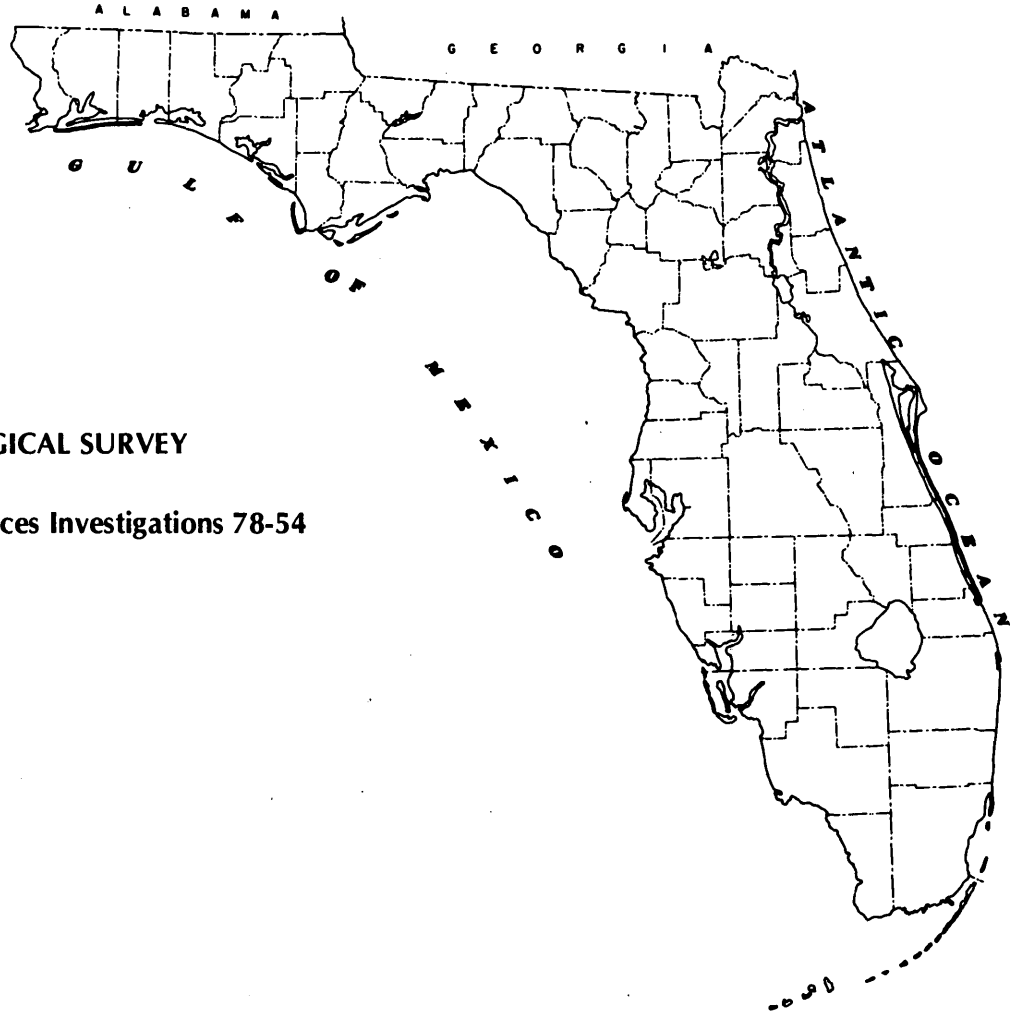
WRI 78-54

EVALUATION OF A DIGITAL MODEL FOR ESTUARINE WATER QUALITY SIMULATION IN WASTE ALLOCATION STUDIES



U.S. GEOLOGICAL SURVEY

Water-Resources Investigations 78-54

Prepared in cooperation with
FLORIDA DEPARTMENT OF ENVIRONMENTAL REGULATION

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16. Abstracts Hydrologic and water-quality data were collected on 4 estuaries in Pasco, Citrus, and Pinellas counties, Florida, to evaluate modeling results. Current and predicted waste loading of the four estuaries was simulated by use of a two-dimensional steady-state, intertidal-condition model. Concentrations of DO, carbonaceous and nitrogenous BOD, and chloride were simulated as averages over a tide cycle. General equations for the model are based on the law of conservation of mass. Assumption of steady-state required that water-quality data for calibration be averaged over an appropriate time cycle with respect to volume and cross-section. Diurnal DO fluctuation was determined in 2 estuaries for evaluating the influence of photosynthesis and respiration. The estuary model is best applied by calibrating it for a particular set of observed conditions, and then using this calibrated model for sensitivity analyses without attempting to verify the chosen parameter values against a second set of conditions. Sensitivity analyses performed included dispersion coefficient, decay rates, photosynthesis, and respiration.

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WATER QUALITY SIMULATION IN WASTE ALLOCATION STUDIES

By

G. E. Seaburn, M. E. Jennings, and M. L. Merritt

ABSTRACT

Four estuaries along the west coast of peninsular Florida were chosen to make an evaluation of an estuarine model application. Constituents simulated were dissolved oxygen (DO), carbonaceous biochemical oxygen demand (BOD), total Kejldahl nitrogen (TKN), and chloride. Current and predicted waste loading of the four estuaries is also described. The model was developed for well-mixed, steady-state, intertidal conditions. Thus, simulated concentrations of substances are computed as average values over a tide cycle. The general equations for the model are based on the law of conservation of mass.

The assumption of steady-state requires that water-quality data for calibration be averaged over a tidal cycle. The model use of concentration averages for reaches required that water-quality measurements be averaged in volume as well as in cross-section. It was determined that data collection to support calibration should include all four constituents computed and should be done in all reaches modeled. To determine the magnitude and influence of photosynthesis and respiration in two estuaries, a field study was made to determine the fluctuation of DO throughout the greater part of a day.

The most appropriate way to use the estuary model is to calibrate it for one set of observed conditions, and then verify the calibrated parameters using one or more sets of independent data. The observed conditions used for calibration and verification should resemble as closely as possible the worst-case situation to be analyzed by the model. Owing to limited resources and because the study was designed for evaluation purposes, the calibration parameters developed in this study have not been verified. In addition, only one set of water-quality measurements, at low-slack tide, were made to represent average conditions. Several sensitivity analyses involving model parameters such as dispersion coefficient, decay rates, photosynthesis, and respiration, were made in order to assess the applicability of model use. Verification of model parameters is recommended prior to use for waste-load allocation studies.

INTRODUCTION

The then Florida Department of Pollution Control (1973), now the Florida Department of Environmental Regulation, in satisfaction of requirements of the Federal Water Pollution Control Act Amendments of 1972 (Public Law 92-500), adopted water-quality criteria for intrastate, interstate, and coastal waters specifying the minimum quality conditions for all classes of waters within the State. For recreational purposes, including body-contact activities, and for the maintenance of well-balanced fish and wildlife populations the concentration of dissolved oxygen (DO) shall not average less than 5 mg/L (milligrams per liter) in a 24-hour period and never be less than 4 mg/L. Except for naturally DO-deficient waters, the DO concentrations in estuaries and tidal tributaries shall not be less than 4 mg/L.

As a preliminary to their program for issuing waste effluent permits according to PL 92-500, the Florida Department of Environmental Regulation entered into a cooperative study with the U.S. Geological Survey to evaluate the utility of simplified mathematical models for use in evaluating the impact of current and projected waste loads on receiving estuaries on the coasts of Florida. Waste loads are defined as effluent discharges from public and private sources, including municipal sewage treatment plants and industrial and commercial operations. The permitting process requires that waste-load allocation studies be made. Four estuaries of the west coast of peninsular Florida were chosen to make an evaluation of the results of model application for use in waste-load allocation studies. These are Crystal River, Homosassa River, Cross Bayou, and Anclote River. Consitiuents simulated were DO, carbonaceous biochemical oxygen demand (BOD), total Kejldahl nitrogen (TKN), and chloride.

PURPOSE AND SCOPE

The purpose of this report is to evaluate the applicability of a steady-state, intertidal estuary model, developed by Thomann (1972), for use in evaluating the impact of predicted future waste loads on receiving estuaries on the coasts of Florida. The report includes a description of the estuaries studied, their current waste loadings, and predictions of future waste load inputs. A brief discussion of the model equations and the basic assumptions upon which they are based, along with the data-collection program required to support model calibration is also included. Only one set of water-quality data, taken at low-slack tide, was used in model calibration. Recommendations concerning the use of the calibrated model for waste-load allocation studies conclude the report.

The development of a verified model, including a set of verified model coefficients established using an independent set of data not used in model calibration, is outside the scope of this study. In addition results of the operation of the calibrated model for waste-load simulations to provide support of official policy in permitting decisions were not a part of this study.

A brief description of each of the subject areas is given in the following pages.

ACKNOWLEDGMENTS

This study was proposed by the Florida Department of Pollution Control, now part of the Department of Environmental Regulation. The Bureau of Environmental Programs, with Dr. Timothy Stuart as Chief, was the liaison group that collaborated with U.S. Geological Survey personnel. Randall Armstrong of the Department of Environmental Regulation participated with Geological Survey field staff in the data-collection effort in the southwest Florida area.

* * * * * * *

For use of those readers who may prefer to use metric units rather than U.S. customary units, the conversion factors for the terms used in this report are listed below:

U.S. customary	Multiply by	Metric
acres	0.00405	square kilometers (km^2)
cubic feet per second (ft^3/s)	.02382	cubic meters per second (m^3/s)
cubic feet (ft3)	.02832	cubic meters (m^3)
cubic feet per second per square mile ($(ft^3/s)/mi^2$)	.0109	cubic meters per second per square kilometer ($(m^3/s)/km^2$)
feet (ft)	.3048	meters (m)
feet per second (ft/s)	.3048	meters per second (m/s)
gallons (gal)	3.785	liters (L)
gallons per minute (gal/min)	.06309	liters per second (L/s)
inches (in)	25.4	millimeters (mm)
miles (mi)	1.609	kilometers (km)
million gallons per day (mgal/d)	.04381	cubic meters per second (m^3/s)
square miles per day (mi^2/d)	2.59	square meters per second (m^2/d)
pounds (lb)	.4536	kilograms (kg)

SYMBOLS

A	=	Cross-sectional area, ft^2
a	=	Weighting factor
b	=	Weighting factor
BOD	=	Biochemical oxygen demand, mg/L
CBOD	=	Concentration of carbonaceous BOD, mg/L
C's	=	Oxygen saturation, mg/L
DO	=	Dissolved oxygen concentration, mg/L
H	=	Mean depth, ft
E	=	Longitudinal tidal dispersion coefficient, mi^2/d
K	=	Reaction rate coefficient, 1/d
K_a	=	Atmospheric reaeration coefficient, 1/d
K_d	=	Carbonaceous BOD oxidation constant, 1/d
K_n	=	Nitrogeneous BOD removal constant, 1/d
K_r	=	Carbonaceous BOD removal constant, 1/d
L	=	Segment length, mi
P	=	Oxygen production by photosynthesis, mg/L-d
Q	=	Freshwater flow, ft^3/s
R	=	Oxygen consumption by respiration, mg/L-d
S	=	Concentration of substances, mg/L
T	=	Temperature, °C
t	=	Time, tidal cycles
TKN	=	Total Kjeldahl Nitrogen (organic and ammonia nitrogen), mg/L
Um	=	Mean tidal velocity, ft/s
V	=	Volume, ft^3
W	=	Mass of source and sink material, lb/d
x	=	Longitudinal distance, mi
y	=	Lateral distance, mi

DESCRIPTION OF THE ESTUARIES

The four estuaries are located in an area (see fig. 1) characterized by sand-covered flatlands dotted with cypress swamp depressions. Along the coast, tidal marshes and mangrove swamps predominate. Commercial activity near the coast includes fishing, seafood processing, boat building, and tourism. Historically, land-based activities have been cattle ranching, citrus farming, and tree farming. In recent years, construction of single- and multiple-family housing has dominated in some of the coastal areas. In the Anclote River-Cross Bayou subarea, numerous new and growing subdivisions have been built in a 5-mile strip paralleling the coast. Homesites have been constructed along parts of Crystal and Homosassa Rivers; many housing developments are currently underway and others have been proposed. Large industries include a chemical plant near the mouth of the Anclote River and large thermal power plants at the mouths of the Anclote and Crystal Rivers.

The climate is characterized by warm, humid summers and mild, dry winters. Average annual rainfall is about 55 inches, with more than half occurring from June to September in the form of intense rainfall, associated either with thunderstorms or with tropical depressions and hurricanes. Air temperature ranges from 72°F to 90°F in the summer and from 55°F to 75°F in the winter. Losses by evapotranspiration are about 70 percent of the rainfall, with nearly 60 percent of this loss taking place during June-September (Cherry and others, 1970).

Crystal River

Freshwater flow in the Crystal River originates as ground water that discharges from a group of springs near the city of Crystal River and flows westward about 7 mi to the Gulf of Mexico (fig. 2). Only a small amount of storm runoff, mostly from the streets of the surrounding community, contributes to the flow.

The average daily discharge of Crystal River from 1964 to 1972, measured just upstream from the confluence with Salt River, was 868 ft^3/s (cubic feet per second). The discharge measured on April 15, 1974 during the data collection phase of this study was about 900 ft^3/s. The stream channel in the headwaters is 400 to 2,000 ft wide, 3 to 10 ft deep. The density of weed growth diminishes toward the Gulf. The entire channel is tide affected and water levels normally fluctuate 1.5 to 2.0 ft at the measuring site.

Data collected for this study at low-slack tide indicate that the chloride concentration of the water ranges from about 19 mg/L near the headwaters to about 640 mg/L near the mouth. Cherry and others (1970) reported chloride concentrations ranging from 320 mg/L at the springs to about 3,000 mg/L near the mouth at high tide.

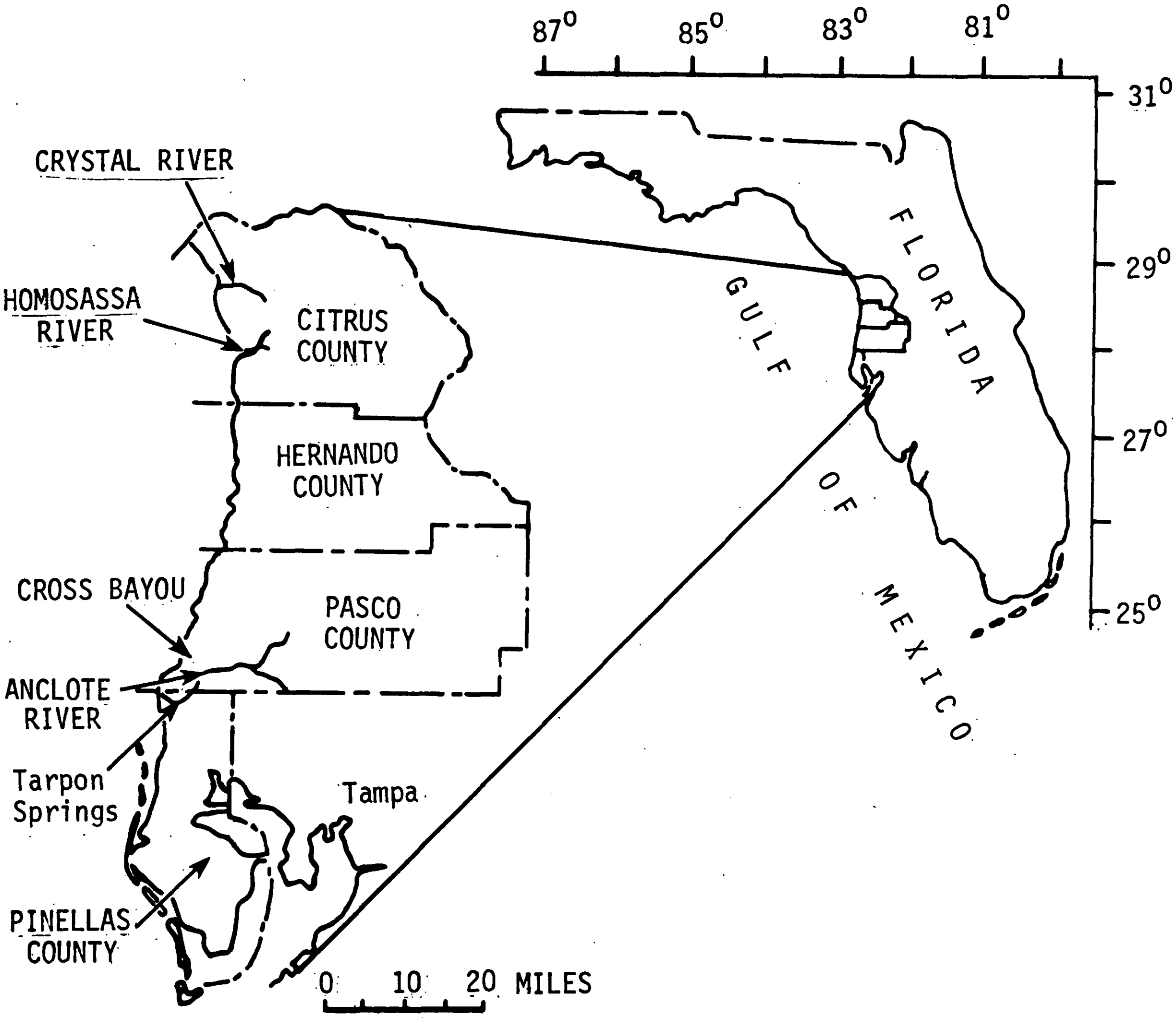


Figure 1.--Location of estuaries used in this study.

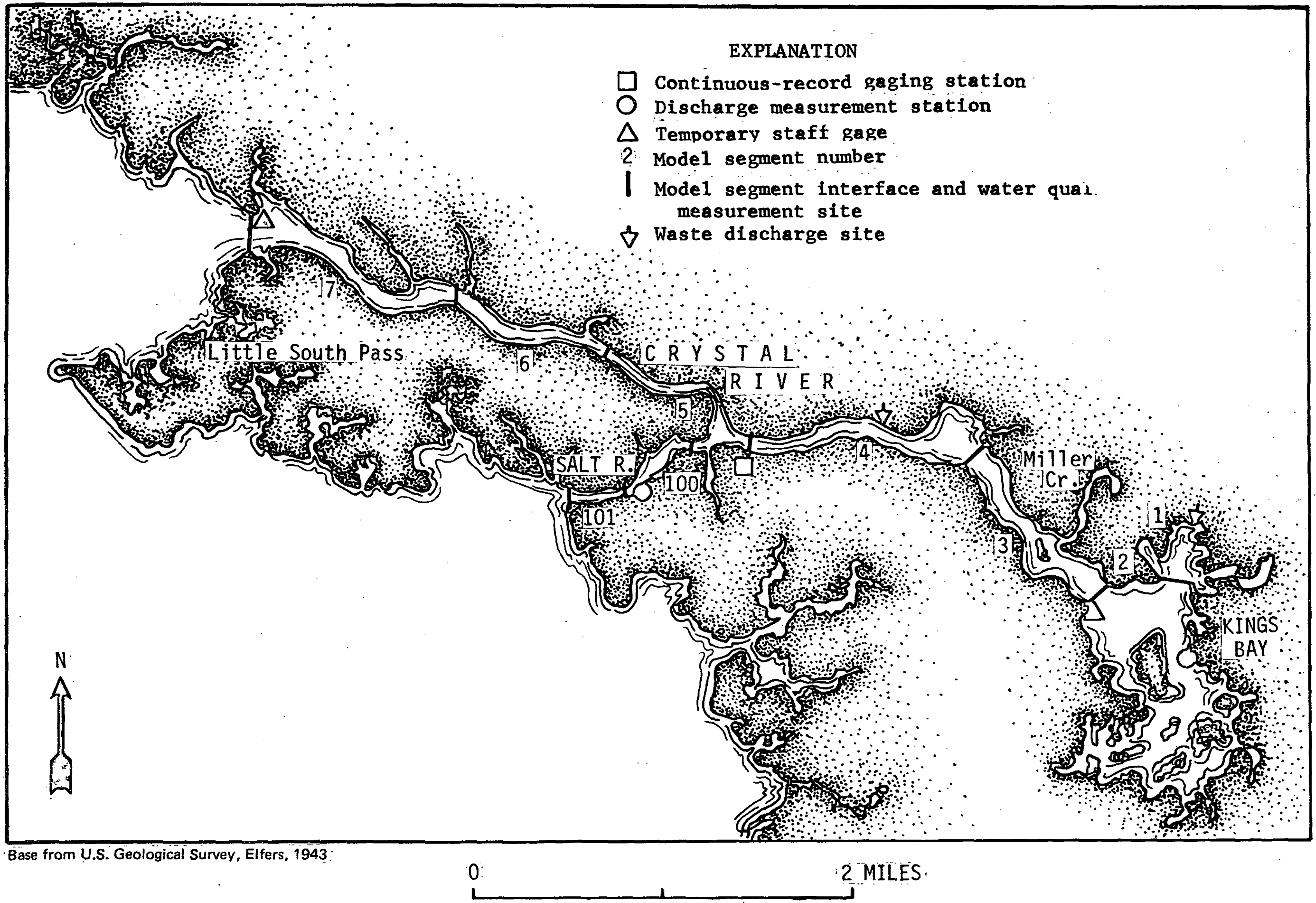


Figure 2.--Crystal River showing model segments, waste sources, and data collection sites.

Data collected in April 1974 demonstrated some chloride stratification at some sample points during part of the day but little DO stratification. Data collected in August 1974, however, indicated DO stratification at some points at certain times during the tidal cycle.

Homosassa River

Flow discharging from Homosassa Springs combines with flow from Halls River (fig. 3) to form the freshwater discharge in Homosassa River. It moves through 6 mi of swampy lowlands to the Gulf. At the village of Homosassa, flow has ranged about from 125 ft^3/s to 780 ft^3/s. Discharge data collected on April 16, 1974 show that the net outflow from Homosassa Springs was about 145 ft^3/s. Flow from Halls River was about 55 ft^3/s; thus the combined discharge is about 200 ft^3/s. Additional net outflow contributed from the swampy area provided a total freshwater discharge at the mouth of Homosassa River of about 280 ft^3/s. Cherry and others (1970) reported an average flow of about 390 ft^3/s of which 220 ft^3/s came from Homosassa Springs and 170 ft^3/s from Halls River.

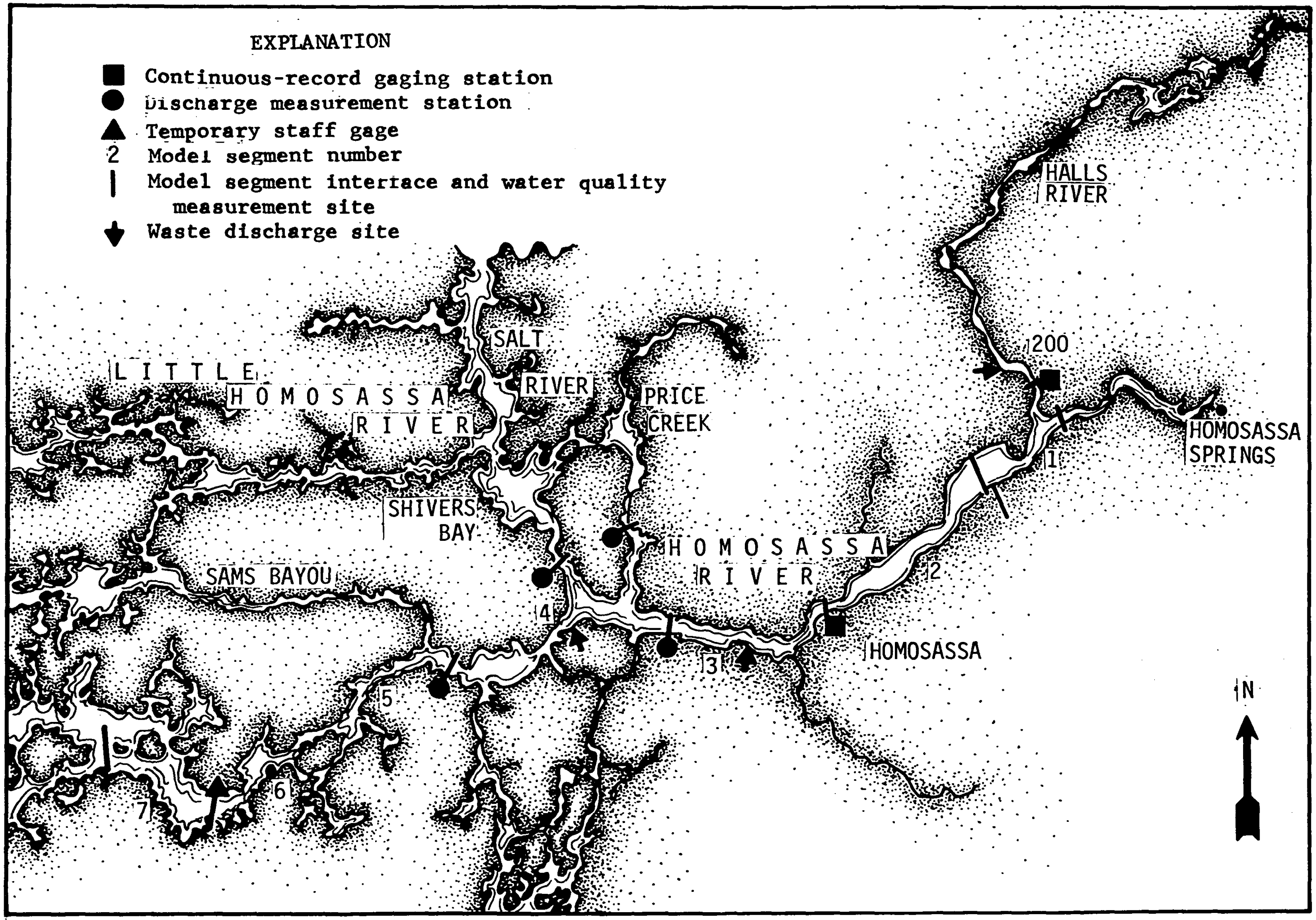
The stream channel is about 200 to 700 ft wide and about 5 ft deep in the springs area and is about 1,000 ft wide and 15 to 20 ft deep towards the Gulf. The upper reaches of the channel are weed choked during parts of the year with the density of weeds diminishing downstream. The entire length of the channel is tide affected, and water levels normally fluctuate 1.5 to 2.0 ft at a tide gage near the village of Homosassa.

Chloride concentration of water sampled at low-slack tide on April 16, 1974 was 580 mg/L in the spring area, 2,500 mg/L in Halls River and 3,200 mg/L at the mouth. Cherry and others (1970) reported chloride concentrations at high tide of 565 mg/L in the springs, 2,050 mg/L in Halls River and 3,900 mg/L at the mouth. Data collected in April 1974 indicated some chloride stratification in some sections, varying diurnally. Little or no DO stratification was in evidence at this time.

Cross Bayou

The freshwater discharge in Cross Bayou (fig. 4) is very small (less than 1 ft^3/s) and is derived from ground-water seepage. The only other inflow to the estuary is discharge from two sewage treatment plants. The estuary is about 1.5 mi long and lies entirely in swampy lowlands. The channel ranges in width from about 30 ft in the upper reaches to about 600 ft at the mouth. The channel bottom is covered with grass but is not weed choked. The entire estuary is tide affected; at low tide the channel depth averages about 0.5 ft and at high tide about 3 ft.

Analyses of water samples indicate that chloride concentrations do not fluctuate appreciably in the estuary. The concentrations at the estuary mouth and head were 12,400 mg/L. The concentration midway in the channel was about 11,600 mg/L. Measurements made on August 30, 1974, show significant DO stratification in some sections. These observations, made at high tide, show that at a depth of 2 to 3 ft, at



Base from U.S. Geological Survey, 1954

Figure 3.--Homosassa River showing model segments, waste sources, and data collection sites.

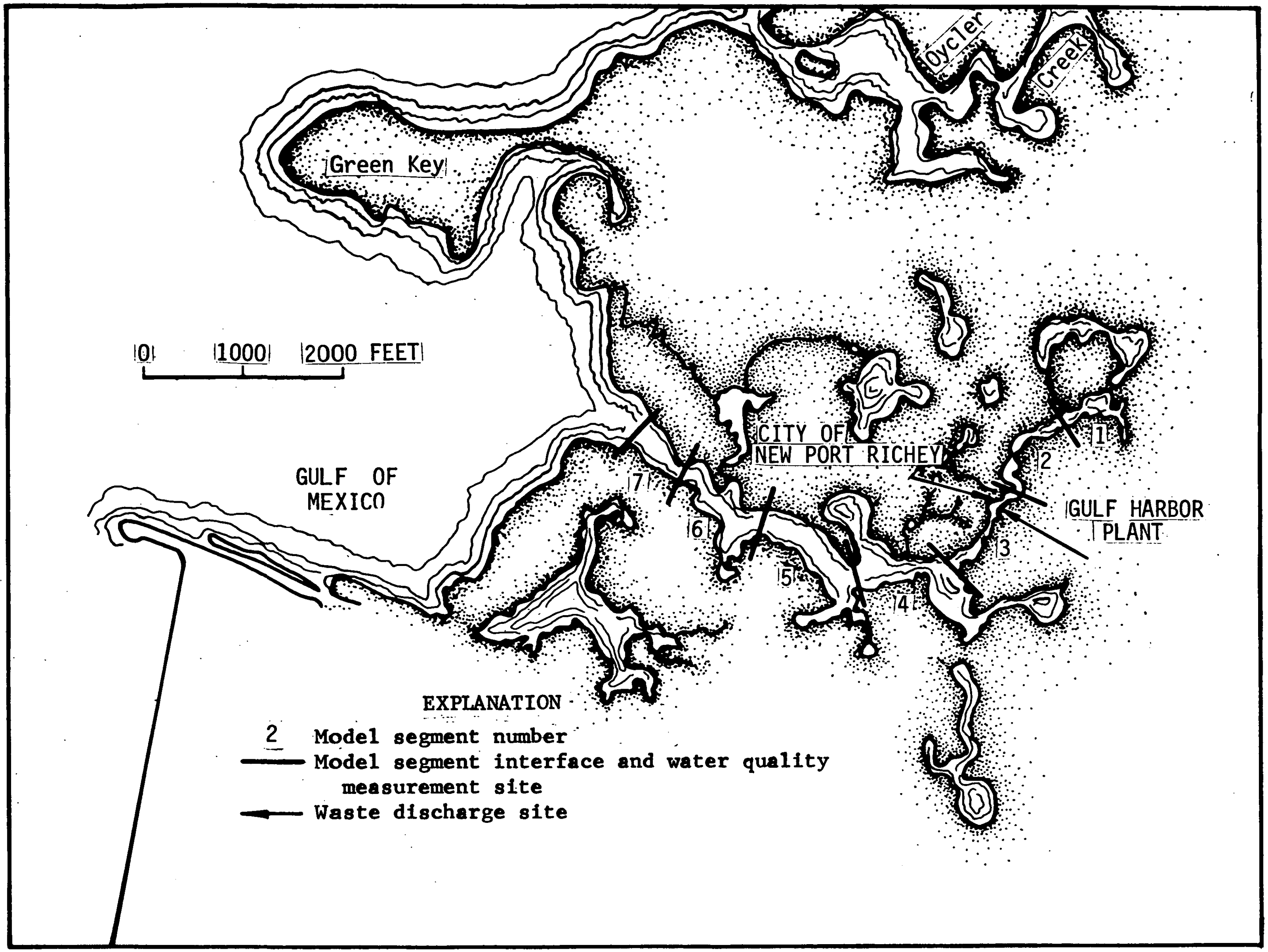


Figure 4.--Cross Bayou showing model segments, waste sources, and data collection sites.

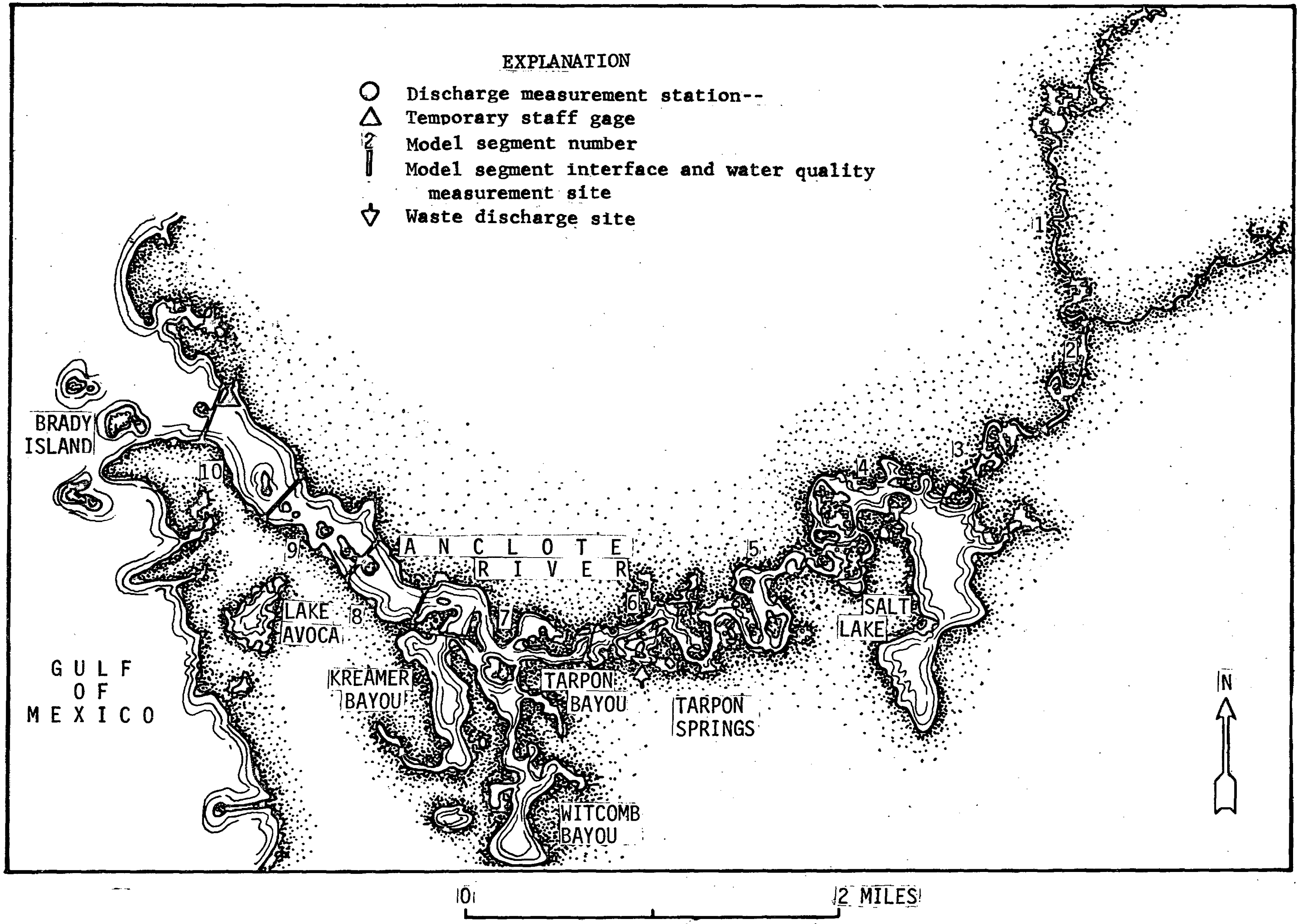


Figure 5.--Anclote River showing model segments, waste sources, and data collection sites.

the bottom of the channel, the DO was 0.4 to 1.8 mg/L less than the DO at the surface in those sections.

Anclote River

Freshwater discharge in the Anclote River (fig. 5) is derived from surface runoff and ground-water seepage. The river is about 18 mi long and meanders through swampy lowlands before discharging into the Gulf near the city of Tarpon Springs. The average discharge from 1946 to 1972, measured at a gage about 12 mi upstream from the mouth was 81 ft^3/s. The freshwater discharge measured above Tarpon Springs about 2.5 mi upstream from the mouth on April 19, 1974 was about 50 ft^3/s. Additional ground-water seepage and spring flow into the river from Kreamer and Whitcomb Bayous was estimated to be about 10 ft^3/s.

In the upper reaches, the stream channel is 10 to 50 ft wide and 3 to 7 ft deep. The stream meanders through a wide swampy area in the reach between Salt Lake and a point about 2 mi upstream from the mouth of the river. A ship channel, averaging about 14 ft deep, has been dredged from the mouth of the river to the city of Tarpon Springs--a distance of a little more than 2 mi. Except for this dredged channel, the river averages about 3 ft deep and about 1,500 ft wide in this reach.

The river is affected by tidal fluctuation as far as 14 mi upstream from the mouth. Chloride concentration of the water ranged from 3,000 mg/L at a point about 8.5 mi upstream from the mouth to 18,000 mg/L at the mouth. Cherry and others (1970) reported a similar variation in chloride concentration over the same reach. Data collected in April 1974 indicated a small degree of chloride stratification in some of the upstream reaches. The data also indicated some diurnally varying DO stratification in some reaches.

WASTE-WATER DISCHARGE

A description of current and predicted waste loading to the four estuaries provides for identification of waste sources required in model operation. The sources and amounts of waste discharging into the four estuaries in 1974 are listed in table 1. The location of each discharge point is shown in figures 2-5. All treatment plants except the one at Tarpon Springs provided secondary treatment in 1974 and the Tarpon Springs plant was upgraded to secondary treatment in 1975.

Predicted waste loads for 1975, 1980, and 1985 were computed by the Florida Department of Pollution Control (written commun., 1974, Randall Armstrong, biologist) assuming:

1. Projected population trends correctly indicate that future points of waste discharge will remain the same as present discharge points.
2. Population estimates for 1975, 1980, and 1985 were made using 1972 census data and population growth rates for that year.

Table 1.--Current and projected sources and amounts of wastes discharging into the estuaries.

Source	Year	Discharge from plant (Mgal/d) Design	Actual	Type of treatment	Receiving body	5-day BOD (lb/d)	Plant ownership
City of Crystal River	1974	0.25	0.26	Secondary	Crystal River	44.0	Municipal
	1975	.35				--	
	1980	.50				67.0	
	1985	.60				79.0	
Crystal River Mobile Home Park	1974	.005	.0033	Secondary	Crystal River	.55	Private
	1975	.007				2.1	
	1980	.009				4.0	
	1985	.026				3.0	
Riverside Villas (Homosassa Springs, No. 3 Plant)	1974	.012	.005	Secondary	Homosassa River	1.0	Private
	1975	.015				6.0	
	1980	.020				7.0	
	1985	.065				8.0	
Springs Village Mobile Home Park	1974	.003	.004	Secondary	Homosassa River	.68	Private
	1975	.003				1.0	
	1980	.006				2.0	
	1985	.002				3.0	
J. G. Coin Laundry	1974	.0075	--	Secondary	Homosassa River	1.0	Private
	1975	.110				34.0	
	1980	.137				44.0	
	1985	.420				57.0	
City of New Port Richey	1974	.35	.80	Secondary	Cross Bayou	125	Municipal
	1975	1.3				172	
	1980	1.7				229	
	1985	2.5				304	
Gulf Harbor	1974	.30		Secondary	Cross Bayou	27	Private
City of Tarpon Springs	1974	.75	1.1	Primary	Anclote River	865	Municipal
	1975	1.5		Secondary		195	
	1980	1.7				220	
	1985	2.0				224	

3. Influent loads were determined on the basis of a per capita flow of 125 gallons per day and a 5-day biochemical oxygen demand of 0.17 lb per day per capita.
4. Plant efficiency is 90 percent BOD removal.

Table 1 shows design flows and projected 5-day BOD loadings for the selected estuary in each of the design years. Projected flows and waste loadings for the Gulf Harbor sewage-treatment plant were assumed to remain unchanged because the plant currently operates at design capacity. If the model were used to study waste-loading alternatives, the present waste loading would be used in the calibration phase; subsequently, projected loadings could be used to determine the resulting DO profiles.

DESCRIPTION OF MATHEMATICAL MODEL

The mathematical model used in this study was adapted from Shindala, Zitta, and Cory (1973) who used concepts given in Thomann (1972). The model has been applied to a number of estuarine studies, including the Delaware estuary and the tidal zone of the Pascagoula River, Mississippi. The model was developed for two-dimensional, steady-state, intertidal conditions to simulate longitudinal and lateral variations in concentrations of both conservative and nonconservative substances. The model is intertidal in the sense that it attempts to portray water-quality profiles over a sequence of tidal cycles. Conservative substances are those that, for all practical purposes, do not decay with time or disappear from the water by processes such as settling or sorption. In the present studies, the main stem and each tributary are assumed to be one-dimensional linkages of segments, each encompassing the entire width of the channel; thus, the two-dimensional capability of the model is used only to join tributaries with a main stem.

As indicated, simulated concentrations of substances are averages over a tide cycle. In the Tampa Bay Area, mixed tides are the rule, with both solar and lunar effects contributing significantly to tides, so averages are based on a complete tide cycle of about 24 hours (two highs and two lows). The assumption of steady-state conditions is not necessary as unsteady-state models exist, (Najarian and Harlemen, 1977), that follow time and space variations in estuarine variables. However, unsteady-state models have large data and computer time requirements. Because of time and money constraints, a steady-state model was selected for initial evaluation. It was believed that considerable insight into estuarine behavior could be obtained for the study sites using such a model.

The general equations for the model are based on the law of conservation of mass. Each estuary was divided into segments, each with a finite volume (fig. 6), and the equations applied to each non-boundary segment and the two, three, or four adjoining segments. The criteria considered in segmenting each estuary include the method of numerical solution, changes in channel geometry, discontinuities in flow due to waste-water discharges or tributary flows, and changes in reaction coefficients.

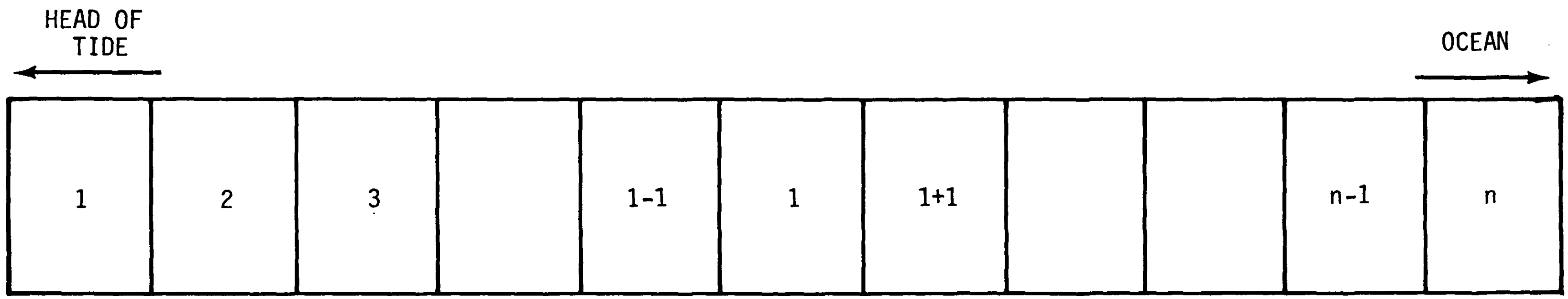


Figure 6.--Finite section segmentation for a one-dimensional estuary model.

Data required to characterize each segment of the estuaries include channel geometry, flow data, water-quality data, and waste-water data. The collection and use of these data are discussed in detail later in this report. In following paragraphs the development of the equations used in the mathematical model are briefly discussed.

Based on a mass-balance analysis, the partial differential equation for one-dimensional mass transport (O'Connor, 1960, 1965; Thomann, 1972) is:

$$\frac{\delta S}{\delta t} = \frac{1}{A}\frac{\delta}{\delta x}(EA\frac{\delta S}{\delta x}) - \frac{1}{A}\frac{\delta}{\delta x}(QS) - KS + S_d \quad (1)$$

where: S is the concentration of a conservative and(or) non-conservative substance that obeys the first-order decay law. A is the cross-sectional area of the estuary; Q is the freshwater flow; E is the longitudinal dispersion coefficient; K is the first-order decay coefficient for the substance; t is time; x is the longitudinal distance; and S_d represents inputs and removals not represented by the dispersion, advection, or reaction terms (first, second, and third terms, respectively on the right-hand side of equation 1). In the finite-segment model developed for this study, the estuary was divided into segments and magnitudes of Q, A, and E were assigned to each interface.

The assumption of steady state was used to develop the model for this study. The assumption of steady-state means that $\delta S/\delta t = 0$.

Mass transport in single constituent systems

Several water pollution control problems involve the discharge of waste material containing conservative substances such as dissolved solids and chloride. The decay rate coefficient for conservative substances is zero (K = 0). Other materials such as BOD and coliform bacteria are nonconservative substances. Although the dilution of concentrations may be affected by many different mechanisms and factors, the assignment of a first-order decay coefficient is a reasonable approximation.

The form of equation (1) that describes the concentration of non-conservative substances under the condition of steady state is,

$$0 = \frac{1}{A}\frac{d}{dx}(EA\frac{dS}{dx}) - \frac{1}{A}\frac{d}{dx}(QS) - KS + S_d \quad (2)$$

For conservative substances under steady state conditions equation (2) is the same except that the term KS is omitted.

Mass transport in coupled systems

Many water-quality problems involve reactions of substances such that the concentration of the substance is dependent on the output of a preceding reaction. These are called coupled systems or consecutive reactions. A common example of a consecutive reaction is the biological or chemical oxidation of oxygen-demanding material producing a change in DO concentration.

Under steady-state conditions, the differential equations for the concentration of two reactants in a coupled system are:

$$0 = -\frac{1}{A}\frac{d}{dx}(QS1) + \frac{1}{A}\frac{d}{dx}\left(ES\frac{dS1}{dx}\right) - K_{11}\,S1 + S_d \tag{3}$$

and

$$0 = -\frac{1}{A}\frac{d}{dx}(QS2) + \frac{1}{A}\frac{d}{dx}\left(EA\frac{dS2}{dx}\right) - K_{22}\,S2 + K_{12}\,S1 + S_d \tag{4}$$

where S1 and S2 are the concentrations of the particular substances, such as BOD and DO; K_{11} is the decay coefficient associated with concentration of S1 and acts as a sink in a typical first-order decay phenomenon; K_{12} is a reaction coefficient, and together with S1 acts as a source for S2; K_{22} is the decay coefficient associated with variable S2. For the case of the DO-BOD coupled equations, S1 represents the carbonaceous BOD or TKN, K_{11} represents the BOD decay rate (which includes oxidation and settling). K_{12} is the deoxygenation coefficient and will be negative, S2 is DO, and K_{22} is the reaeration rate constant. Equation (3) must first be solved for the concentration of BOD in order to provide input to equation (4) to solve for DO concentration.

The numerical scheme developed to solve these equations for single or coupled systems involves a finite-segment approach somewhat similar to finite-difference approximations. In this scheme, an estuary is divided into segments. (A one-dimensional diagram of hypothetical segments and typical notation for them is shown in fig. 6.) A material balance is then written for each segment, with terms representing inputs or outputs through interfaces with adjacent segments and within the central segment itself. Each segment is considered to contain vertically mixed water, that is, no vertical concentration gradients exist within the segment. The longitudinal concentration gradients are estimated linearly in the dispersion terms and are determined by weighting factors in the advective terms. Decay terms use the average concentration values for each reach. For a one-dimensional steady-state system, a mass balance for S in segment i including flows in and out of the segment and all source and sink terms are set up. Included in the mass balance equation are advection and dispersion terms, carbonaceous BOD and nitrogenous TKN reaction terms, community photosynthesis and respiration terms and the reaeration source term. When all segments including boundary segments are specified, a series of simultaneous linear equations (Thomann, 1972) is obtained. Solution requires specification of DO at upstream and downstream boundaries and the prior solution for BOD quantities at all segments. The set of linear equations is then solved by matrix algebra techniques to obtain the concentrations, S_i, in all non-boundary segments. The matrix solution technique used in this study is the Gauss-Seidel method.

The equations described above are for the one-dimensional case, but an extension to the two-dimensional case can be easily made by adding similar terms corresponding to additional interfaces with the central segment. Two-dimensional equations are required for application to wide tidal bodies or to simulate junctions with tributaries.

DATA REQUIREMENTS FOR MATHEMATICAL MODEL

Before using the mathematical model for predictive purposes, all relevant parameters must be specified. Some may be estimated or computed from field measurements, such as channel geometry data and flow and velocity data. Some parameters can only be determined by calibrating the model against field water-quality measurements. One model parameter, waste-load input, falls into both categories, because naturally occurring waste loads can be determined by calibrating against field water-quality measurements, whereas manmade waste loads can be determined directly through field measurements.

Each estuary was divided into segments and field data were collected at either the interface between segments or the midpoint of each segment. Time-averaged data of all types are required by the steady-state assumption of the model. The model assumes cross-sectional uniformity of flow and velocity data, and the model's use of average concentration values in each reach require water-quality measurements to be averaged not only in cross-section but also along the length of each reach. Whereas concentrations may actually be vertically stratified in an estuary, computed concentration, as well as measured concentrations, are treated in the model as cross-sectional averages.

The data collection program is described in detail in the following four sections. Because only one set of water-quality data was taken at low-slack tide, additional data collection might be useful in future studies to supplement the one described. It might be useful to conduct tracer studies in one or several reaches to directly measure tidal dispersion coefficients. These data would then allow unique determintion of the dispersion coefficients partially derived through calibration on the basis of chloride data.

Channel Geometry

The model assumption of steady-state requires that the geometric parameters used for running the model be averaged over a complete tidal cycle. Channel geometry includes depth, segment length, cross-sectional area, and segment volume. All geometric data were collected at approximately high tide and were adjusted to represent average tidal conditions.

Channel depth was measured at high tide along the thalweg using an echo-sounding device or sounding pole to identify any nonuniformities in the channel. At the interface between segments a depth profile was obtained by taking fathometer readings from a boat moving from one bank to the other. Mean depth was calculated by averaging the fathometer profile. At very narrow points, sounding was used in place of the fathometer. The mean depth for an entire stream segment was computed by averaging the mean depths at the ends of the segment. The length of each segment was measured from aerial photographs or topographic maps. Where channels were less than 200 ft wide and where boat traffic permitted, the channel width was measured with a steel tape. Maps and aerial photographs were used to determine widths where the channel was more than 200 ft wide and where boat traffic was heavy. Cross-sectional areas were computed at the interfaces between segments from the channel widths and mean depths. An average cross-sectional area was computed for each segment and multiplied by the segment length to determine the segment volume. In some cases, segment volumes were increased to account for the estimated additional volume of some irregular-shaped channels and lateral bayous. For example, the volume of Segment 2 of Crystal River was increased about 125 percent to account for the storage in Kings Bay (fig. 2).

Data on channel geometry are summarized in table 2 segments for each estuary.

Flow and Velocity Data

Use of the steady-state model requires that the average net freshwater flow at each interface be determined. Discharge was measured periodically during a half tidal cycle during daylight hours at selected locations along each estuary. Hourly discharge measurements were made beginning and ending at about low-slack tide (a period of about 12.5 hours) either from bridges by standard current-meter technique (Buchanan and Somers, 1969) or by the moving-boat technique (Smoot and Novak, 1969). The net freshwater discharge was determined as the difference between the ebb-tide discharge and the flood-tide discharge at each measuring site and was interpolated to obtain input data for all segments.

The net freshwater discharge measured at selected cross sections on Crystal, Homosassa, and Anclote Rivers is listed in table 2. Except for sewage treatment-plant effluent, net freshwater discharge from Cross Bayou was negligible during field measurements.

Mean tidal velocities are required by the digital model to estimate the reaeration rate coefficient, K_a using the O'Connor-Dobbins equation, $K_a = 12.9\ U_m^{1/2}/H^{3/2}$ where K_a is the coefficient in 1/days, U_m is the mean tidal velocity in feet per second, and H is the mean channel depth, in feet (O'Connor and Dobbins, 1958).

The usual method of computing mean tidal velocity is to average flood tide and the ebb-tide velocities over a complete tide cycle.

Table 2.--Summary of channel geometry and discharge data.

Name	Segment	Channel geometry: Length (mi)	Depth (ft)	Cross sectional area (ft^2)	Volume (ft^3)	Discharge: Measured flow (ft^3/s)	Velocity (ft/s)	Low flow (ft^3/s)
Crystal River	1	0.35	7.5	3,300	10,240,000	50	0.015	6
	2	1.25	7.5	5,300	133,700,000	850	.16	94
	3	1.00	11.0	5,680	29,120,000	900	.16	100
	4	1.35	14.0	5,312	39,000,000	900	.16	100
	5	.90	18.0	4,800	24,000,000	850	.17	94
	6	.92	17.0	6,360	27,000,000	850	.14	94
	7	1.23	18.0	9,274	50,800,000	850	.09	94
	100	.44	5.0	684	1,780,000	50	.07	6
	101	.36	5.0	864	2,380,000	50	.06	6
Homosassa River	1	.85	6.0	1,135	5,090,000	145	.13	14
	2	.91	7.5	4,459	12,480,000	200	.04	20
	3	.96	11.0	1,914	16,150,000	200	.10	20
	4	.90	9.5	3,422	12,750,000	225	.07	20
	5	1.18	13.0	3,740	22,311,000	250	.07	20
	6	.96	14.0	1,885	14,268,000	280	.15	20
	7	1.09	11.0	7,125	25,950,000	280	.04	20
Cross Bayou	1	.25	3.0	152	304,000	0	0	0
	2	.19	3.0	168	160,000	0	0	0
	3	.19	3.0	245	206,500	2.63	.011	2.63
	4	.19	3.0	378	623,000	2.63	.007	2.63
	5	.19	3.0	522	675,000	2.63	.005	2.63
	6	.19	3.0	538	530,000	2.63	.005	2.63
	7	.19	3.0	440	538,000	2.63	.006	2.63
Anclote River	1	1.42	7.0	301	2,010,000	50	.17	2.3
	2	1.23	8.0	759	3,445,000	50	.07	2.3
	3	1.40	8.0	450	4,473,000	50	.11	2.3
	4	.97	9.0	1,639	5,350,000	50	.03	2.3
	5	1.16	9.0	1,200	8,660,000	50	.04	2.3
	6	1.01	11.0	2,100	8,811,000	50	.02	2.3
	7	1.20	12.0	5,108	22,710,000	60	.01	3.0
	8	.40	14.0	6,285	12,200,000	60	.01	3.0
	9	.56	13.0	5,233	16,800,000	60	.01	3.0
	10	.57	13.0	5,270	15,900,000	60	.01	3.0
	100	.70	5.0	1,550	39,150,000	10	.006	0.7

However, because velocity measurements were not available for all segments, mean tidal velocities were computed by dividing the net freshwater discharge through each segment by the average cross-sectional area of each segment.

The procedure recommended by the Environmental Protection Agency (Florida Department of Environmental Regulation, oral commun., 1976) in applying mathematical models in waste allocation studies is to use the average 7-day low-flow condition that can be expected to occur on the average once every 10 years (7Q10) as an estimated worst-case condition to ensure that minimum water-quality conditions are maintained at all times. In modeling estuaries, applying this statistic to net freshwater inflow provides what may be an estimate of worst-case conditions, because the amount of fresh dilution water is thereby minimized. For this reason, this is the general procedure used in this study. The 10-year, 7-day, low flows in the present study were estimated from available discharge records. In future studies, model calibration should be based upon some observed freshwater low-flow conditions, and 7Q10 freshwater flow conditions should be used in the model to predict the effect of waste loading on the estuaries.

The streamflow record at Crystal River was inadequate for the calculation of a meaningful 10-year, 7-day low flow. Thus, an arbitrary "low flow" (not statistically determined) was selected equal to about 10 to 15 percent of the freshwater discharge measured during this study, or 100 ft^3/s. The values assigned to the various reaches are listed in table 2.

The Anclote River is gaged 12 mi from its mouth. The 10-year, 7-day low flow at this site is 1.7 ft^3/s or 2.3×10^{-2} $(ft^3/s)/mi^2$. The low flow at the mouth of the river was calculated, from the total drainage area and a unit low flow for this locality, to be about 3 ft^3/s, including about 0.7 ft^3/s from Kreamer and Whitcomb Bayous (fig. 5).

Sufficient record is not available for the Homosassa River to determine 10-year, 7-day low flow. Therefore, an arbitrary "low flow" value of 10 percent of the discharge measured during the study or 20 ft^3/s at the mouth was assumed for low-flow conditions.

Cross Bayou currently has no freshwater discharge, except for surface and ground-water runoff in its lower part, and low flow was assumed to be zero in the inland segments and zero near the mouth.

Water-Quality Data

The assumption of steady-state upon which the model is based requires that water-quality data for calibration be averaged over an appropriate time cycle, which may be a tidal cycle or a 24-hour period, depending upon the pattern of time variation of the data types. The model assumption of cross-sectional mixing requires that depth and lateral variation in water-quality data be measured and used to formulate cross-sectional averages. The model use of concentration averages for reaches requires that water-quality measurements be averaged in volume, as well as in cross-section. This suggests that segmentation be done so as to minimize concentration variations along the chosen reaches.

Data collection to support calibration should include all four parameters computed: Chloride, CBOD, TKN, and dissolved oxygen, and should include all reaches modeled. The first three should be collected over a complete tidal cycle. In the Tampa Bay area, this is approximately a 24-hour period, with two highs and two lows, owing to the mixed tide effect in the area. Dissolved oxygen should be collected over a 24-hr period because of the typical diurnal variation in dissolved oxygen. Time-averaged water-quality data are necessary for calibration because this steady-state model computes time-averages. Depth-integrated measurements are particularly important for dissolved oxygen and chloride because of possible seasonal and diurnal stratification.

In addition to water-quality data collected for model calibration, diel DO data from any DO-stratified sections, collected in the same time period as other data, would support an independent determination of the amount of photosynthesis and respiration. In swiftly flowing narrow sections, and in very saline reaches, there is generally little plant life, and diurnal data collection may not be necessary if photosynthesis and respiration are negligible.

The analytical data summarized in table 3 represent average conditions in each segment at low-slack tide. These are not the tidal-averaged data required for calibration, but are included to provide a quantitative picture of the example estuaries. On-site measurements were made for water temperature, specific conductance, and DO, using direct-reading instruments. Some measurements were made at several depths in each cross section. Water samples were also collected at several depths and analyzed in the laboratory for chloride, nitrogen, and BOD_5 (5-day BOD). Some high concentrations of DO were measured which considerably exceeded saturation concentration. This indicated that the plant communities in the estuaries were producing much DO by photosynthesis. To determine the magnitude and influence of photosynthesis and respiration in two estuaries, a field study was made to determine the fluctuation of DO throughout a day. Measurements of DO in the Crystal River were made over a period of about 19 hours on August 15, 1974 for this purpose. The field data are shown in table 4. The minimum DO concentration in each segment was recorded about 1.5 hours after sunrise and ranged from 2.1 to 6.2 mg/L. The concentration of DO was maximum late in the afternoon and ranged from 8.5 to 10.5 mg/L.

Table 3.--Summary of water-quality data.

[Analyses by U.S. Geological Survey Field Data[1/]]

Name	Date of collection	Segment	Temperature (°C)	Specific conductance (micromhos at 25°C)	Dissolved oxygen (mg/L)	Chloride (mg/L)	KKN[2] (mg/L)	5-Day BOD (mg/L)	20-Day BOD (mg/L)
Crystal River	04/17/74	1	24.0	240	9.6	19	1.8	1.70	--
		2	24.0	1,600	10.7	340	0.60	0.20	1.4
		3	24.0	1,600	10.3	410	.50	.20	--
		4	24.5	1,800	9.9	440	.50	.50	--
		5	24.5	2,000	9.5	500	.21	.50	--
		6	25.0	2,100	9.3	530	.28	.30	--
		7	25.0	2,500	9.0	640	.20	.40	1.5
		100	25.0	10,500	10.5	2,800	.37	.60	--
		101	24.5	14,000	11.1	4,400	.47	.60	--
Homosassa River	04/18/74	1	24.0	2,500	10.3	580	.13	.40	--
		2	24.0	3,800	8.9	1,100	.18	.80	--
		3	23.7	3,800	8.5	1,100	.24	.80	--
		4	23.5	4,000	7.7	1,100	.24	1.10	--
		5	23.3	6,000	7.9	1,800	.31	1.30	--
		6	23.5	7,200	7.2	2,100	.33	.80	--
		7	23.5	10,500	6.8	3,200	.41	.60	--
		200	24.0	8,000	10.6	2,500	.24	.60	--
Cross Bayou	08/14,22, 28,30/74	1	32.0	35,400	19.5	12,000	3.00	7.1	--
		2	32.0	35,400	17.5	12,000	3.00	7.1	--
		3	32.0	33,000	15.0	12,000	2.31	7.9	--
		4	32.0	33,000	16.0	12,000	2.31	7.9	--
		5	32.0	35,600	17.0	12,000	2.41	7.5	--
		6	32.0	35,600	18.0	12,000	2.41	7.5	--
		7	32.0	36,800	21.5	12,000	2.42	8.5	26.3

Table 3.--Summary of water-quality data. (continued)

[Analyses by U.S. Geological Survey Field Data[1/]]

Name	Date of collection	Segment	Temperature (°C)	Specific conductance (micromhos at 25°C)	Dissolved oxygen (mg/L)	Chloride (mg/L)	KKN[2] (mg/L)	5-Day BOD (mg/L)	20-Day BOD (mg/L)
Anclote River	4/19/74	1	24.0	23,000	4.3	8,100	0.61	1.70	--
		2	24.0	28,500	5.1	9,800	.55	1.40	--
		3	23.5	32,300	5.6	12,000	.50	1.70	--
		4	23.5	35,000	5.2	13,000	.60	1.20	--
		5	23.0	38,500	6.0	15,000	.69	1.60	--
		6	23.0	40,700	6.5	15,000	.76	1.80	--
		7	22.5	42,500	8.0	16,000	.73	2.60	5.7
		8	22.0	43,000	8.0	17,000	.81	2.10	--
		9	21.5	43,000	7.8	18,000	.69	1.80	--
		10	21.0	43,000	8.0	18,000	.74	1.60	3.8
		100	22.0	40,100	6.0	16,000	.65	2.00	--

1/ Data represent average values in the segment.
2/ TKN is the sum of the concentration of ammonia and total organic nitrogen.

Table 4.--Diurnal dissolved oxygen data at Crystal River, August 15, 1974.

Segment	Time	Temperature (°C)	Conductivity (micromhos at 25°C)	Dissolved oxygen (milligrams per liter)
1	0800	24.0	220	2.5
	1140	28.0	260	3.6
	1250	28.5	220	5.4
	1550	27.5	260	6.2
	1715	27.0	210	8.5
	2010	26.0	220	7.0
	2240	25.5	60	6.0
2	0624	25.0	630	2.6
	0745	24.5	1,060	2.5
	0845	25.0	840	2.1
	1115	29.0	860	4.3
	1305	28.5	750	5.8
	1540	28.0	980	8.5
	1730	27.5	475	10.5
	2000	27.0	860	7.7
	2225	26.0	260	6.3
3	0638	26.0	1,400	6.9
	0900	25.5	720	3.4
	1100	28.5	950	5.5
	1320	29.0	1,140	7.7
	1530	30.0	1,200	8.2
	1745	28.0	800	8.6
	1940	28.0	1,360	9.4
	2215	27.0	590	8.4
4	0700	26.0	950	6.7
	0910	26.0	-	5.1
	1050	28.0	1,040	6.4
	1340	30.0	2,250	7.8
	1510	30.5	2,900	8.2
	1755	28.5	1,300	8.6
	1920	27.5	950	8.6
	2200	27.5	1,430	8.7
5	0710	26.0	1,050	7.3
	0920	26.5	1,030	6.2
	1035	28.5	1,250	6.9
	1355	30.5	7,700	7.1
	1455	31.5	8,500	7.1
	1820	29.0	1,450	8.8
	1900	28.5	1,230	8.8

NOTE: Sunrise occurred at about 0645; sunset about 1930.
DO measurements are corrected for chloride concentration.

Data from a similar field study made at Cross Bayou are shown in table 5. Because the freshwater flow through the estuary is small, the residence time of water and wastes in the estuary is long. This results in the development of large populations of algae that produce oxygen during the daylight hours and respire all of the time. The concentration of DO was minimum shortly after sunrise and ranged from 0.6 to 1.4 mg/L in the different segments. The concentration of DO was maximum late in the afternoon, and ranged from 5.6 to 18.4 mg/L.

An analysis of these field data was made to compute the average daily rate of photosynthesis and respiration. The computation was made according to procedures described by Slack and others (1973).

The average daily rates are shown in table 6 for each segment of the main channels of Crystal River and Cross Bayou. Because the results were for a time period that differs from that of the data collected for model calibration, they can be used in the calibration process only as approximate values for the time of year. Because daily fluctuations in photosynthesis and respiration rates are often striking, the computed rates were regarded as initial values and were varied as calibration parameters.

Waste-Water Data

Current waste-water discharges from all sources are one type of water-quality data required for the calibration of the model. In the four estuaries studied, all manmade waste loads (point sources) are from municipal or private plants treating mainly domestic wastes; no industrial wastes are being discharged into any of the estuaries. Points of waste-water discharge into each of the estuaries studied are shown in figures 2-5. Average daily effluent discharges are shown in table 1. Water samples were collected at the outfall of each treatment plant and chemical analyses of the effluents from each source are listed in table 7. Except for the Tarpon Springs sewage treatment plant, all wastes received secondary treatment at the time of collection. The Tarpon Springs treatment plant was upgraded from primary to secondary treatment in 1975.

The magnitudes of BOD loads reported in table 7 are similar to the estimated design BOD loads shown in table 1. For this reason, the design BOD loads would best be used in the estuary model rather than the measured ones because they represent the average steady-state conditions better than the one-time samples collected.

Table 5.--Diurnal dissolved oxygen data at Cross Bayou, August 28, 1974.

Segment	Time	Temperature (°C)	Conductivity (micromhos at 25°C)	Dissolved oxygen (milligrams per liter)
1	0912	27.0	12,000	1.1
	1057	28.0	do.	3.0
	1230	29.0	do.	5.6
	1354	30.0	do.	13.6
	1705	30.5	do.	18.4
	1800	30.0	do.	17.2
2	0910	27.0	12,000	1.4
	1054	28.0	do.	3.4
	1225	31.0	do.	4.0
	1350	30.5	do.	7.4
3	0900	27.0	12,000	1.2
	1049	28.0	do.	3.7
	1220	31.0	do.	5.6
	1344	30.5	do.	6.4
	1440	32.0	do.	7.8
	1650	31.0	do.	14.8
	1816	31.0	do.	14.0
4	0855	27.0	12,000	1.1
	1045	28.0	do.	3.2
	1213	31.0	do.	8.6
	1340	31.0	do.	6.2
	1443	33.0	do.	7.4
5	0850	28.0	12,000	1.3
	1040	28.0	do.	3.1
	1209	31.0	do.	7.0
	1335	31.0	do.	7.4
	1446	32.0	do.	8.6
	1730	30.5	do.	5.6
6	0845	27.0	12,000	0.6
	1035	29.0	do.	3.0
	1206	32.0	do.	4.6
	1330	31.0	do.	8.4
	1452	32.0	do.	10.0
7	0840	28.0	12,000	0.7
	1030	29.5	do.	2.7
	1203	33.0	do.	4.1
	1325	30.0	do.	6.6
	1458	32.0	do.	11.4

NOTE: Sunrise occurred about 0700; sunset about 2000.

Table 6.--Calculated average daily photosynthesis and respiration rates in Crystal River and Cross Bayou

Estuary	Segment	Photosynthesis (mg/L)/d	Respiration (mg/L)/d
Crystal River	1	9.4	11.4
	2	11.8	10.4
	3	4.3	2.7
	4	2.90	1.7
	5	2.5	1.4
	6	1/ 2.0	1/ 1.0
	7	1/ 2.0	1/ 1.0
Cross Bayou	1	42.8	13.8
	2	33.4	13.0
	3	33.2	17.9
	4	32.4	12.4
	5	35.9	13.2
	6	39.5	14.8
	7	44.2	14.1

1/ Estimated.

APPLICATION OF MATHEMATICAL MODEL

The parameters in the model are variables representing the quantitative effect of the various hydrological processes occurring in the estuary. Calibration, the process of choosing applicable model parameters, is necessary before use of the model in sensitivity analyses and simulation can be done. Sensitivity analysis is defined as a procedure in which a perturbation is imposed upon an individual selected model parameter while other model parameters are kept unchanged. The perturbation simulates a variation in the quantitative effect of a natural estuarine process represented, and the model user observes the resultant change in the computed concentrations values.

Calibration of this model is achieved by varying physically realistic estimates of selected parameters in a series of computer runs until computations match the existing field-measured profiles.

Some parameters are known, or measured, or can be computed from measurements by means other than by calibrating a model. On the other hand, some parameters cannot be independently estimated and can only be determined for the time period of data collections by varying them freely within a realistic range in the process of calibrating the model to match computed with observed data. These, then, become the calibration parameters.

Model calibration parameters should be considered unique to the data-collection period unless further testing proves otherwise. If parameters can be shown to be invariant for the system at other periods representing different estuarine conditions, we say the model has been verified for the different conditions. Ideally, several sets of data representing varied estuarine conditions, including "worst-case" conditions, should be obtained and used in model verification prior to simulations for waste-load allocation analysis. Because of time and money constraints, model verification using more than one set of data was not possible during this study.

In lieu of additional data for verification, the most appropriate way to use the estuary model in this study is to calibrate for a particular set of observed conditions, then use the calibrated model for sensitivity analyses for variations in the chosen parameter values for that set of conditions. Sensitivity analysis in this case provides clues as to the probable range of errors to be expected if the model is used for prediction.

The observed conditions used for calibration should resemble as closely as possible the worst-case situation to be analyzed by the model in order to minimize the effect of model parameters changing from their calibrated values as a result of changes in measured parameters. This was the case for the four estuaries analyzed in this study.

Table 7.--Laboratory analysis of sewage treatment plant effluent

[Analysis by U.S. Geological Survey]

Plant	Conductivity (micromhos at 25°C)	Chloride (mg/L)	TKN[1] (mg/L)	BOD 5-day (mg/L)	BOD 20-day (mg/L)	Remarks
City of Crystal River	825	26	9.6	0.4	0.8	
Crystal River Mobile Home Park						Not sampled
Riverside Villas						Not sampled
Springs Village Mobile Home Park						Not sampled
J.G. Coin Laundry						Not sampled
City of New Port Richey	1,260	200	34	21	-	
Gulf Harbor	8,200	2,400	13	5.0	50	
City of Tarpon Springs	5,100	1,400	26	6.0	25	

1/ TKN is the sum of the concentration of ammonia and total organic nitrogen.

Calibration Chloride

Model computations for chloride may be calibrated by using the dispersion coefficient as a calibration parameter. In fact, dispersion is the only unknown parameter influencing the chloride concentration profile in an estuary. It is best to simulate chloride first, as the other calculated concentrations are dependent upon dispersion coefficient as well as other parameters not yet determined.

Because dispersion varies with freshwater flow, initial dispersion values in this study were calculated from the approximate relationship:

$$E = 0.333\ Q^{0.48} \qquad (8)$$

where E is the dispersion coefficient in square miles per day (mi^2/d) and Q is freshwater flow in cubic feet per second (ft^3/sec) (Shindala, Zitta, and Corey, 1973). Initial dispersion values were adjusted by comparing the calculated chloride profile with the observed chloride profile and then changing the dispersion values until calculated and observed chloride profiles agreed. Final calibrated values of the dispersion coefficients for each segment used in this study are listed in table 8.

Assigning dispersion coefficients was difficult, for they represent the influence of a set of complex physical phenomena. Future studies should include tracer studies in order to provide firm measurements of dispersion coefficients.

To test the sensitivity of the dispersion coefficient, simulations were made with E equal to one-half and twice the values used for calibration while other parameters were held equal to their calibration values. The effects on the chloride profiles for each estuary are shown in figures 7-10. The computed chloride profiles are somewhat sensitive to changes in E. A change of 100 percent in the value of E results in a change of up to about 25 percnet in the computer chloride concentration in any one segment.

CBOD and TKN

Model calculations for CBOD may be calibrated by adjusting the CBOD decay-rate coefficient. However, this approach has the disadvantage that the CBOD profile in an estuary may not be especially sensitive to variations in the CBOD decay rates. Furthermore, decay rates as determined in the laboratory are sufficiently accurate measures of CBOD oxidation in the prototype that the range of uncertainty does not allow a wide enough range of variation to simulate the observed CBOD concentrations. This means that a close match of the measured CBOD profiles may not be achievable in this way. Therefore care must be taken to ensure that decay rates are not varied in an unrealistic way. Also,

Table 8.--Parameter values used to calibrate the model.

Name	Segment	Dispersion coefficient E (mi^2/d)	Decay-rate coefficients K_d (d^{-1})	K_r (d^{-1})	K_n (d^{-1})	Photo-synthesis P (mg/L)/d	Respira-tion R (mg/L)/d
Crystal River	1	1.5	0.02	0.02	0.05	15.36	11.36
	2	30.0	.02	.02	.05	16.37	10.37
	3	50.0	.02	.02	.05	5.72	2.72
	4	50.0	.02	.02	.05	2.70	1.70
	5	25.0	.02	.02	.05	4.30	1.39
	6	9.5	.02	.02	.05	2.00	1.00
	7	9.5	.02	.02	.05	2.00	1.00
	100	2.0	.02	.02	.05	2.00	1.00
	101	2.0	.02	.02	.05	1.00	--
Homosassa River	1	15.0	0.04	0.04	0.04	0	0
	2	15.0	.04	.04	.04	0	0
	3	8.0	.04	.04	.04	0	0
	4	8.0	.04	.04	.04	0	0
	5	8.0	.04	.04	.04	0	0
	6	8.0	.04	.04	.04	0	0
	7	8.0	.04	.04	.04	0	0
	200	2.0	.04	.04	.04	0	0
Cross Bayou	1	0.6	0.2	0.2	1.0	13.8	30.0
	2	.6	.2	.2	1.0	13.0	30.0
	3	.6	.2	.2	1.0	17.9	30.0
	4	.6	.2	.2	1.0	12.4	30.0
	5	.2	.2	.2	1.0	13.2	30.0
	6	.6	.2	.2	1.0	14.8	30.0
	7	.6	.2	.2	1.0	14.1	30.0
Anclote River	1	8.0	0.04	0.04	0.04	0	0
	2	8.0	.04	.04	.04	0	0
	3	8.0	.04	.04	.04	0	0
	4	8.0	.04	.04	.04	0	0
	5	8.0	.04	.04	.04	0	0
	6	8.0	.04	.04	.04	0	0
	7	8.0	.04	.04	.04	0	0
	8	4.0	.04	.04	.04	0	0
	9	4.0	.04	.04	.04	0	0
	10	4.0	.04	.04	.04	0	0
	100	2.0	.04	.04	.04	0	0

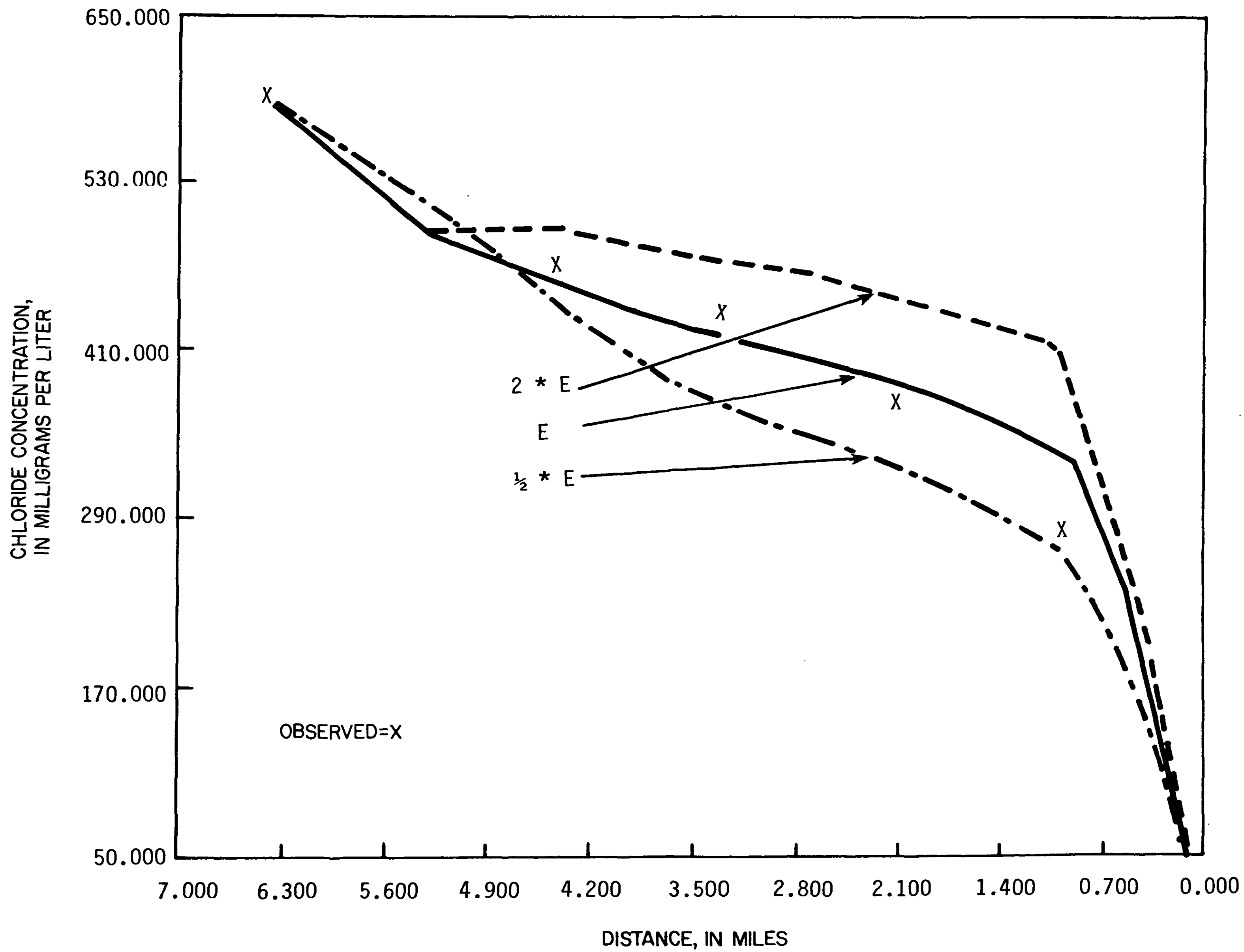


Figure 7.--Effect of changing the dispersion coefficient, E, on the chloride profile of Crystal River.

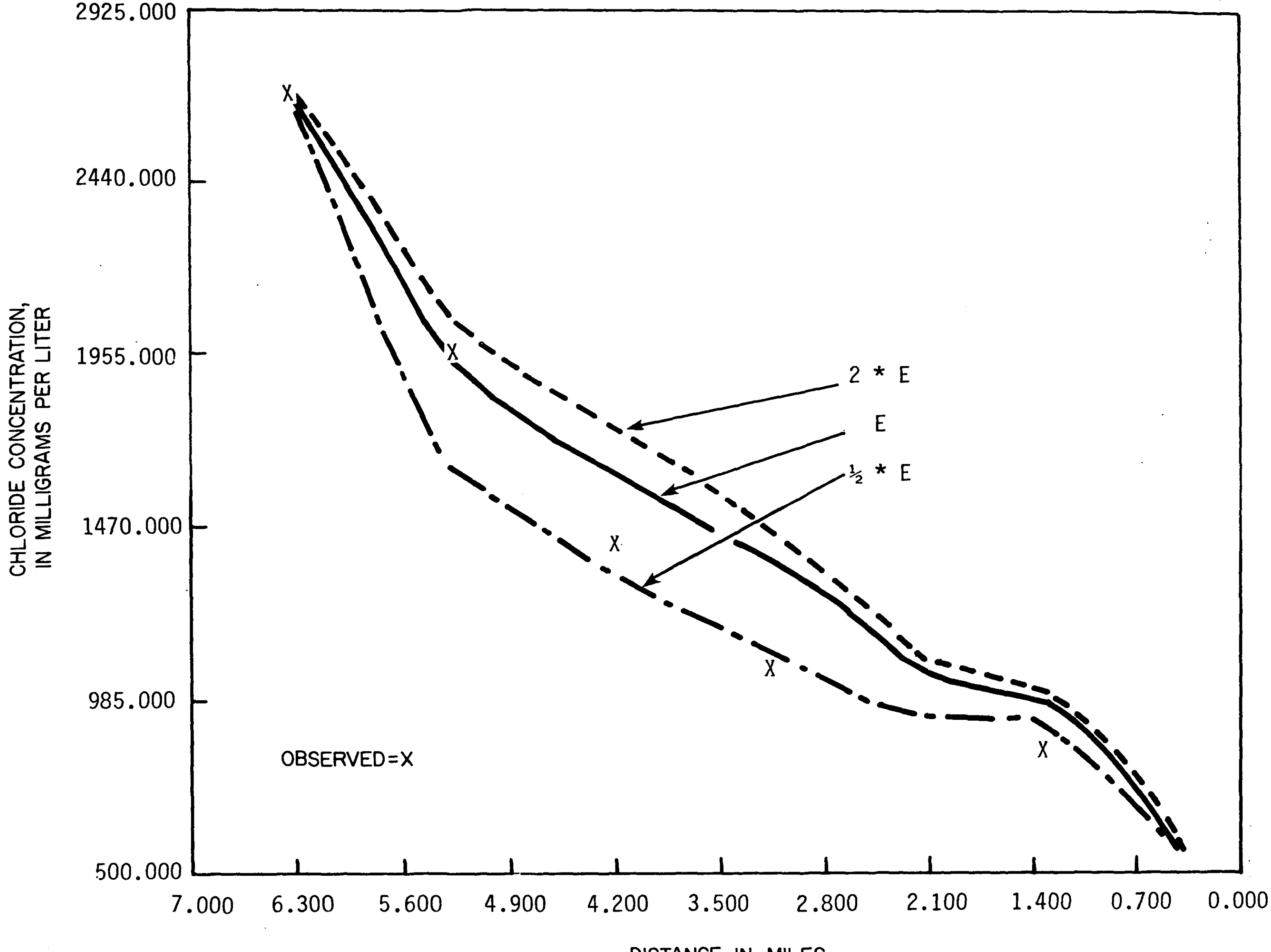


Figure 8.--Effect of changing the dispersion coefficient, E, on the chloride profile of Homosassa River.

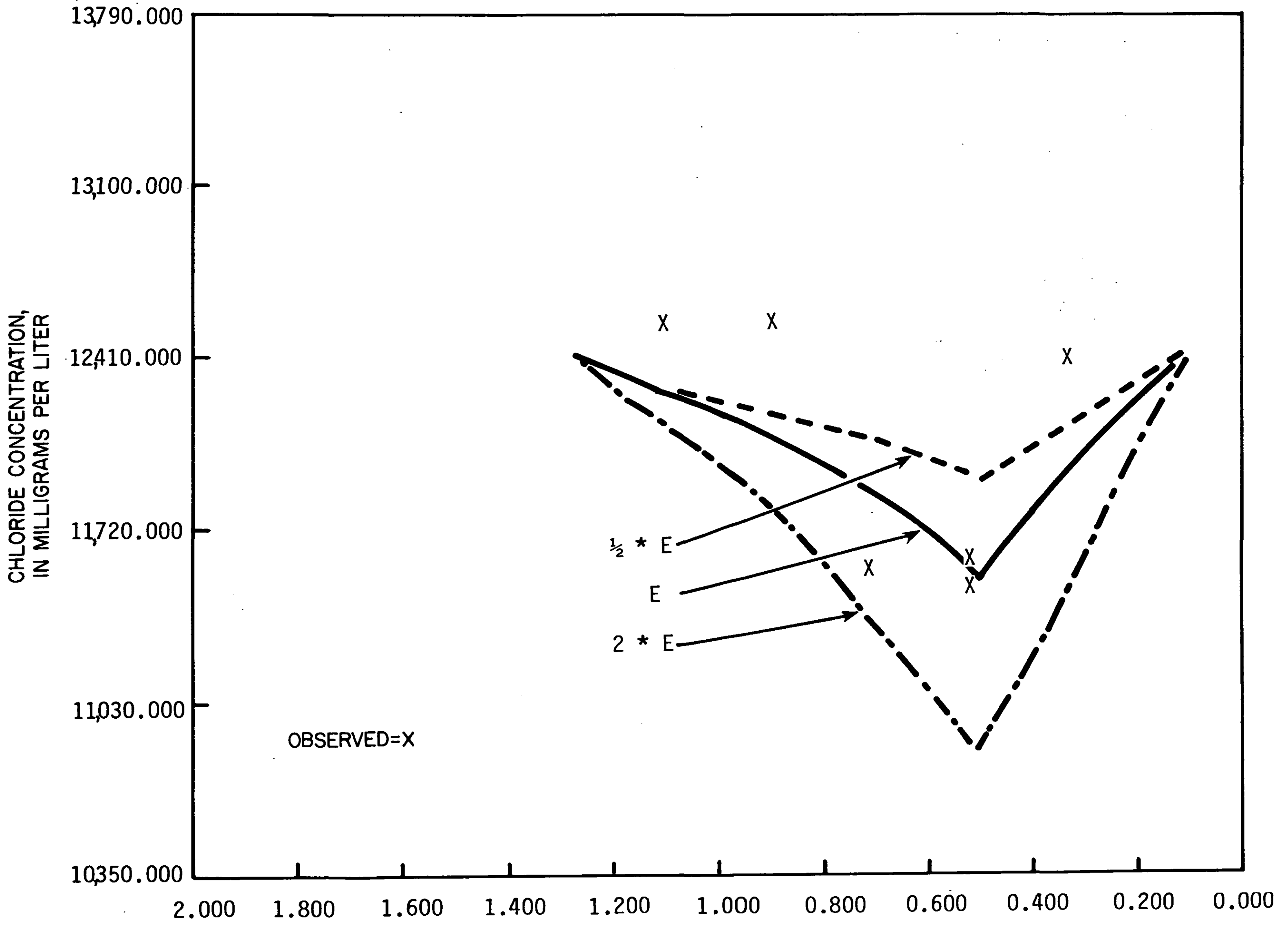


Figure 9.--Effect of changing the dispersion coefficient, E, on the chloride profile of Cross Bayou.

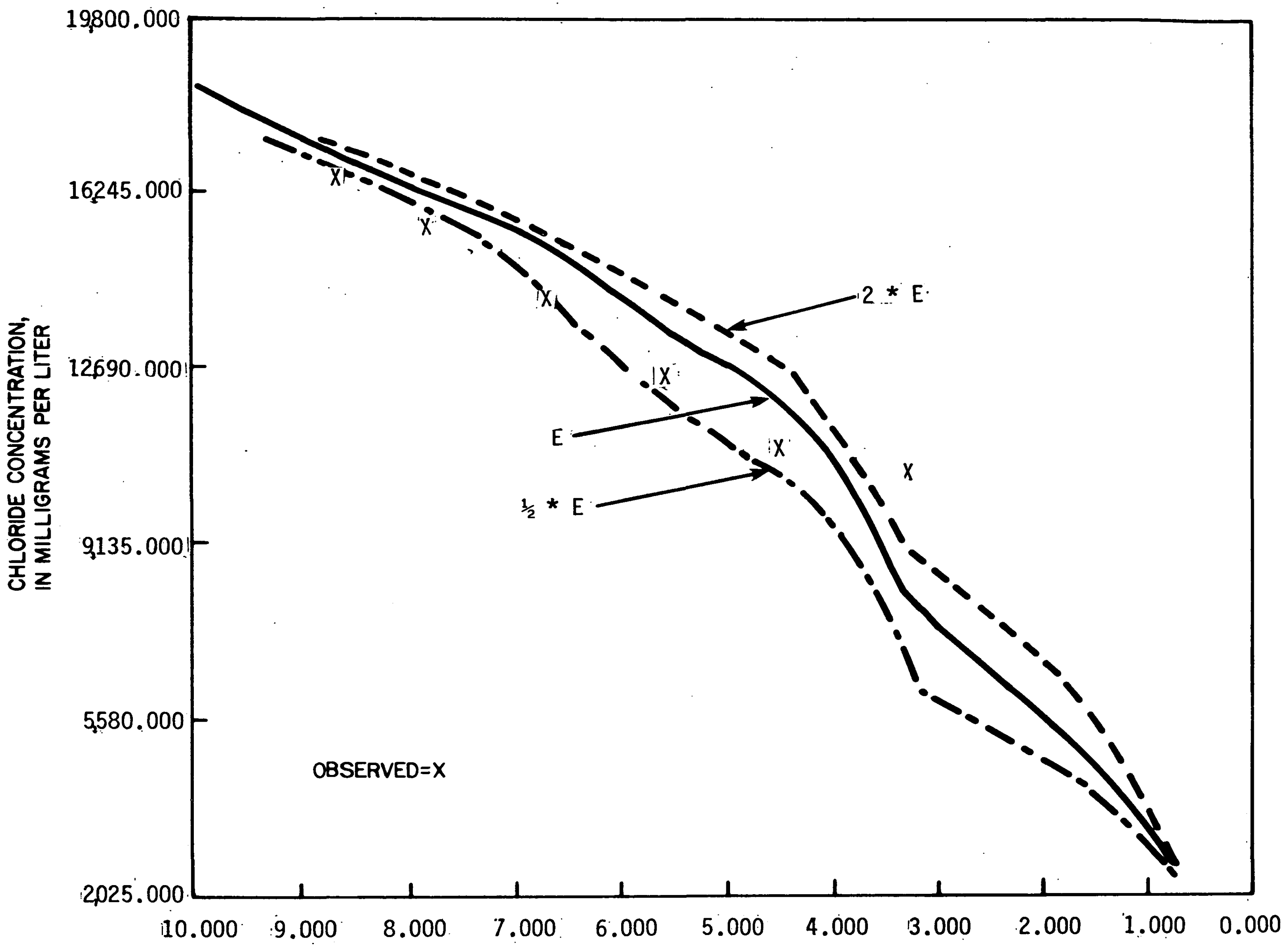


Figure 10.--Effect of changing the dispersion coefficient, E, on the chloride profile of Anclote River.

information on source terms, such naturally occurring non-point CBOD sources, should be accounted for if found to exist.

Model calculations for TKN can be calibrated in the same manner as CBOD.

In this study the decay rates K, K_r, and K_n are temperature-adjusted in the model using field temperature values as supplied to the model. Initial values of K_d and K_r were determined from laboratory analyses for 20-day BOD in the estuary waters. An initial value of K_r was chosen equal to K_d. All values were adjusted to achieve the best possible fit with measured values, but close simulations were not achieved. A summary of the final calibrated decay-rate coefficients used in each estuary is given in table 8.

Sensitivity of the calibrated model to changes in the decay-rate coefficients was studied. For Crystal River and Cross Bayou, the coefficients were changed to one-half and twice the calibration values and to one-fourth and two and one-half times the calibration values for the Homosassa and Anclote Rivers. These changes had virtually no effect on the CBOD and TKN profiles for the Crystal and Homosassa Rivers, and had only minor effects (less than 1.5 percent) on the DO profiles of these estuaries (figs. 11 and 12). The effect of changing the decay-rate coefficients on the Anclote and Cross Bayou estuaries was slightly more pronounced. The maximum deviations of CBOD, DO, and TKN in the Anclote estuary were 6 to 7 percent. In Cross Bayou, the CBOD change was no longer than 10 percent, and the DO and TKN changes were as high as 26 percent. DO profiles are shown in figures 13 and 14 and CBOD profiles in figures 15 and 16, and TKN profiles in figures 17 and 18.

Dissolved Oxygen

Model calculations for dissolved oxygen may be calibrated, following CBOD and TKN calibration, by varying either reaeration rate coefficients or photosynthesis minus respiration (P-R) as a calibration parameter. Reaeration rate coefficient may be estimated by an empirical equation using velocity of flow and temperature. However, the available equations were developed for fast-flowing, well-mixed streams, not tidal water bodies; thus, coefficient values must be considered only approximate.

Photosynthesis and respiration can be directly computed if 24-hour oxygen data are available for all sections where significant amounts of photosynthesis and respiration are occurring and for the same time period as other data collected for the study. Computations were made using a computer program developed by Stephens and Jennings (1976).

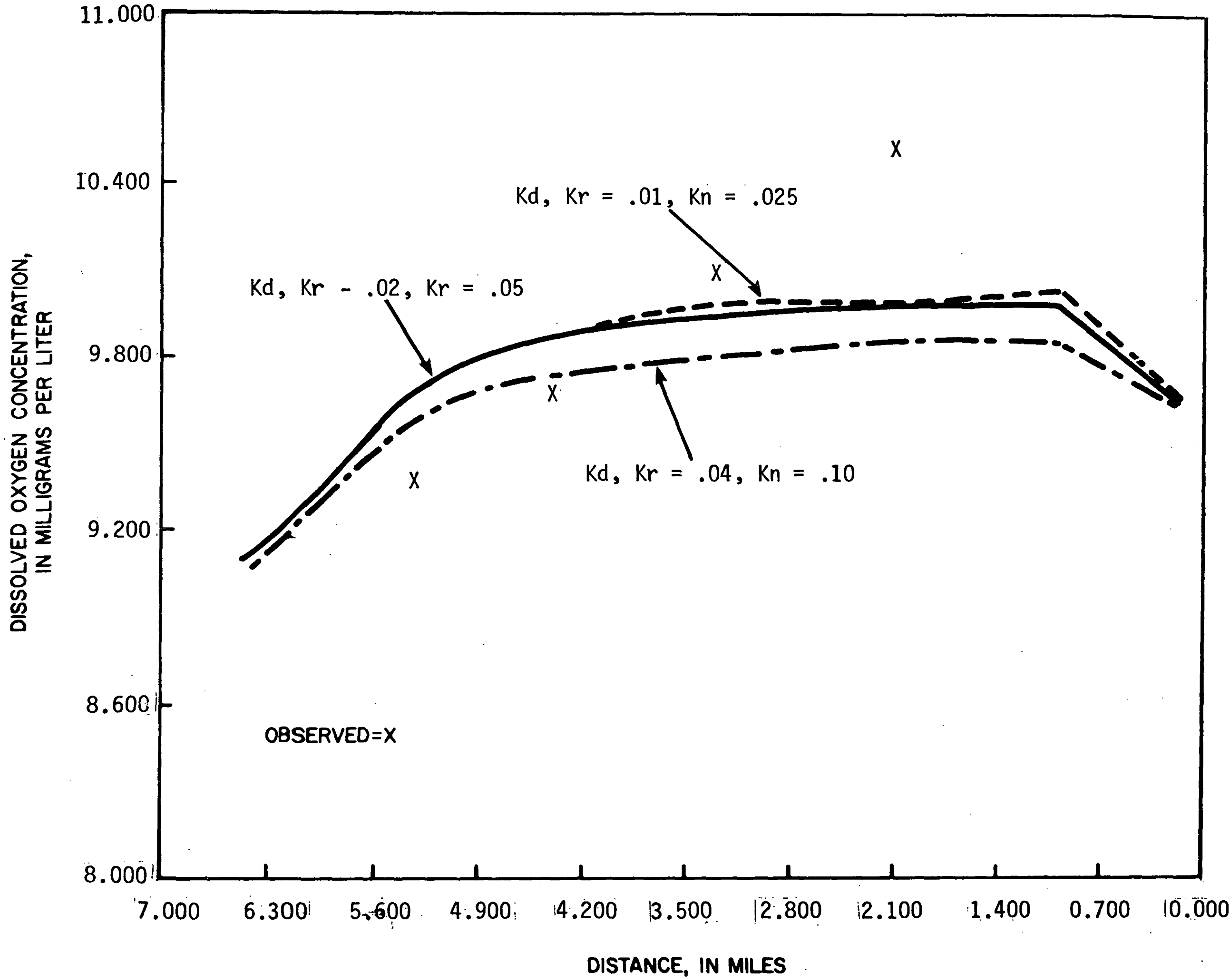


Figure 11.--Effect of changing the decay-rate coefficients Kd, Kr, and Kn on the DO profile of Crystal River.

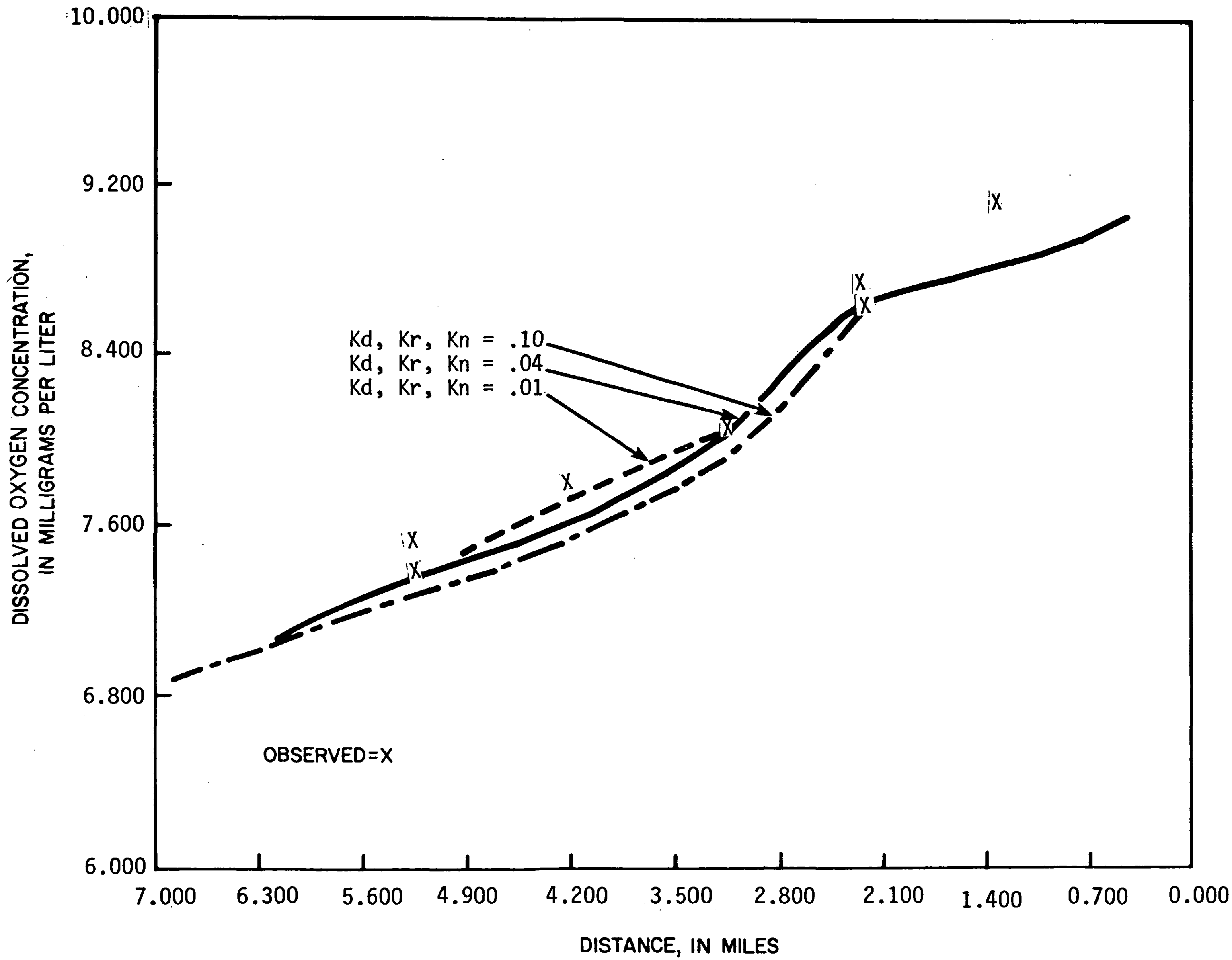


Figure 12.--Effect of changing the decay-rate coefficients Kd, Kr, and Kn on the DO profile of Homosassa River.

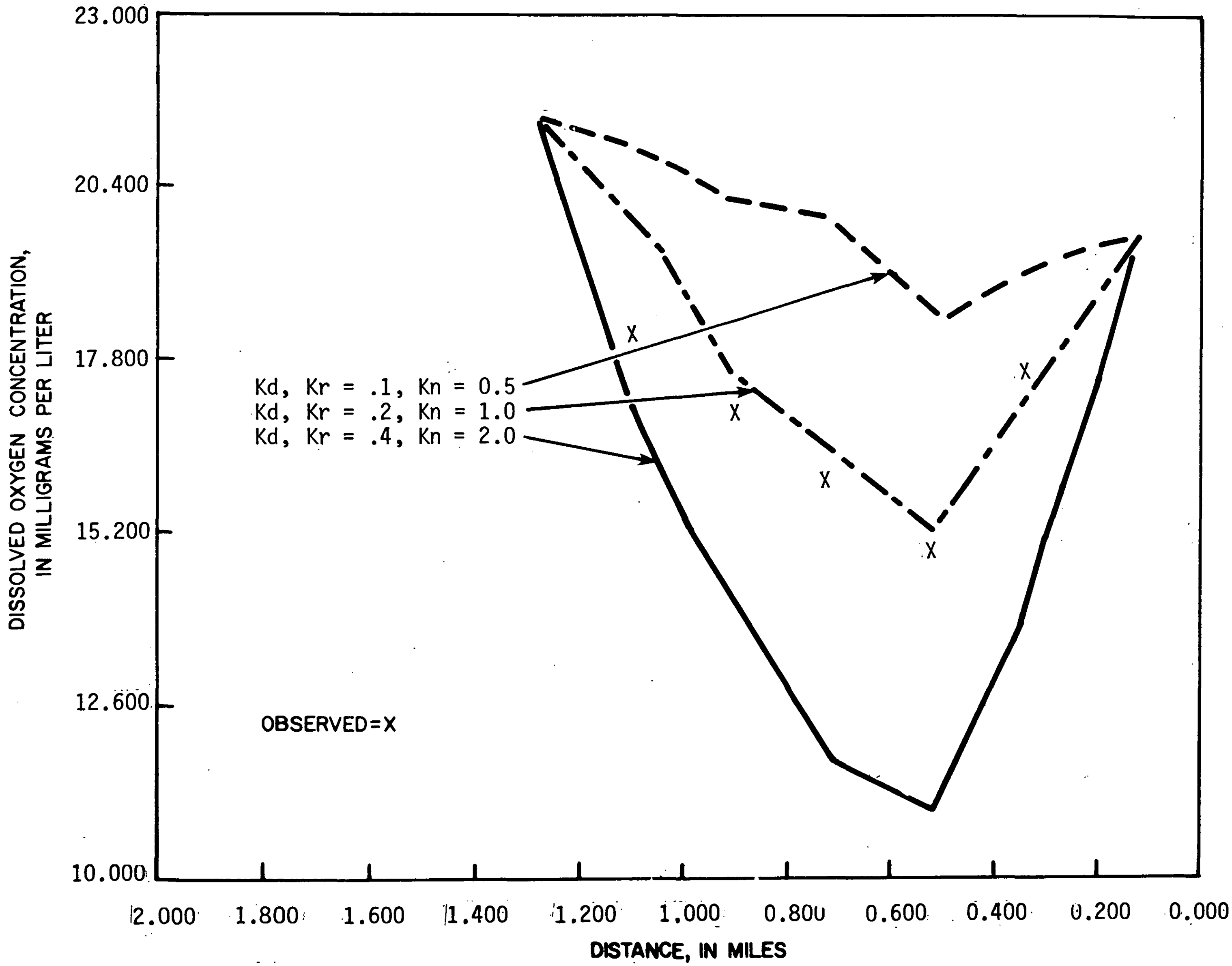


Figure 13.--Effect on changing the decay-rate coefficients Kd, Kr, and Kn on the DO profile of Cross Bayou.

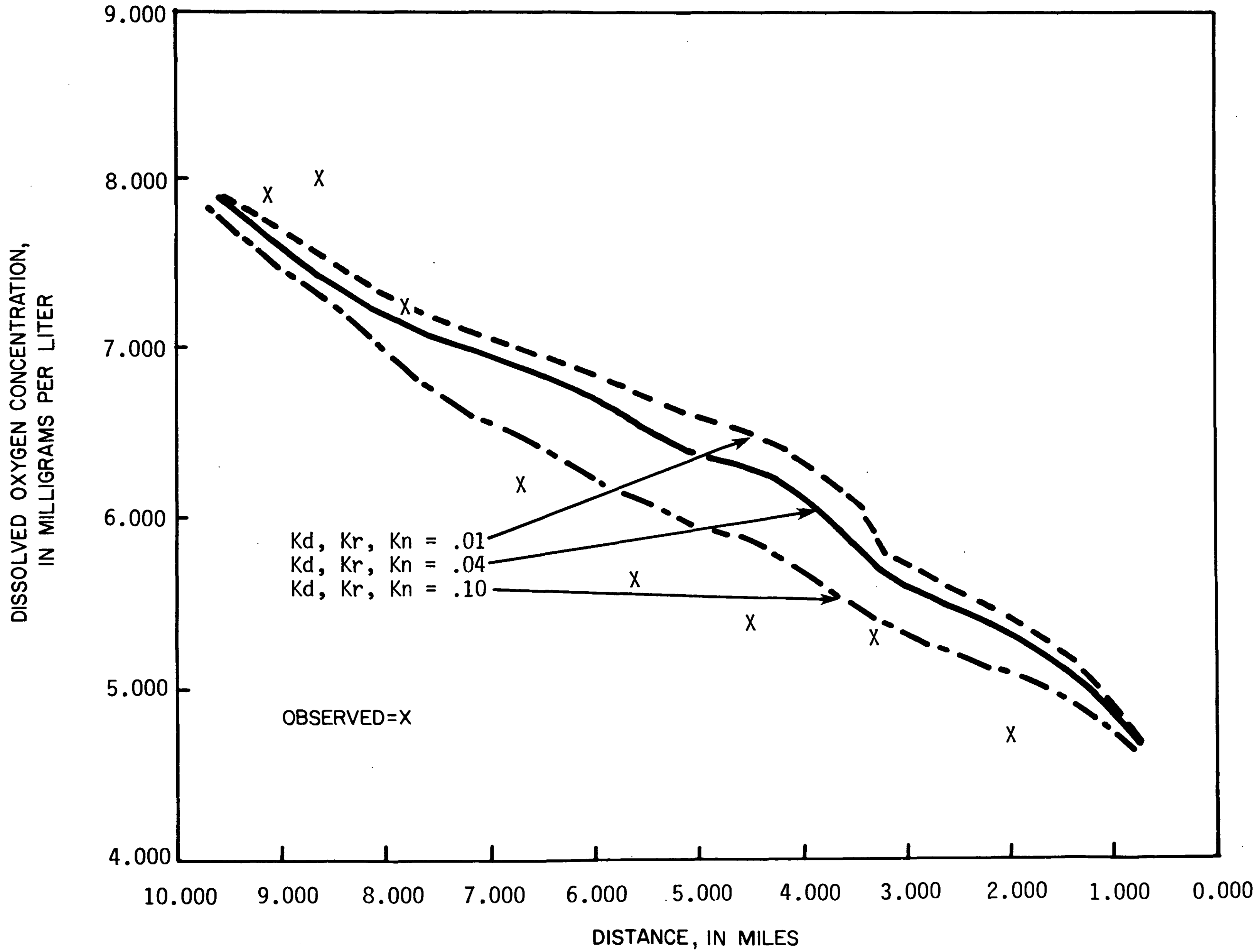


Figure 14.--Effect of changing the decay-rate coefficients Kd, Kr, and Kn on the DO profile of Anclote River.

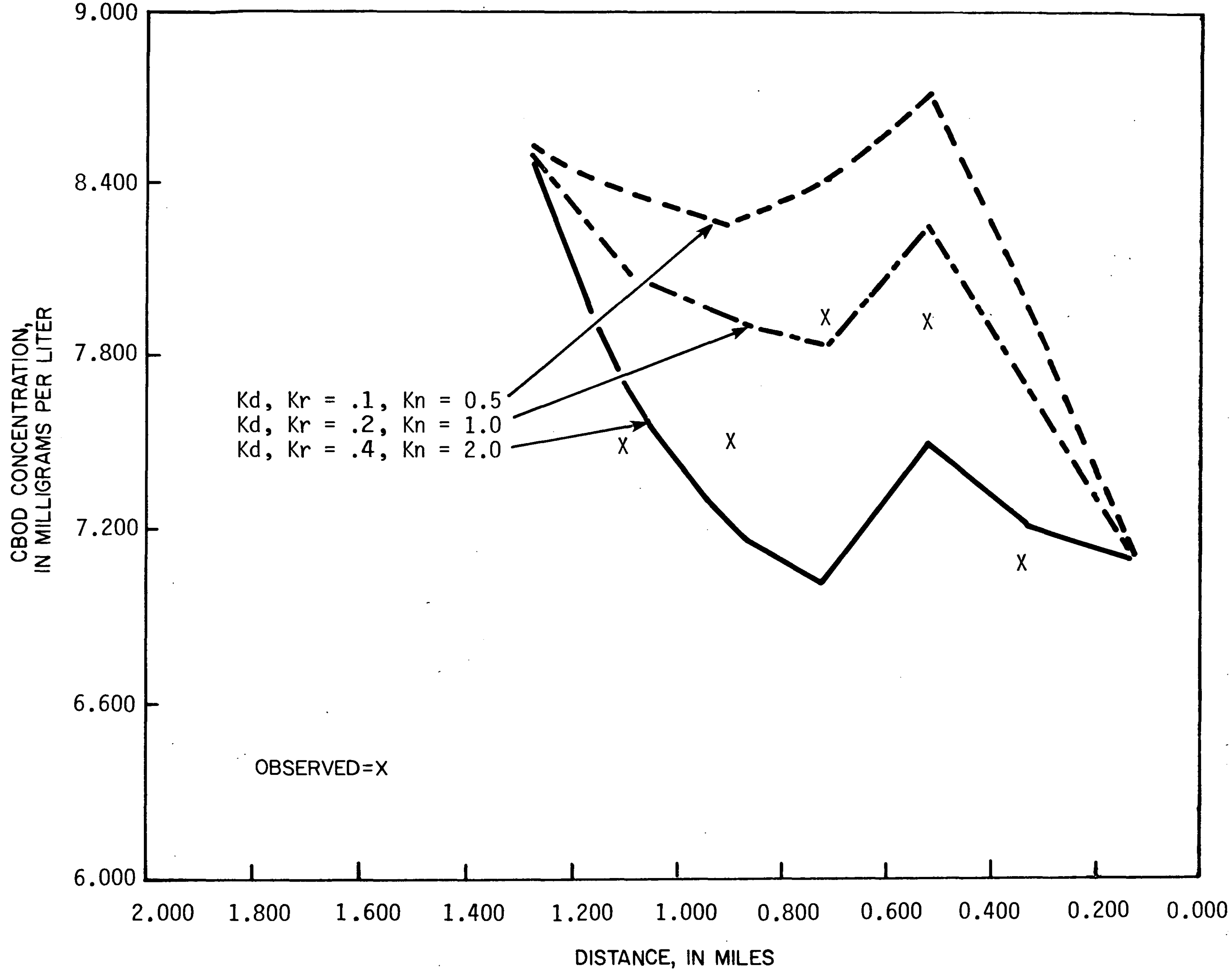


Figure 15.--Effects of changing the decay-rate coefficients Kd, Kr, and Kn on the 5-day BOD profile of Cross Bayou.

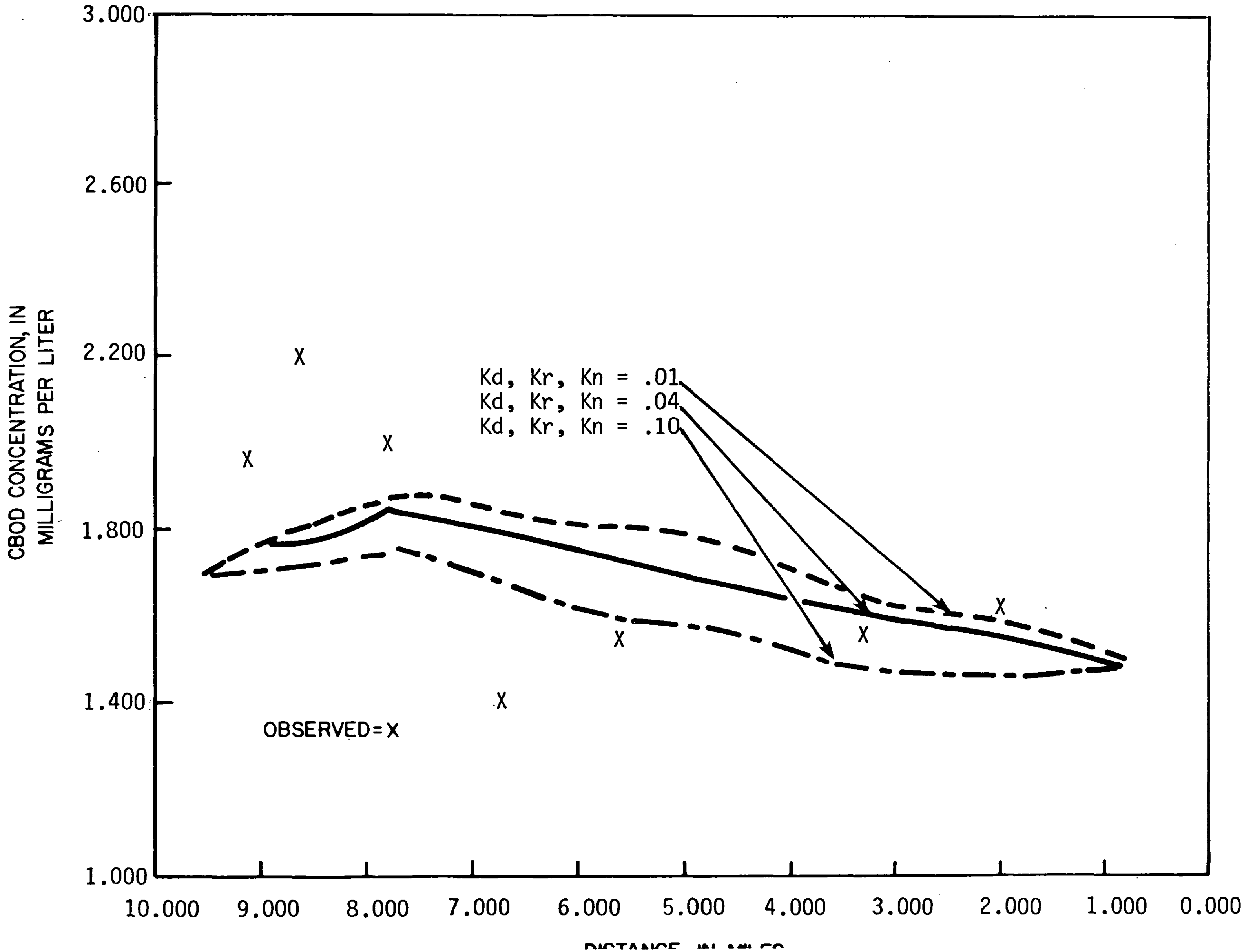


Figure 16.--Effect of changing the decay-rate coefficients Kd, Kr, and Kn on the total nitrogen profile of Cross Bayou.

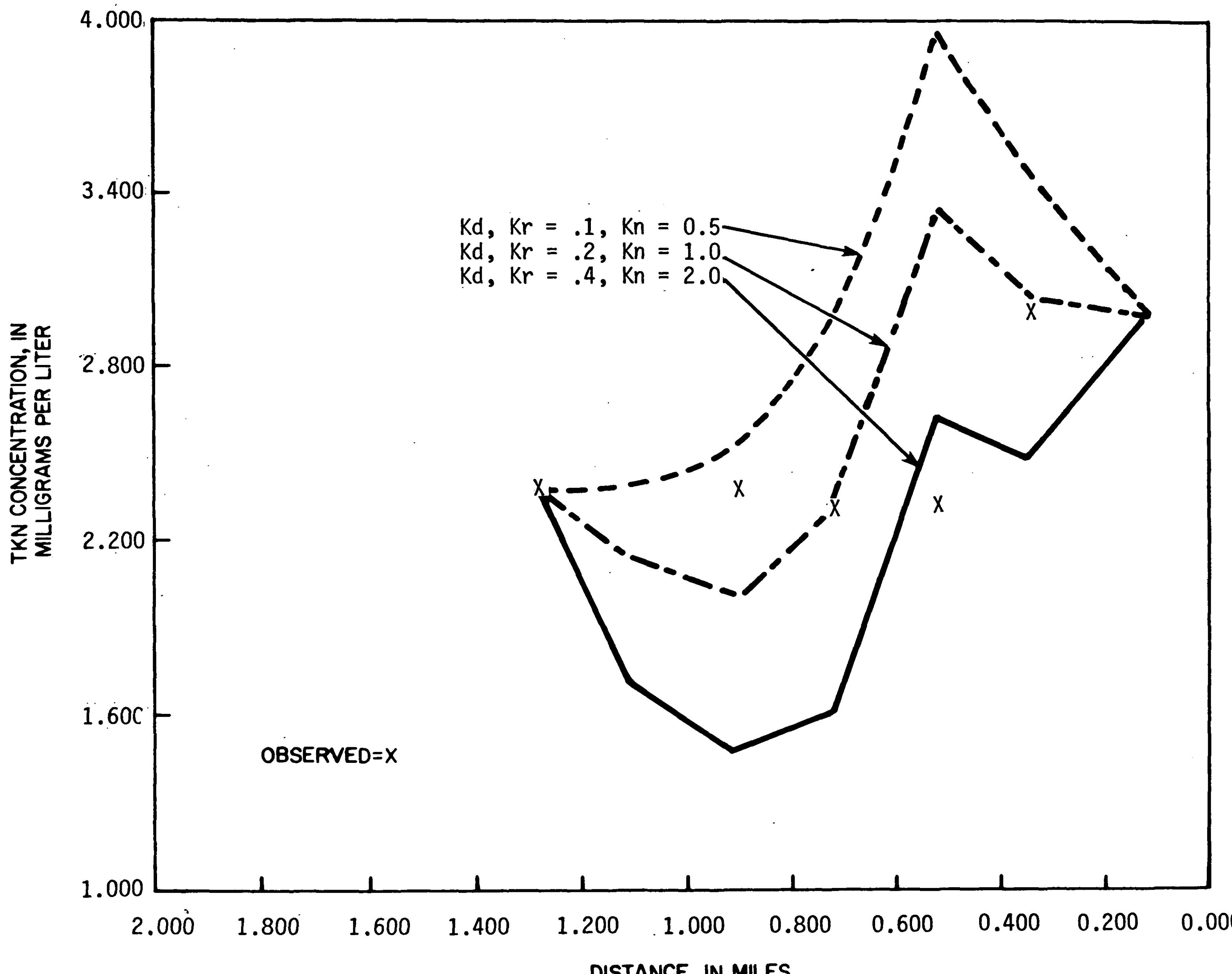


Figure 17.--Effect of changing the decay-rate coefficients Kd, Kr, and Kn on the total nitrogen profile of Cross Bayou.

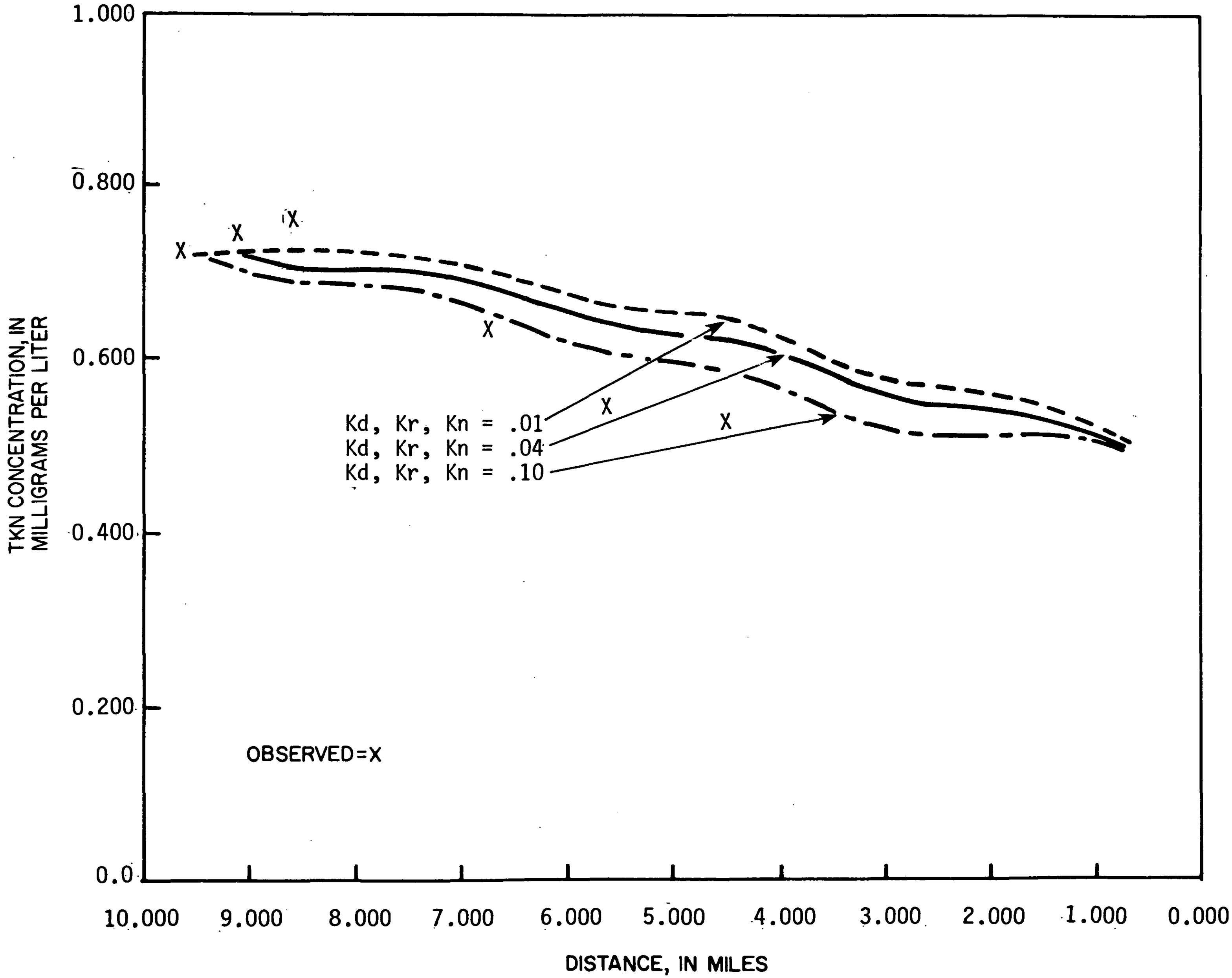


Figure 18.—Effect of changing the decay-rate coefficients Kd, Kr, and Kn on the total nitrogen profile of Anclote River.

Dissolved oxygen data from another time period were available and were used to make an initial estimate of the photosynthesis minus respiration occurring on the day of the collection of the bulk of the field data.

After adjustment of initial values of photosynthesis and respiration, computed values of DO agreed reasonably well with the observed values. The resulting values of photosynthesis and respiration are listed in table 8 for Crystal River and Cross Bayou. Respiration and photosynthesis were found to be about equal in magnitude in the Homosassa and Anclote Rivers and were, therefore, set equal to zero.

Because photosynthesis and respiration can have a significant effect on the DO profiles when the values of the two parameters differ, simulations were made with respiration and photosynthesis equal to each other and results were compared with results of a final calibration run for Crystal River and Cross Bayou where the accepted values were not equal. The DO profiles differ considerably as shown in figures 19 and 20, demonstrating the sensitivity of the model, and of the prototype system, to this parameter.

Weighting Factors

The effect of the weighting factors, which govern the method used in the numerical solution of the model (see Thomann, 1972), was studied. A central difference scheme was selected for use in this study. A sensitivity study was made to determine the effect of a forward difference scheme and a backward difference scheme. All of the schemes resulted in virtually the same numerical solution.

Imposed Stress Conditions

It is often desirable to investigate the effects of waste loads during low-flow conditions. Thus, data should be collected for model calibration during field conditions representative of tidal-averaged low flow, as was the case in this study. The calibration parameters then represent low-flow conditions, and the model user has the option of simulating waste loads in the model generated only by lowering the flow values by a small amount to represent, for example, 10-year, 7-day low flows.

For simulations such as waste-load allocation studies, boundary conditions (pre-specified concentration values at physical and model grid boundaries), for all water-quality variables computed, must be specified. If the hypothetical natural prototype conditions which the model is to be used to simulate, in order to study physical stresses on the system closely resemble the calibration conditions, then calibration period consitiuent values may be effectively used as boundary values

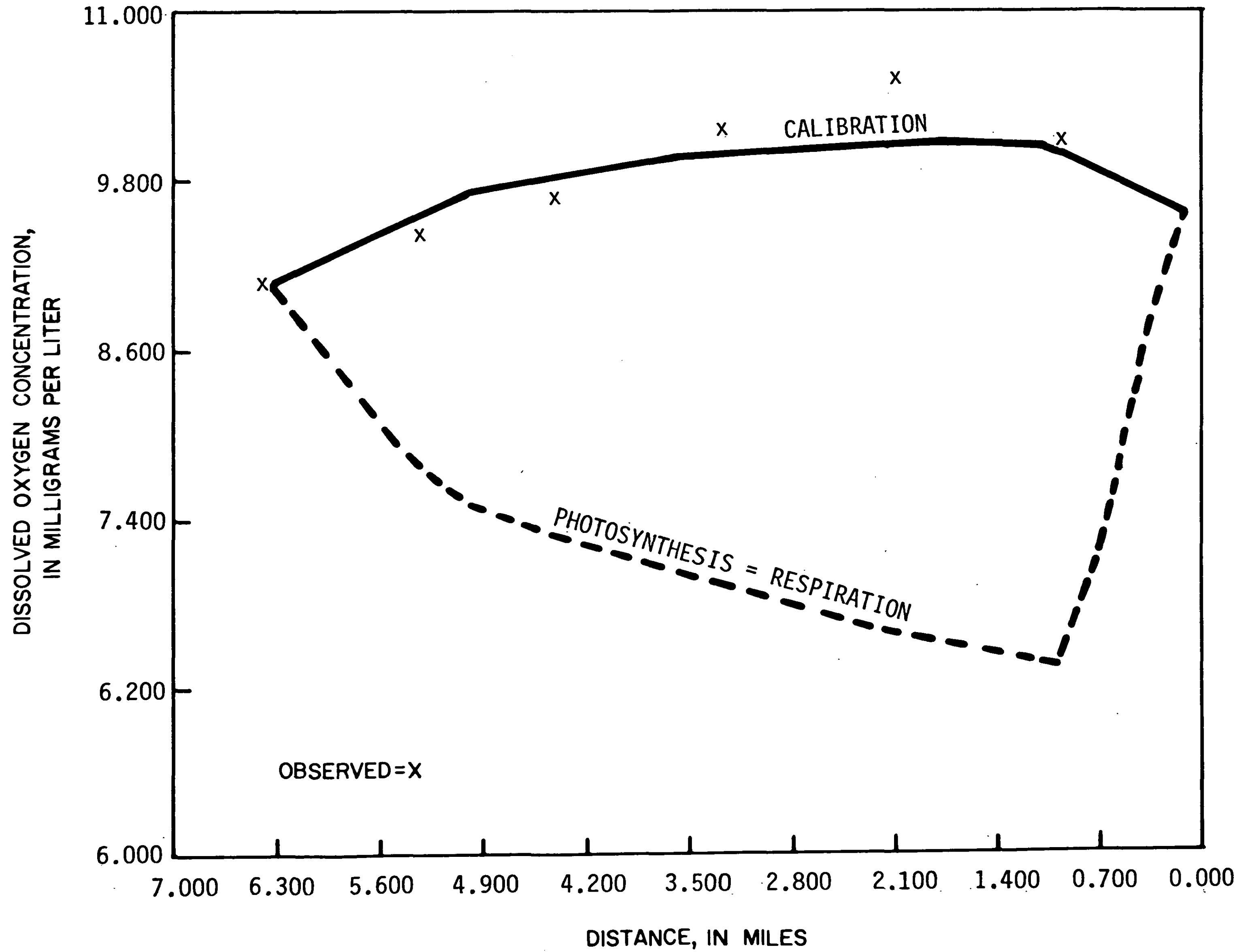


Figure 19.--Effect of changing the amount of photosynthesis occurring in the Crystal River on the DO profile.

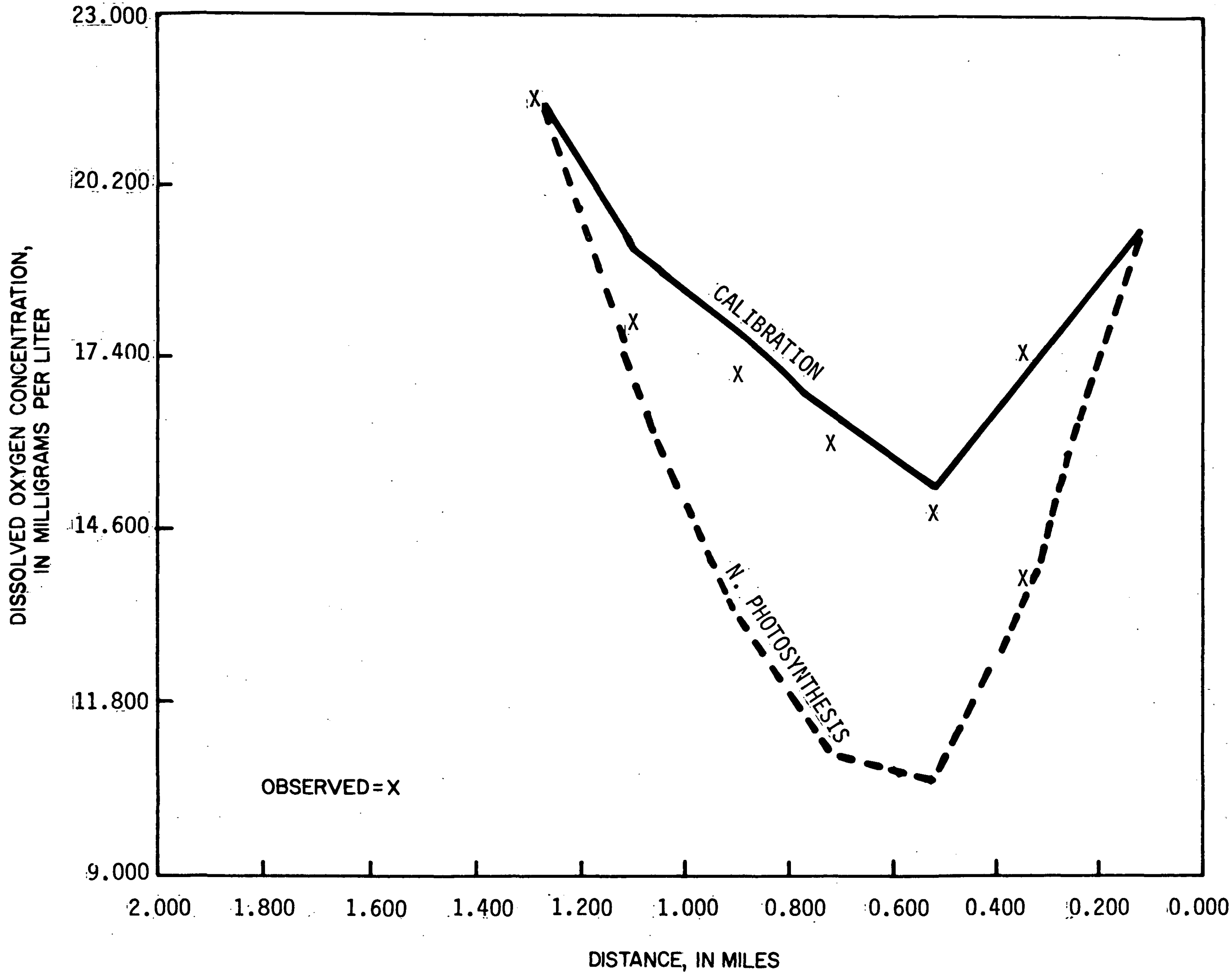


Figure 20.--Effect of changing the amount of photosynthesis occurring in the Cross Bayou Estuary on the DO profile.

under the stress conditions to be simulated. Boundaries should be selected a sufficient distance away from the location within the modeled area of stress so that the boundary values may be expected to remain unchanged by the imposition of the stresses in model operation.

Conclusions and Limitations

The calibration of the model in this study was only roughly accomplished owing to a limited data base. The resultant parameters are therefore, unverified and should be used with caution in model simulations except as initial estimates prior to model verification studies. Additional data collection, as described in the preceding sections, to strengthen model calibration and provide for model verification, is recommended before the model may be used to analyze the effect of stresses upon the system and to generate the type of concrete conclusion which might serve as a basis for management decisions.

Much knowledge and experience concerning how best to apply this model was acquired in this study, and a thorough model evaluation has been done. Because parameter sensitivity analyses can often yield insight into the importance of model parameters on final results, several sensitivity analyses were performed involving model parameters such as dispersion coefficient, decay rates, photosynthesis, and respiration.

It should be re-emphasized that model computations described in this report generate average values of DO for estuarine water bodies, and provide no basis for estimating the magnitude of daily fluctuations about this average. A more complex model, perhaps with non-steady state capability, would be required to produce this type of information.

In conclusion, the feasibility of the use of this mathematical model for estuarine waste allocation studies depends upon the match between model assumptions and actual estuarine conditions, the use of the best methods of calibration, and the support of an intensive and properly designed data collection program. User familiarity with the model and its requirements and limitations is strongly recommended.

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