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RECALIBRATION OF PAGAN RIVER
WATER QUALITY MODEL

by
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A Report to
Smithfield Foods, Inc.

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INTRODUCTION

Two water quality models of the Pagan River were developed in the 1970s by the Virginia Institute of Marine Science. The first model was developed under the CSA (cooperative state agencies) program (Kuo, Lewis and Fang, 1976). It simulated the oxidation of organic matter and the effect that, and reaeration, had on the dissolved oxygen regime of the river. The model included four water quality parameters: salinity, dissolved oxygen, carbonaceous oxygen demand and nitrogenous oxygen demand. A later model, developed as part of the Hampton Roads 208 studies, was an expansion of the first one. It included the nitrogen and phosphorus cycles, algal dynamics, and fecal coliform bacteria. It was calibrated and verified with field data collected in the summer of 1976 (Rosenbaum, Kuo and Neilson, 1977). Both models have been used by the Virginia Water Control Board in the establishment of permit limits for point source discharges to the river.

Since the model study, the two major point source dischargers, the Smithfield Packing and Gwaltney, have improved their waste treatment facilities. As a result, it is expected that the river water quality condition should be significantly different from that in 1976, with which the model was last calibrated. Recent surveys (Guy and Davis, 1986 and 1987) indicated that the combined CBOD (carbonaceous oxygen demand) loadings from the two major discharges have decreased by an order of magnitude, from nearly 5000 lb/day in 1976 to about 500 lb/day in 1986. The nitrogen and phosphorus loadings remained roughly the same, however, more than two-thirds of nitrogen was discharged in oxidized form, i.e., nitrate. In 1976, almost 100% of nitrogen was discharged in unoxidized form. The surveys also showed that the sediment oxygen demand in the upper reach of the river had decreased significantly in response to the decrease in carbon loadings. In the section of the river upstream from the Smithfield Packing outfall, the SOD decreased from 3.8 $gm/m^2/day$ in 1976 to 1.9 $gm/m^2/day$ in 1985. Near the mouth of the river, the SOD remained relatively constant around 1.9 $gm/m^2/day$. In view of these changes, it is imperative to recalibrate the water quality model if it is to be used as a tool for assessing the waste assimilation capacity of the river. This report describes the recalibration of the model using the data collected by Smithfield Foods, Inc. (SFI) in the summers of 1985 and 1986 (Guy and Davis, 1986 and 1987; hereafter referred to as the Report).

I. Period of Model Simulation

Smithfield Foods, Inc. conducted 7 and 8 slackwater surveys in 1985 and 1986 respectively. Salinity, temperature and pH were measured. Water samples were collected in each survey at 13 sampling stations along the river. The samples were analyzed for dissolved oxygen, BOD, TKN, ammonia nitrogen, nitrite nitrogen, nitrate nitrogen and chlorophyll. However, not all parameters were determined at all stations in every survey. The Report provides the data and a full description of the surveys. Figures 1 and 2 show the dates of slackwater surveys, and the basin total daily discharges from July to September of 1985 and 1986, respectively.

To calibrate the water quality model, a period of time preceeding one slackwater survey should be chosen for model simulation. The period should be longer than the flushing time of the river system so that the water quality conditions at the end of simulation are independent of those at the beginning. The freshwater flows into the river during this period should be low since the model is to be used for waste load allocations under low flow conditions. Furthermore, there should be no significant surface runoff within the drainage basin during the simulation period. Otherwise, the river water quality conditions will be dominated by nonpoint sources, which have not been quantified in the Report.

The 1985 data sets are not adequate for model calibration because of their deficiency in the monitoring of the phytoplankton population. Photosynthesis plays an important role in the dissolved oxygen regime of the Pagan River. The 1985 surveys monitored chlorophyll 'a' at only three stations, all of them were located downriver of Smithfield Packing's outfall. Both the historical data and data of 1986 show that majority of phytoplankton population resided upriver from Smithfield Packing's outfall. Without chlorophyll 'a' data in this reach of the river, no calibration of phytoplankton-related coefficients may be made.

The flushing study conducted using the model as calibrated in 1976 (Appendix B of the Report) shows that under low flow conditions (about 3 cfs at the upstream end), it takes about 20 days to flush out 90% of materials introduced into the river. Thus, a model simulation of 20 days would be appropriate for calibrating the model. Figure 2 shows that the two periods proceeding August 6 and September 24 are suitable for model calibration. There was one month of low flow preceeding August 6, even though a small runoff event occurred around July 26. There was no runoff event for at least 20 days preceeding September 24 even though the flow was not low in the early part of the month.

The attempt to simulate the period preceeding August 6, 1986 was abandoned because of inconsistency of the August 6 data set (pages A-5 and A-30 of the Report). The data showed little chlorophyll 'a' (3.3 μg/l at mile 4.0 and 0.5 μg/l at mile 3.0) in the lower half of the river, however, the dissolved oxygen was super-saturated there. The model can not reproduce these conditions without excessive reaeration. The wind data of August 6 and the preceeding days did not justify any additional reaeration. Therefore, the period preceeding September 24, was chosen for model simulation.

Ideally, the calibration should be conducted by using the observation collected in the September 12 or August 25 slackwater survey as initial conditions in a model simulation of the period from September 12 or August 25 to September 24. Unfortunately, there was a big runoff event (Fig. 2) from August 26 to 30, the model simulations starting August 25 would be complicated by non-point source contributions. If the model simulation starts on September 12, then the simulation period would be shorter than the flushing time of the river (about 20 days), and the model predictions on September 24 would significantly depend on the initial conditions. A compromise was made by starting model simulation on September 3, halfway between August 25 and September 12. This allowed model simulation of 21 days during which time the freshwater discharge decreased monotonically. For initial conditions, the concentrations of water quality parameters at the beginning of model simulation were specified using the average values of the slackwater surveys of August 25 and September 12 (pages A-6, A-7, A-31 and A-32 of the Report). The model was run to simulate the period from September 3 to 24. Model predictions for the last two tidal cycles were then compared with the slackwater survey data collected on the same day. In successive model runs, calibration parameters were adjusted until agreement was achieved between the model prediction and the data.

II. Data Conversion

All of the water quality data used for model calibration are presented in the report by Guy and Davis. To allow comparison between the data and the model results, several of the parameters reported by the laboratory must be converted to a more useable form. The formulae used in these conversions are described below.

1. TKN to organic nitrogen, NI

As analyzed by the laboratory, total Kjeldahl nitrogen includes ammonia nitrogen, dissolved and detrital organic nitrogen, and the nitrogenous portion of the algal biomass. To obtain organic nitrogen, as utilized by the model, the ammonia and algal fractions must be subtracted from the TKN via the following relationship:

N1 = TKN ammonia nitrogen - a_n * Ch

where Ch is the chlorophyll 'a' concentration in μg/l and a_n is the nitrogen to chlorophyll ratio, calibrated to be 0.005 mg of nitrogen per μg chlorophyll 'a'. For the samples for point source effluents, no adjustments for algal biomass were made.

2. BOD_5 to CBOD

The majority of the BOD analyses are five-day biochemical oxygen demand (BOD_5). These must be scaled-up to ultimate carbonaceous biochemical oxygen demand (CBOD) and corrected for the respiration and decay of algae entrapped in the BOD bottle. The long-term BOD analyses with nitrification inhibition may be used to establish the relationship between ultimate and five-day CBOD. Figures 3 and 4, reproduced from the Report, represent two typical results of long-term BOD analyses with nitrification inhibition. The data in Fig. 3 follow closely the first order decay curves (with decay rate of

0.1/day), however those in Fig. 4 do not. If it is restricted to the data with incubation periods less than or equal to 30 days, a good fit of the data in Fig. 4 to the first order decay curves may still be achieved. Fig. 4a presents the least square fit of the data. It shows that a second stage decay becomes effective after 30 days of incubation. It was pointed out in the Report (pages 37 and 40) the possibility of nitrogenous BOD becoming effective in a very long-term BOD study. Therefore, it was decided that 30-day CBOD, instead of 60-day CBOD, was a closer representative of CBOD. It should be noted (see Fig. 3) that there is very little change in CBOD values between 30 days and 60 days.

If CBOD follows the first order decay with a constant decay rate, the ratio $CBOD/CBOD_5$ should be a constant for all long-term BOD analyses. Figure 5 presents this ratio for all long-term BOD analyses with nitrification inhibition. The ratios range from 1.7 to 5.3, however, 70% of them fall within the range of 2.0 to 3.0. The mean and median values are 2.91 and 2.60 respectively. To minimize the weight of a few outliers with high ratio, the median value was chosen to convert $CBOD_5$ to CBOD.

Incorporating the adjustment for algal biomass, the following formula may be used for conversion,

$$CBOD = 2.60 * CBOD_5 - 2.67 * a_c * Ch$$

where a_c is carbon to chlorophyll ratio, calibrated to be 0.025 mg carbon per µg chlorophyll 'a'. However, all of the five-day BOD analyses of the 1985 and 1986 surveys were performed without nitrification inhibition. Therefore, BOD_5, instead of $CBOD_5$, was used for the above formula. The BOD_5 values include $CBOD_5$ and that portion of nitrogenous BOD which exerts its demand within the first five days of sample incubation. For the samples from point-source effluents it is expected that BOD_5 may approximate $CBOD_5$. For river water samples, there is no definite relationship between the two except that BOD_5 is greater than or equal to $CBOD_5$, and the difference increases with concentration of unoxidized nitrogen.

III. Preparation of Input Data Set

To conduct the simulation, the model requires data on ambient conditions and external inputs to the system, and evaluation of a number of constants and coefficients. The manner in which these are obtained and the values employed are as significant as the achievement of calibration itself. Therefore, the model inputs and coefficients are presented before the calibration results.

1. Freshwater discharge

Daily discharges from 3 to 24 September 1986 at Wrenn's Mill Pond (page D-26 of the Report) were used as model input at the most upstream segment of the model. The lateral inflows from tributaries and overland flow were computed internally by the model assuming the flow is proportional to drainage area. The total basin flows computed by the model were seven times those at the most upstream segment. This ratio agrees well with the data presented on page D-26 of the Report. The freshwater discharges at Wrenn's Mill Pond decreased from 5.6 cfs on September 3 to 1.6 cfs on September 24.

2. Solar radiation

Solar radiation was measured by VIMS at Gloucester Point, Virginia. Daily values were input to the model. They ranged from 240 to 570 langleys/day during the period of simulation.

3. Water temperature

Water temperature decreased from 25°C to 23°C during the period of simulation. The model assumed a constant temperature of 23.7°C throughout the period. The value is the average water temperature on September 24 (page A-8 of the Report).

4. Downstream boundary conditions

Ideally, the concentrations of water quality parameters at the mouth of the river should be specified as boundary conditions for each day of the simulation period. In reality, no such data exist. The conditions at the boundary are dominated by the James River and are relatively insensitive to the conditions in the Pagan River. Since the James is a much larger water body, the water quality conditions there should vary within a narrow range over the low flow simulation period. For the purpose of model calibration with respect to September 24 slackwater survey data, the boundary conditions were specified with constant values estimated from those data collected at the most downstream station (Table I).

TABLE 1. Downstream boundary and freshwater inflow concentrations used in the model calibration simulation

Parameter mg/l except as noted	Downstream Boundary	Freshwater Inflow
Salinity (ppt)	17.5	0.1
Organic Nitrogen	0.60	1.2
Ammonia - N	0.30	0.01
Nitrite + Nitrate-N	0.10	0.01
Organic Phosphorus	0.11	1.2
Inorganic Phosphorus	0.027	0.045
Chlorophyll 'a' (μg/l)	10.0	80 (100*)
CBOD	3.0	12.0
DO	8.5	6.3 (10.6*)

* The value used for 1977 model calibration.

5. Upstream boundary conditions and nonpoint source input

Upstream boundary conditions are not specified for the model. Only the amount and quality of the fresh water flowing into the most upstream segment is specified. The freshwater inflow to all segments is assumed to have the same quality as that flowing into the most upstream segment.

Since the model simulated a period of relatively low freshwater discharge, the contribution from nonpoint sources was less significant. The base conditions and nonpoint sources were input to the model through the specification of the concentrations of freshwater flows (Table 1). The values used for previous model calibration (Rosenbaum, Kuo and Neilson, 1977) were used for all parameters except for DO and chlorophyll which were adjusted to reflect the monitored conditions on September 24, 1986.

6. Point source inputs

Three point source discharges were included in the model simulation. They are Town of Smithfield, Smithfield Packing, and Gwaltney. The values of point source discharges were calculated from the data reported on September 12 and 24 (page I-21 of the Report) except for the phosphorus loadings. The phosphorus loadings were derived from HRSD nutrient removal study conducted in 1987. Since the algal growth was not phosphorus limited, the phosphorus loadings had no impact on other water quality parameters. The model assumed the point source discharges to be constant from September 3 to September 17, using the values reported on September 12. Then the discharges were changed to the values reported on September 24 for the remainder of the simulation period. The loadings are presented in Table 2.

TABLE 2. Point source discharges

Loading Rate (lb/day except as noted)	Town of Smithfield	Smithfield Packing	Gwaltney
Flow (mgd)	0.45/0.45 *	1.23/1.29	1.29/1.48
Organic Nitrogen	5.6/5.3	24/63	17/12
Ammonia Nitrogen	0.0/2.8	72/260	6.5/28
Nitrite + Nitrate-N	97/52	783/155	1244/694
Organic Phosphorus	1.0/1.0	8.0/8.0	6.0/6.0
Inorganic Phosphorus	5.1/5.1	386/386	241/241
CBOD	52/.20	279/352	141/137
DO (mg/1)	7.5/7.5	6.2/6.4	6.3/6.4

* The first number is for September 3 to 17, the second number is for September 18 to 24.

7. Sediment oxygen demand

An SOD study was conducted by VIMS in 1985 and 1986. Field data indicated that the spatial distribution of sediment oxygen demand in the Pagan River was roughly uniform and that the mean was 1.9 $gm/m^2/day$ at 20^oC. This value was used for all segments of the model.

IV. Calibration Procedures

The model was run to simulate the river water quality conditions from September 3 to September 24 of 1986. The predicted conditions on the last day of simulation were compared with slackwater survey data of September 24. The average, maximum and minimum concentrations on that day have been plotted as functions of distance from the river mouth. The slackwater survey data are also presented on the plots for comparison (Figs. 6 to 14).

The two semi-empirical constants in the formulation of dispersion coefficient were first adjusted to achieve model calibration with respect to physical transport processes in the river. The constants were adjusted until the predicted salinity distribution agreed with field data. This was a relatively easy and quick process, since theoretical analysis (Wilber and Kuo, 1987) had defined the values of these coefficients within a narrow range. The next stage was to adjust the kinematic coefficients of the water quality model to achieve the calibration with respect to biochemical processes. The first step of the tedious trial and error process was to reproduce the observed chlorophyll 'a' and dissolved oxygen distributions. Then a series of fine tuning runs was made to adjust rate constants which have minor influence on chlorophyll 'a' concentrations. The values of kinetic coefficients employed in the model calibration are listed in Table 3.

V. **Results and Discussion**

The results of model calibration are presented in Figs. 6 to 14. Since the phosphorus species were not measured in the 1985 and 1986 surveys, no field data are available for comparison with model results in Figs. 13 and 14.

The excellent agreement between the field data and the model results on salinity distribution indicates that the model simulates the physical transport processes very well. In the calibration with respect to biochemical processes, the agreement of DO distribution was emphasized since DO is the primary water quality standard. Fig. 7 presents the DO distribution along the river. Again, agreement between field observations and model simulation is good.

Fig. 8 shows that the model reproduces the concentration levels and spatial trend of the chlorophyll distribution, however, it predicts a spatial gradient much weaker than that shown in the field data. Since chlorophyll distribution is usually patchy and fluctuates widely over a diurnal cycle, the samples collected at one instant of time (slackwater) can only represent an order of magnitude. A wide error or confidence band should be placed on the field data and close agreement between model results and field data cannot be expected. Ideally, the chlorophyll concentration should be measured around the clock at each station for the purpose of model calibration.

TABLE 3. Calibration Values of Kinetic Coefficients

Coefficient	Present Calibration	1977 Calibration (if different)
Phytoplankton-Related		
a_c, carbon to chlorophyll ratio	0.025	
a_n, nitrogen to chlorophyll ratio	0.005	
a_p, phosphorus to chlorophyll ratio	0.0005	
PQ, photosynthesis quotient	1.4	
RQ, respiration ratio	1.0	
K_{mn}, half saturation concentration for inorganic nitrogen, mg/1	0.025	
K_{mp}, half saturation concentration for inorganic phosphorus, mg/1	.001	0.005
k_{gr}, base growth rate at 20°C, 1/day	2.0	
a, respiration rate at 20°C, 1/day	0.07	0.10
k_g, grazing rate, 1/day	0.2	0.5
k_{cs}, settling rate, ft/sec	1.0	0.0
I_s, optimum light intensity, langleys/day	250	
Nitrogen-Related		
k_{n11}, settling rate, 1/day	0.0	0.05
k_{n12}, hydrolysis rate, 1/day/°C	0.003	0.0005-0.016
k_{n23}, nitrification rate, 1/day/°C	0.005	0.005-0.025

k_{n33}, denitrification rate	0.05	
Phosphorus-Related		
k_{p11}, settling rate, 1/day	0.0	
k_{p12}, organic to inorganic phosphorus conversion rate, 1/day/°C	0.003	
k_{p22}, settling rate, 1/day	0.2	
CBOD-Related		
k_s, settling rate, 1/day	0.0	
k_1, decay rate 1/day at 20°C	0.05	0.12

Figure 9 indicates that the model under predicts CBOD at the upstream end of the river. The problem of data conversion from BOD_5 to CBOD may, at least partially, be responsible for the discrepancy. As discussed in Section II-2, the values of calculated CBOD data are likely to be higher than actual CBOD and, furthermore, the amount of the overestimate is particularly high in the upriver segments where the nitrogenous oxygen demands are high. The concentrations of organic and ammonia nitrogen in this reach of the river suggest that the CBOD concentration may be over estimated by as much as 10 mg/l.

The model predicts a general increasing trend in the upriver direction for organic nitrogen (Fig. 10). This trend is in agreement with the data sets from most of the slackwater surveys. The September 24 survey data have organic nitrogen concentrations much higher than those predicted by the model in the reach of the river between miles 5 and 7. Examination of other slackwater survey data reveals, however, that the existence of peak concentration in this reach of the river is more an exception than a norm.

Both the distributions of ammonia nitrogen and nitrate nitrogen are dominated by point sources (Figs 11 and 12). The agreement between the ammonia nitrogen data and model prediction is quite good; however, the model over predicts nitrate nitrogen concentration. This is due to the unusually large discharges of nitrate nitrogen from point sources computed from data reported on September 12. According to page I-21 of the Report, Smithfield Packing and Gwaltney had a combined discharge of 2027 pounds per day of nitrate nitrogen over the 3-day period from September 10 to 12. The combined discharge reported for the other periods ranged from 400 to 800 pounds per day.

The large discharge of nitrate nitrogen from September 10 to 12 was reflected in the slackwater survey data of September 12 (page A-32 of the

Report), for which the nitrate nitrogen was analyzed by Reed Laboratory. The nitrate nitrogen for September 24 were analyzed by SFI. Inspection of all 1986 data reveals that, when nitrate nitrogen was analyzed by both SFI and Reed Laboratory, the values reported by SFI were much smaller than those reported by Reed Laboratory. A linear regression analysis was attempted to correlate the two sets of nitrate nitrogen data, however, no statistically significant correlation may be obtained. Therefore, instead of adjusting September 24 data (analyzed by SFI), the September 12 data (analyzed by Reed Laboratory) are also presented in Fig. 12 for comparison.

VI. Conclusion

The model of water quality in the Pagan River has been recalibrated to 1986 conditions. The predictions for salinity agree well with field observations giving confidence that the model accurately simulates the physical transport processes at work in the river.

The model also successfully reproduces water quality conditions. The complex interactions occurring and the nature of the available data (e.g. lack of phosphorus data) suggest that this calibration is less quantitative than that for physical processes and somewhat qualitative. The calibration efforts have emphasized the dissolved oxygen distribution because oxygen is a primary indicator of water quality. The distribution of dissolved oxygen is affected by both the oxidation of organic matter discharged to the river and the input of oxygen as a byproduct of photosynthesis. The general trends for organic components, specifically CBOD and organic nitrogen, are accurately portrayed although the predicted values for the downstream reaches are in better agreement than those for upper reaches of the river. Similarly, the general trend for algal biomass, as represented by chlorophyll 'a', is captured but predictions in upriver segments differ somewhat from observations.

In conclusion, we believe that the existing water quality model successfully reproduces present (1986) water quality conditions in the Pagan river and that this re-calibration is essentially equal to that achieved in the mid-1970's.

VII. Sensitivity Analyses

Sensitivity analysis is the process in which the effect on model predictions of alterations in calibration coefficients or input parameters are examined. The analyses herein are based on the September 1986 calibration simulation. In successive model runs, a calibration parameter is altered and the resulting predictions are compared to the base conditions. The sensitivity analyses are directed toward examining those factors which enhance or limit the algal production and/or dissolved oxygen concentration in the river. Parameters towards which the sensitivity of the model is tested include:

algal growth rate
algal carbon-chlorophyll ratio
sediment oxygen demand
CBOD decay rate
ammonia nitrification rates
downstream boundary conditions
chlorophyll and DO concentrations in the freshwater inflow.
nonpoint source inputs

1. Algal growth rate

The model employs a base algal growth rate which is varied in a deterministic manner as a function of temperature and the availability of light and nutrients. The sensitivity of model results to the evaluation of base rate and to natural fluctuations about the base is examined in a pair of runs in which the algal growth rate is altered by plus or minus 20%. The effects on predicted chlorophyll concentrations are presented in Fig. 15. It can be seen that the 20% alterations in base growth rate produce a maximum 24 µg/l alteration in predicted daily average chlorophyll. The most significant implication of this test is that small natural fluctuations in the base growth rate can produce algal population which diverge widely from the model predictions.

It is also illustrative to examine the effects of alterations in algal population on several water quality parameters. Organic nitrogen predictions from the growth rate sensitivity tests are also shown in Fig. 15. It can be seen that the 24 µg/l change in the chlorophyll concentration produces less than 0.25 mg/l change in organic nitrogen. The same alteration in chlorophyll produces approximately 2.5 mg/l change in CBOD.

The most significant effect is on dissolved oxygen (Fig. 15). The 24 µg/l change in chlorophyll results in a maximum 3.5 mg/l change in daily-average dissolved oxygen. Thus, the DO predictions are also sensitive to algal growth rate. Some departure of observations from predictions can be expected due to the natural variability of the base growth rate.

2. Algal carbon-chlorophyll ratio

The algal carbon-chlorophyll ratio employed , a_c = 0.025 mg-carbon/µg chlorophyll 'a', is selected largely on the basis of calibration. To test the sensitivity of the model to the evaluation of this parameter, a model run with a_c = 0.05 was performed. The selection of a_c did not affect the chlorophyll prediction but rather influenced dissolved oxygen and CBOD. The results of the sensitivity test for these two constituents are presented in Fig. 16. It can be seen that the change of a_c produces a maximum change of more than 4.0 mg/l in dissolved oxygen and approximately 5.0 mg/l change in CBOD. Thus, the evaluation of a_c is seen to be an important factor in the prediction of dissolved oxygen in the system.

3. Sediment Oxygen Demand

Sediment oxygen demand (SOD) is variable and difficult to measure. A value of 0.5 to 1.5 gm/m^2/day is typical for a unpolluted estuarine bottom. The Pagan River had SOD values ranging from 1.6 to 3.8 gm/m^2/day when surveys were conducted for 1977 model calibration. The measurements made in 1985 had relatively uniform values with a mean of 1.9 gm/m^2/day throughout the length of the river. A uniform value of 1.9 gm/m^2/day is used for the present model calibration. Sensitivity to this SOD is tested in two model runs. One with uniform value of 1.0 gm/m^2/day, and the other with value of 3.8 gm/m^2/day upriver of mile 6.0 and 1.9 gm/m^2/day downriver.

The alteration of SOD values has effect only on dissolved oxygen concentrations. Results are shown in Fig. 17. It can be seen that the use of the value of SOD, 1.0 gm/m^2/day, produces an approximately 2.5 mg/l increase in daily average dissolved oxygen. If the 1970's SOD value is used, the dissolved oxygen is seen to reduce by 5.0 mg/l. Therefore, SOD plays an important role in DO concentration and attention should be devoted to evaluating its magnitude and effects of natural variability.

4. **CBOD decay rate**

The CBOD decay rate is obtained through calibration of model results to observations. The calibrated value of 0.05/day at 20°C is near the lower limit of literature values. The sensitivity of the model to the decay rate is tested in model runs in which the decay rates 0.1 and 0.15 are used. The effects on CBOD and DO are shown in Fig. 18. The increases in decay rate produce maximum decreases of 3.5 and 5.0 mg/l in predicted CBOD. Daily dissolved oxygen predictions decrease by 1.1 and 1.5 mg/l for the two sensitivity runs.

5. **Ammonia nitrification rate**

As with CBOD decay rate, the nitrification rate of 0.003/day/°C is obtained through calibration of model results to observations. The sensitivity of the model to the nitrification rate is tested in sensitivity runs in which the rates of 0.001 and 0.01/day/°C are used. The effects on model predictions are shown in Fig. 19. It can be seen that the three-fold change in the nitrification rate produces only slight changes in the predicted dissolved oxygen concentrations. The effects on ammonia nitrogen and nitrate & nitrite nitrogen are more pronounced.

6. Downstream boundary conditions

As discussed in Section III-4, the concentrations of water quality constituents at the river mouth are specified such that the calibrated model predictions will agree with field observations at the most downstream station. The sensitivity of the model predictions to these specified values at the downstream boundary are tested in 4 sets of model runs in which the boundary conditions of DO, chlorophyll 'a', CBOD and organic nitrogen are lowered and highered respectively. The results are shown in Figs. 20 to 23. It is apparent that the effects of downstream boundary conditions are limited to the lower few kilometers of the river. Thus it may be concluded that the specification of boundary conditions is not crucial to model predictions.

7. Chlorophyll and DO concentrations in the freshwater flow

The concentrations of water quality constituents in the freshwater inflow are required as input data for each model run. The values used for the calibration run are presented in Table 1. These values are adopted from the model study of 1977, except for the chlorophyll and DO concentrations. Present model calibration sets DO= 6.3 mg/l, and chlorophyll = 80 μg/l, while the 1977 calibration set DO = 10.6 mg/l and chlorophyll = 100 μg/l. The sensitivity of the model results to these two variables is tested in a model run in which the 1977s values are used. The results are presented in Fig. 24. They show that, except for the very upstream segments, the predicted DO and chlorophyll concentrations have no significant difference between the two cases. The lack of sensitivity is due to the fact that the flow rate of freshwater inflow is negligible compared to the volume and tidal prism in the river.

8. Nonpoint source inputs

The nonpoint source inputs are highly transient and difficult to quantify. The bulk of them discharge into the river with surface runoff as a result of precipitation. A dry period with decreasing river flow was chosen for model calibration such that the nonpoint source contribution may be minimized. Two model runs were conducted to test the sensitivity of model predictions to nonpoint source inputs. In the first test, the model is run for 21 days as in the calibration run. Then nonpoint sources are input to the model for one day and the model is run for another 10 days. The nonpoint sources are the results of the 'typical storm' which was used for water quality planning in the Hampton Roads 208 program. The model predictions at 5 and 10 days after the storm are compared with calibration results in Fig. 25. In the second sensitivity test, the average nonpoint source loadings of the summer season are input to the model as a constant source. The model is run with the same conditions as the calibration run except for the addition of nonpoint source loads. The results are presented in Fig. 26. Both sensitivity tests result in similar response. As expected, the nonpoint sources have their most pronounced effects in the upper reach of the river where the river volume is small and tidal flushing is weak. Both dissolved oxygen and chlorophyll 'a' are suppressed by the nonpoint source runoff. The effect on nitrite-nitrate nitrogen is opposite to that on organic and ammonia nitrogens. This is because of the difference between the relative magnitudes of nonpoint source to point source. Most of the point source nitrogen is nitrate, while nitrate nitrogen comprises the smallest portion of nonpoint source nitrogen. The dilution effect of the runoff is greater than the increase due to nitrate nitrogen contributions, thus runoff reduces the concentration of nitrite-nitrate nitrogen in most of the river. Figs. 25a and 26a indicate that nonpoint source loadings could raise the organic nitrogen concentration around river mile 6 to a level of 1.5 to 2.0 mg/l. This is of the same level as the field data in Fig. 10. Therefore, the nonpoint source contribution (i.e., event of August 26 to 30) may account for the discrepancy between field data and calibrated model results (Fig. 10).

REFERENCES

Guy and Davis. 1986. Stream survey report of the Pagan River, summer 1985. A Report to Smithfield Foods, Inc., Guy and Davis, Consulting Engineers, Richmond, VA.

Guy and Davis. 1987. Stream survey report of the Pagan River, summer 1986. a Report to Smithfield Foods.,Inc., Guy and Davis, Consulting Engineers, Richmond, VA.

Kuo, A. Y., J. K. Lewis and C. S. Fang. 1976. Mathematical model studies of water quality of the Pagan Estuary. SRAMSOE 107, VIMS.

Rosenbaum, A., A. Y. Kuo and B. J. Neilson. 1977. Water quality model of the Pagan river. SRAMSOE 148, VIMS.

Wilber, A. and A. Y. Kuo. 1987. Longitudinal dispersion in partially-mixed estuaries. In R. M. Ragan (ed.) Proceedings of the 1987 National Conference on Hydraulic Engineering, ASCE, New York. 499-504.

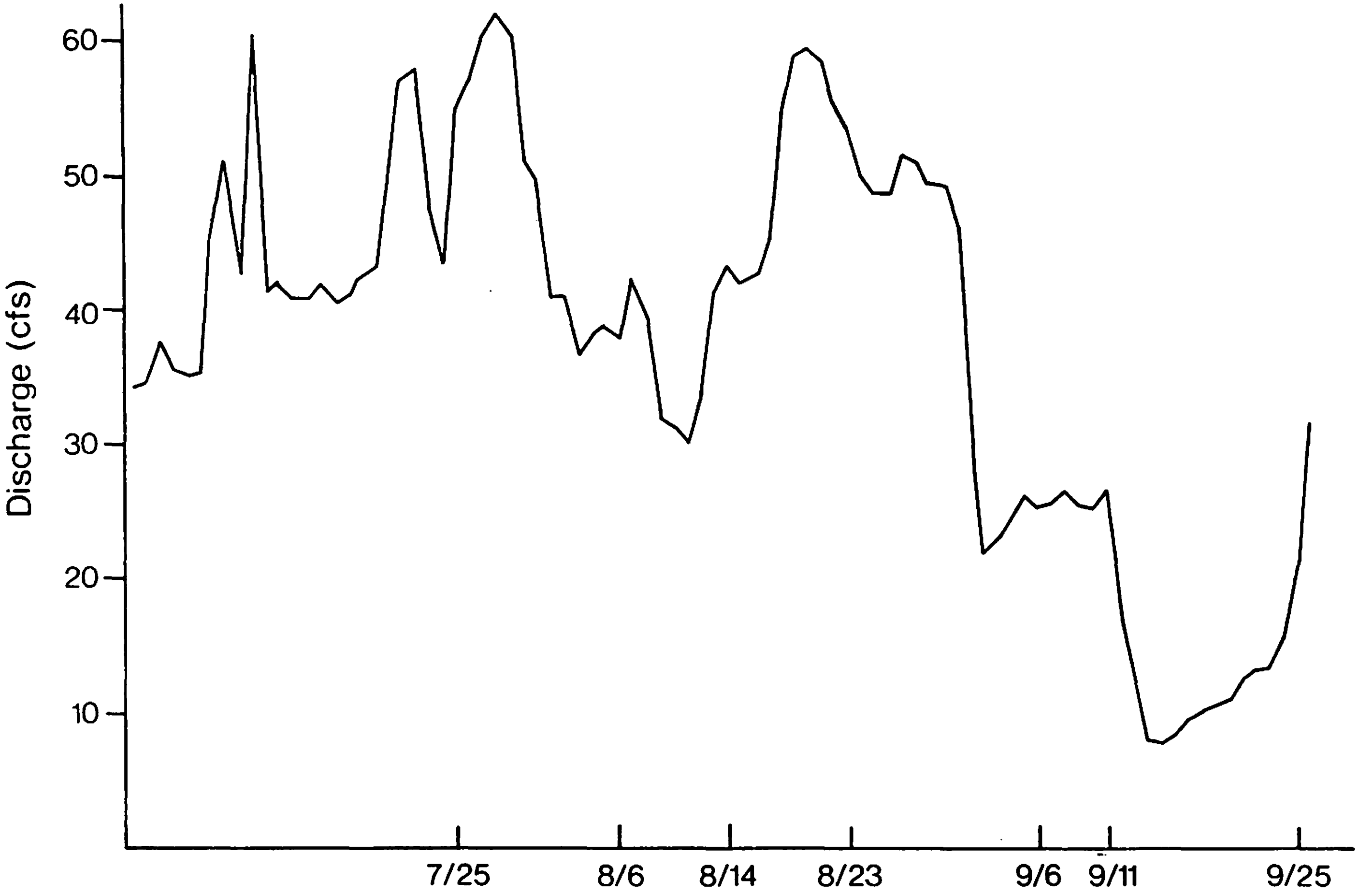


Fig. 1. Basin total discharge, July - September 1985. The dates indicate slackwater survey dates.

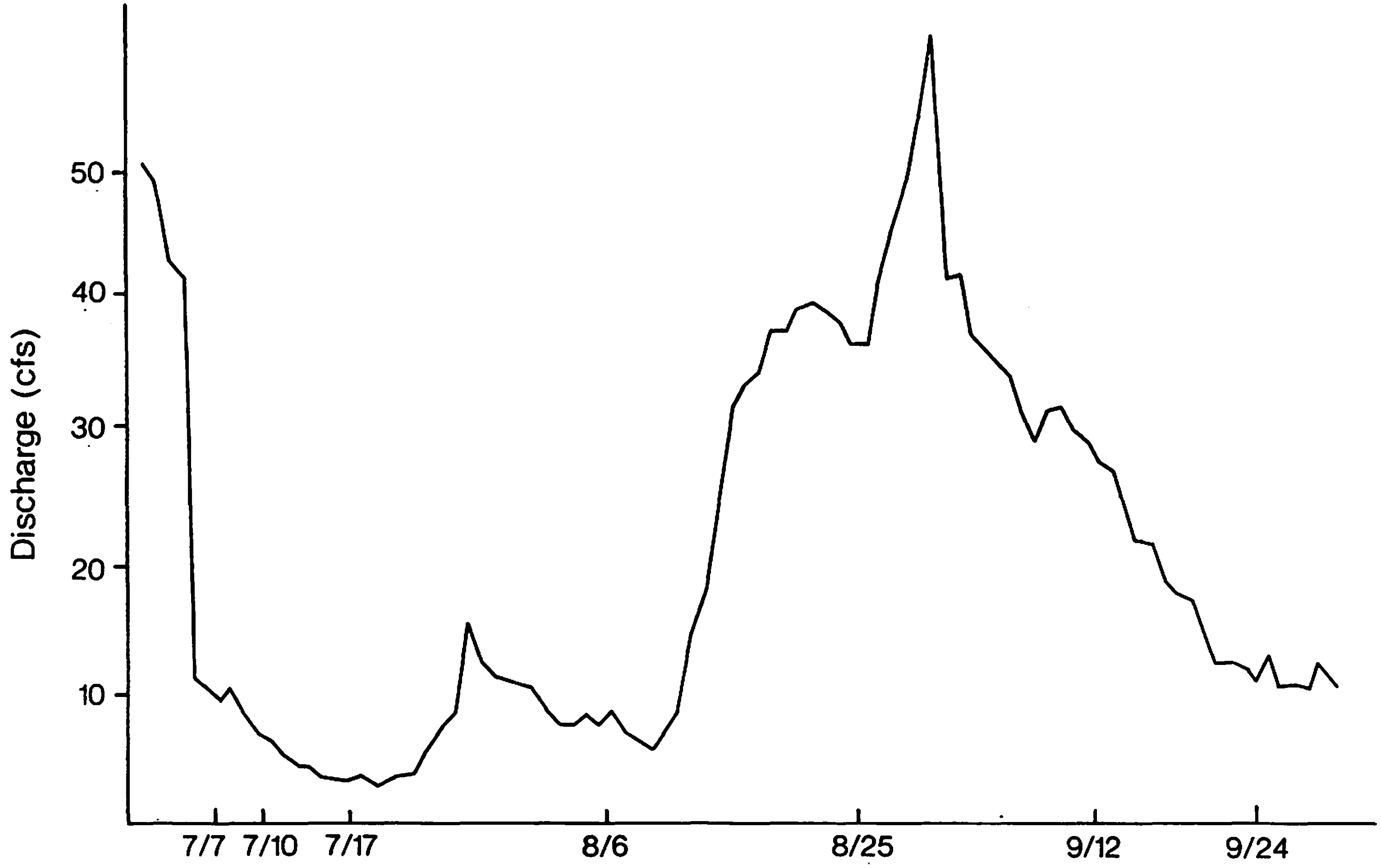


Fig. 2. Basin total discharge, July - September 1986. The dates indicate slackwater survey dates.

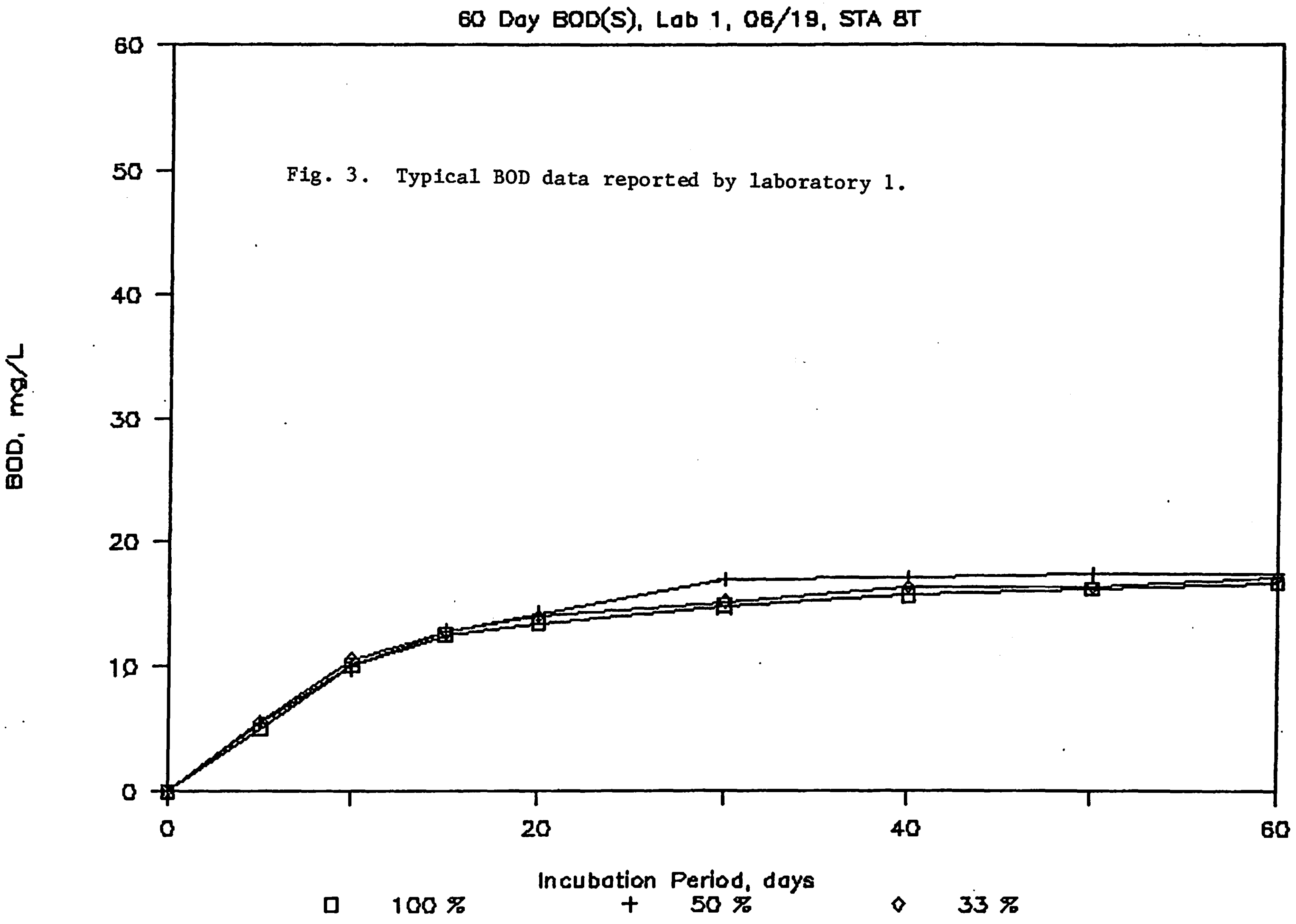


Fig. 3. Typical BOD data reported by laboratory 1.

Figure A - 152

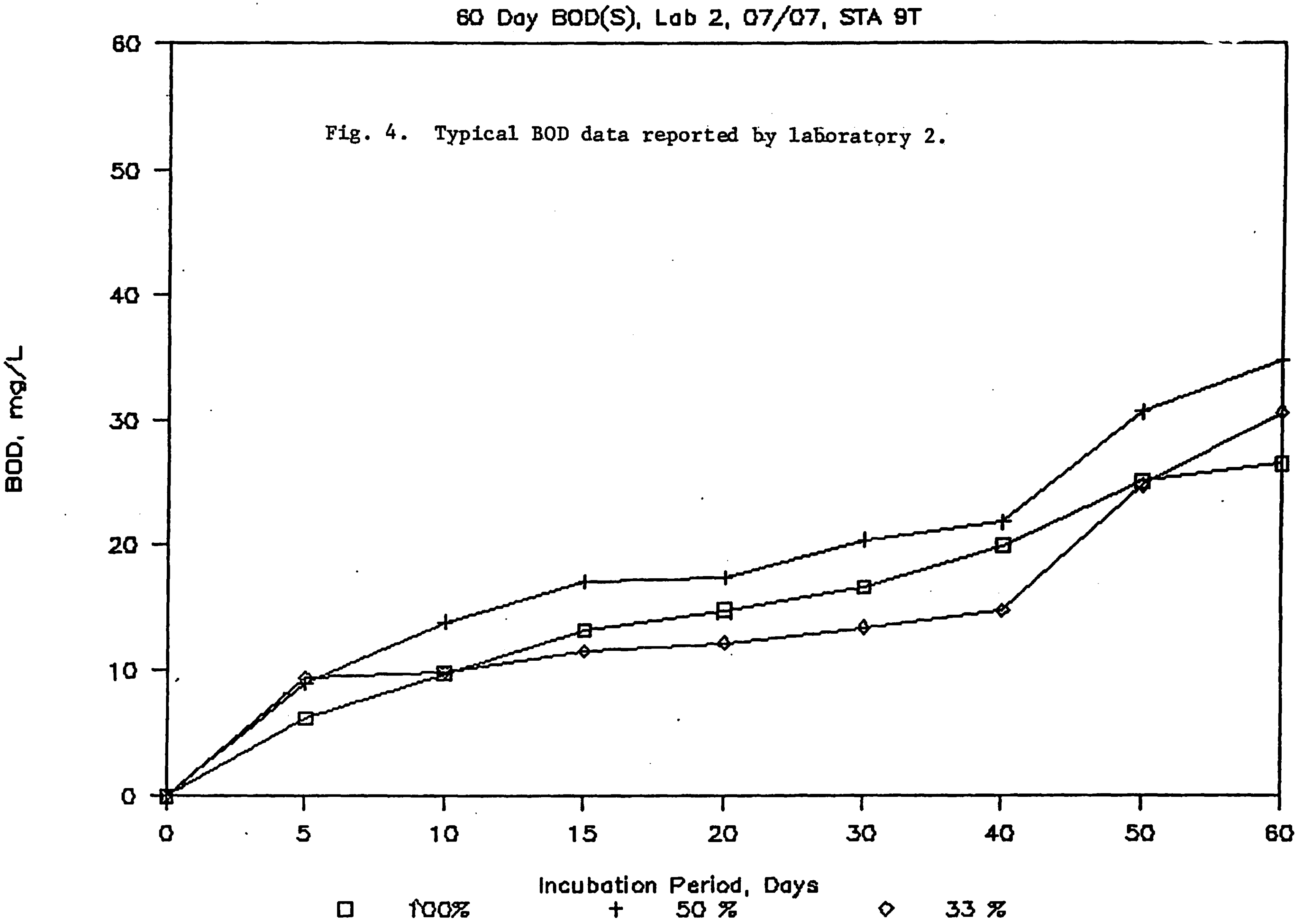


Fig. 4. Typical BOD data reported by laboratory 2.

Figure A - 169

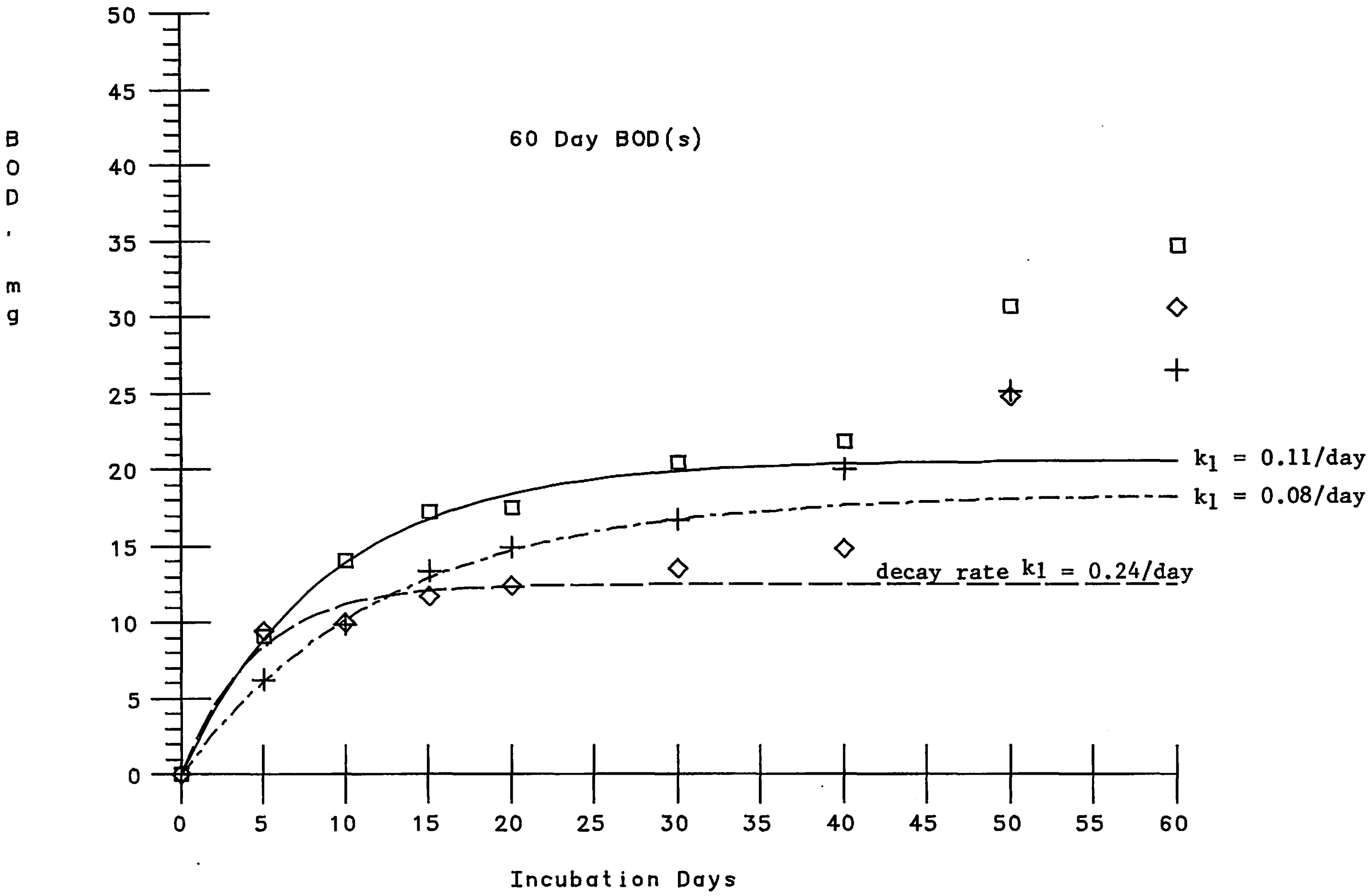


Fig. 4a. Least square fit of BOD data with first order decay curve.

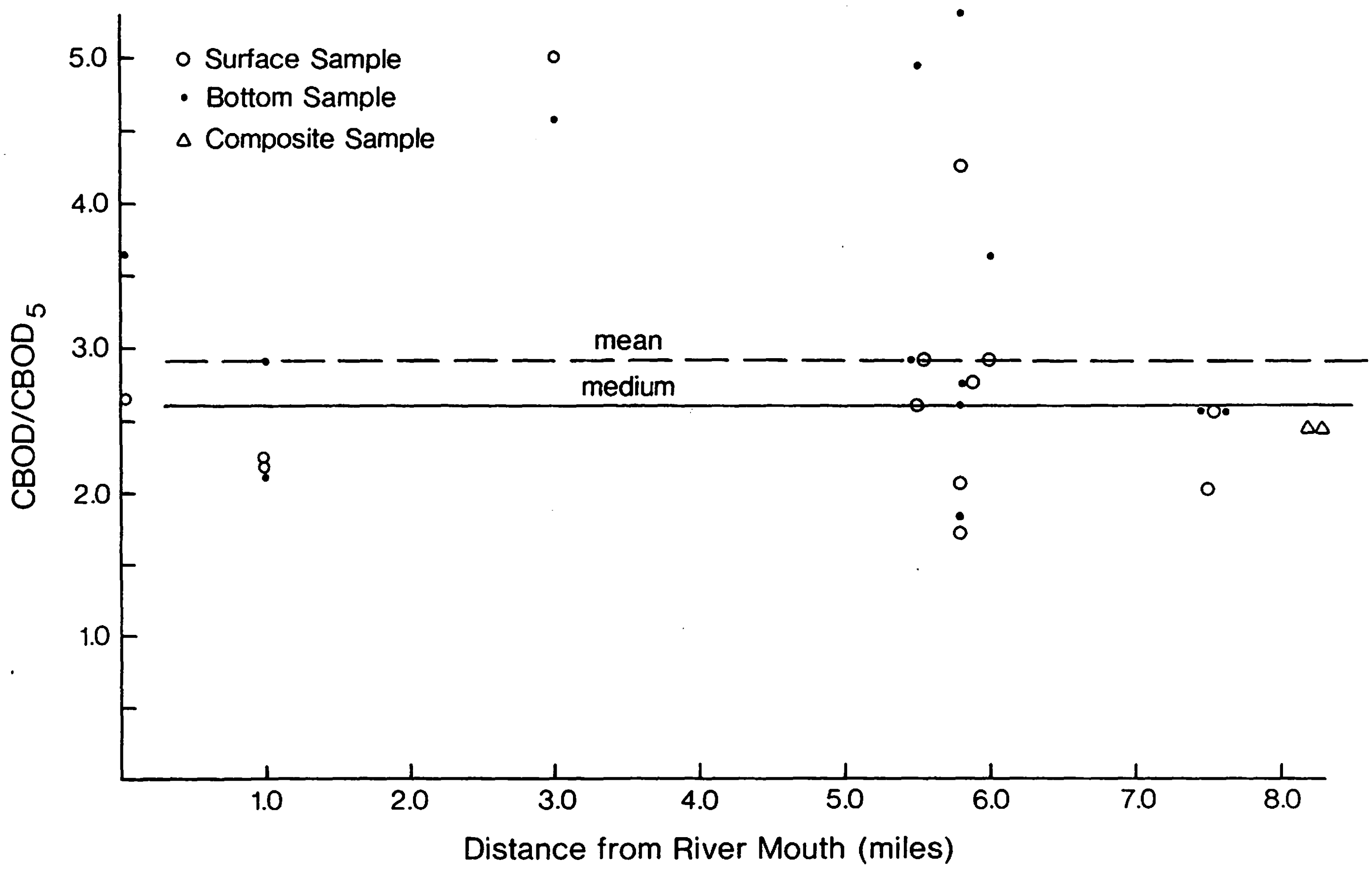


Fig. 5. Ratio of CBOD to $CBOD_5$ for nitrogen-inhibited BOD samples.

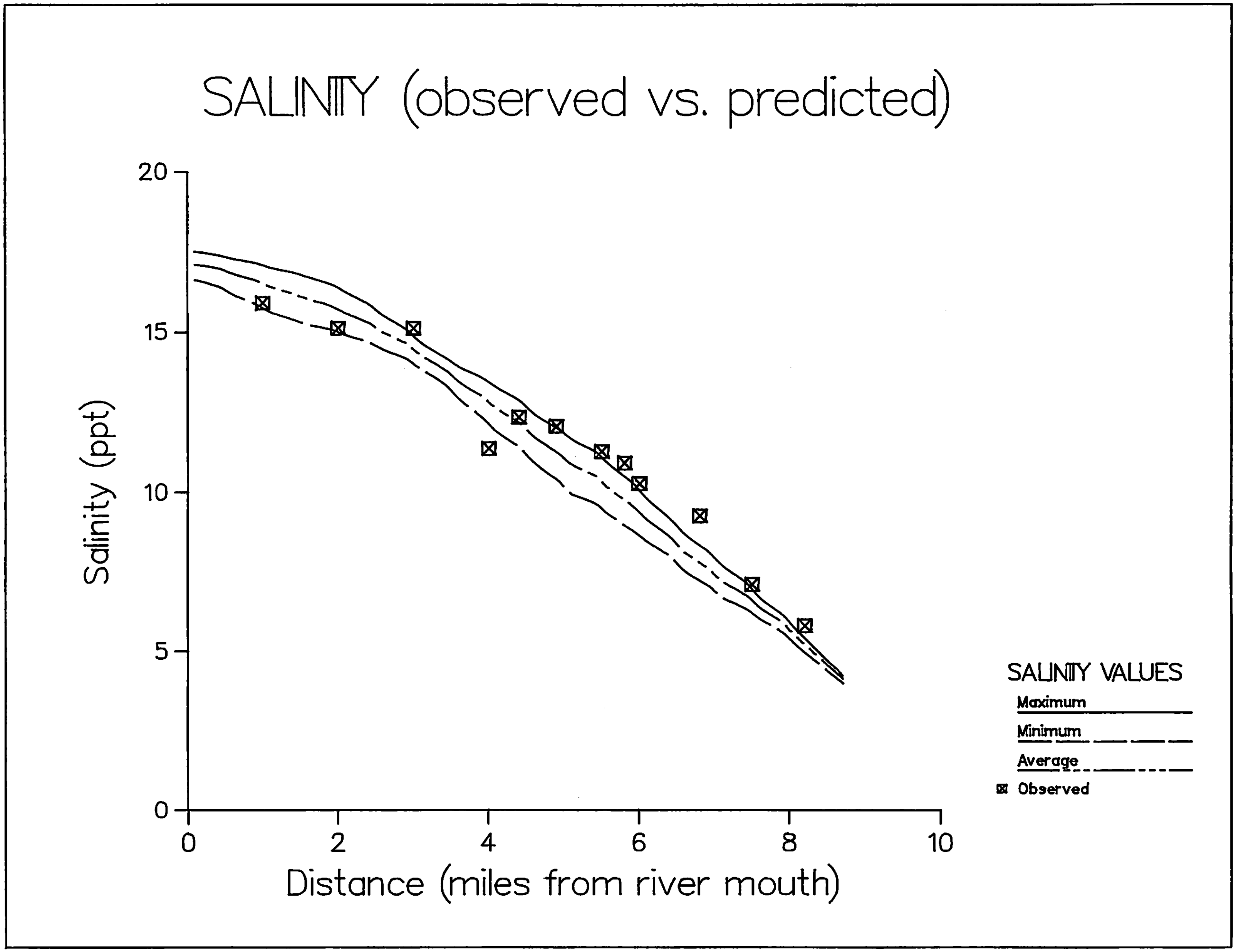


Fig. 6. Calibration of salinity.

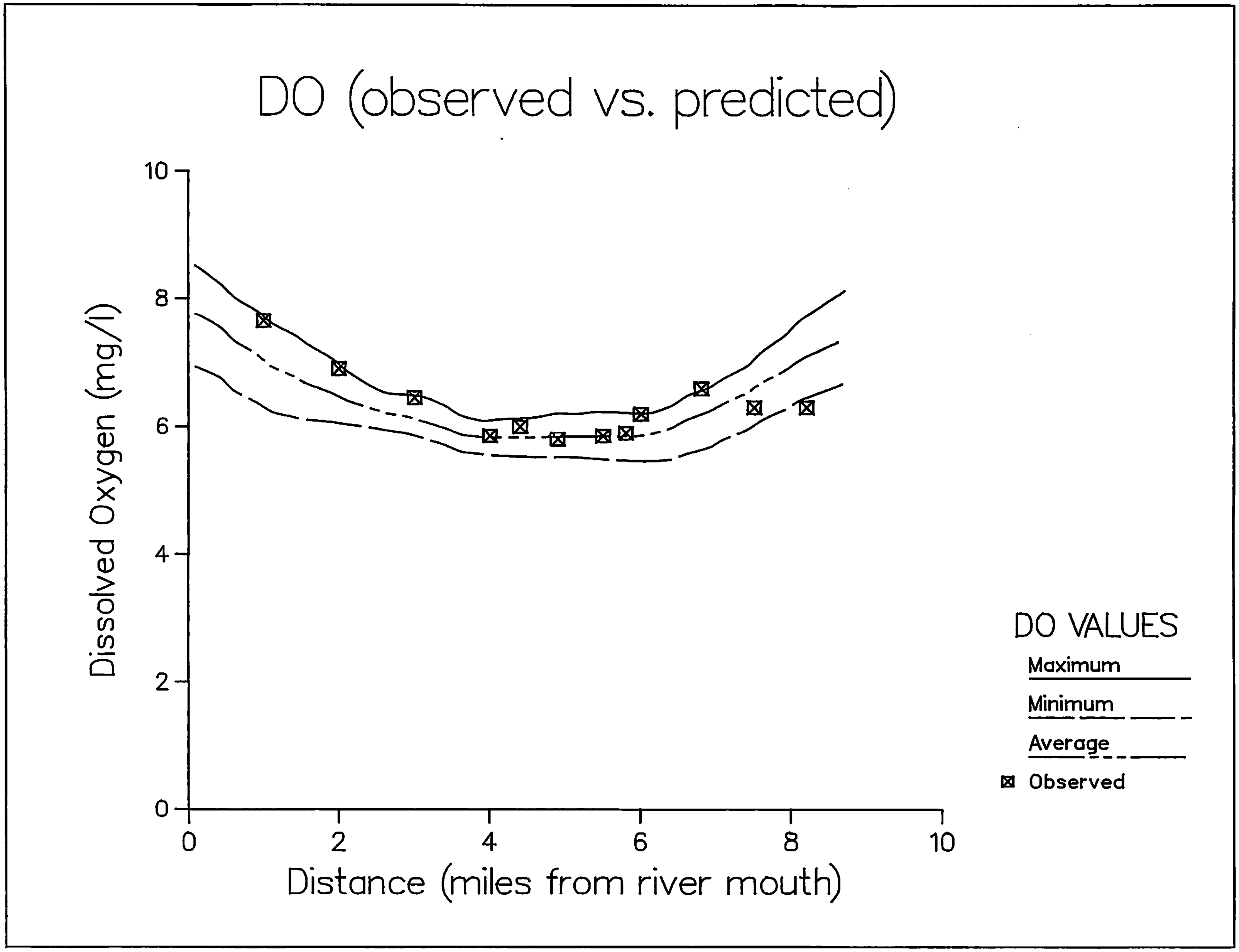


Fig. 7. Calibration of dissolved oxygen.

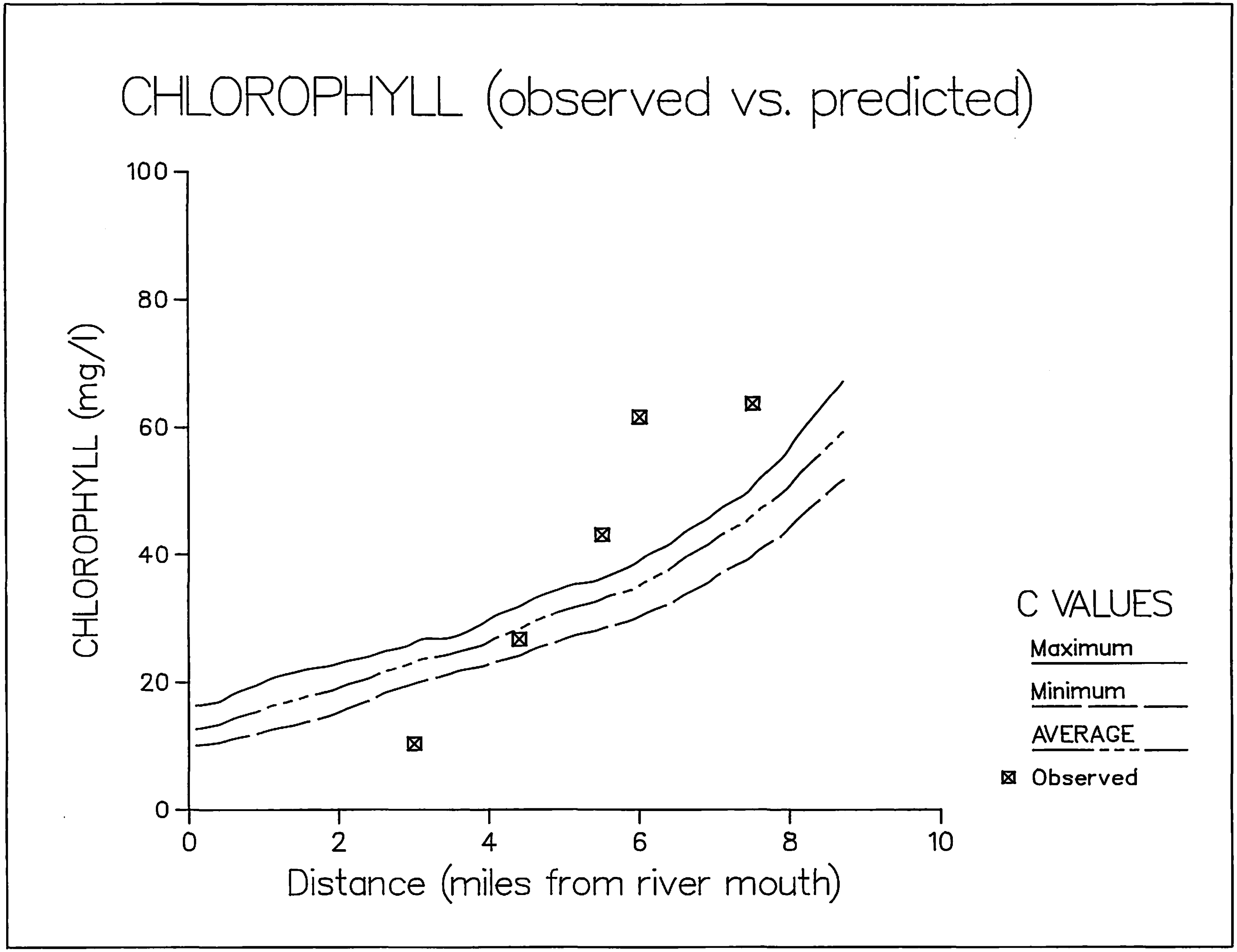


Fig. 8. Calibration of chlorophyll 'a'.

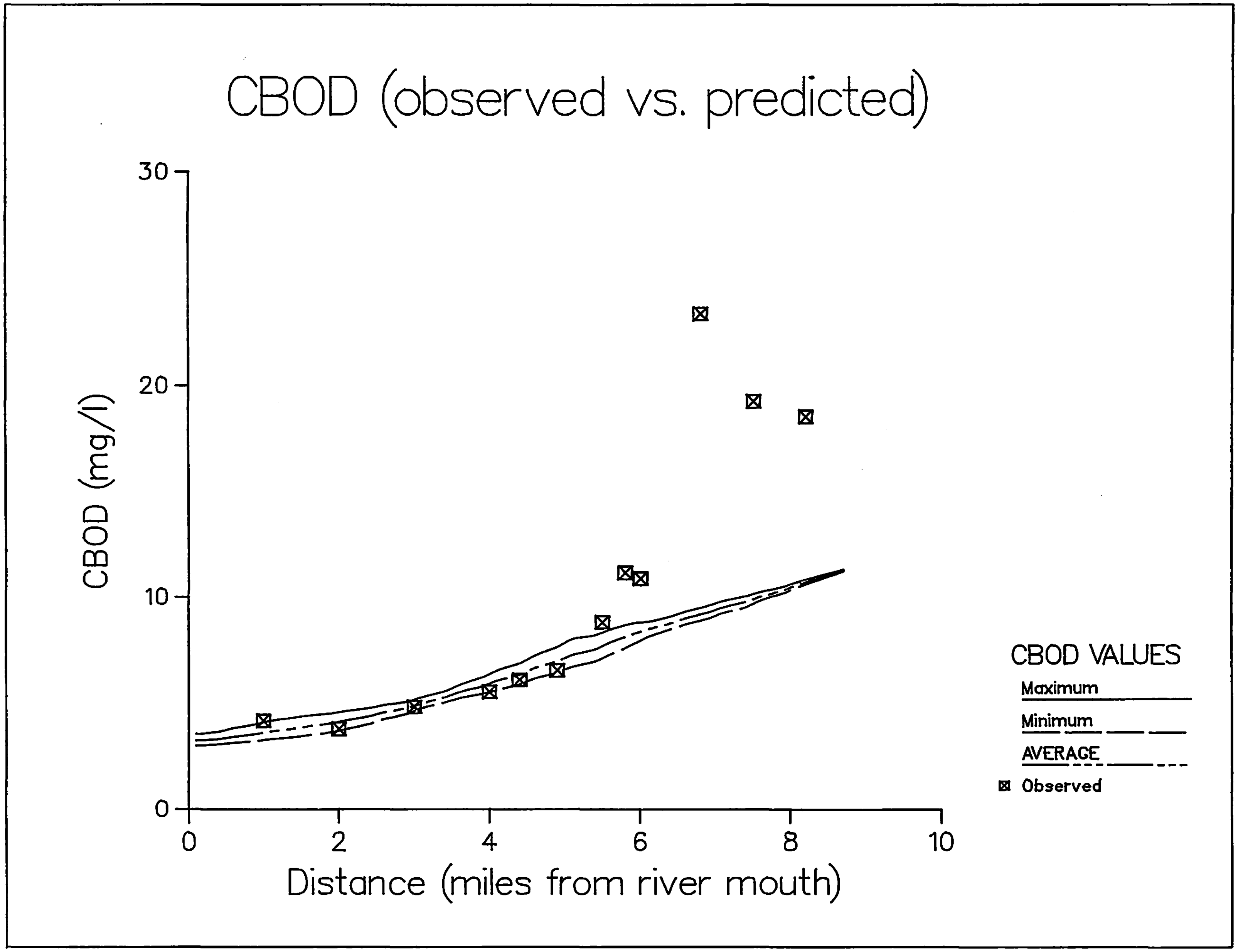


Fig. 9. Calibration of CBOD.

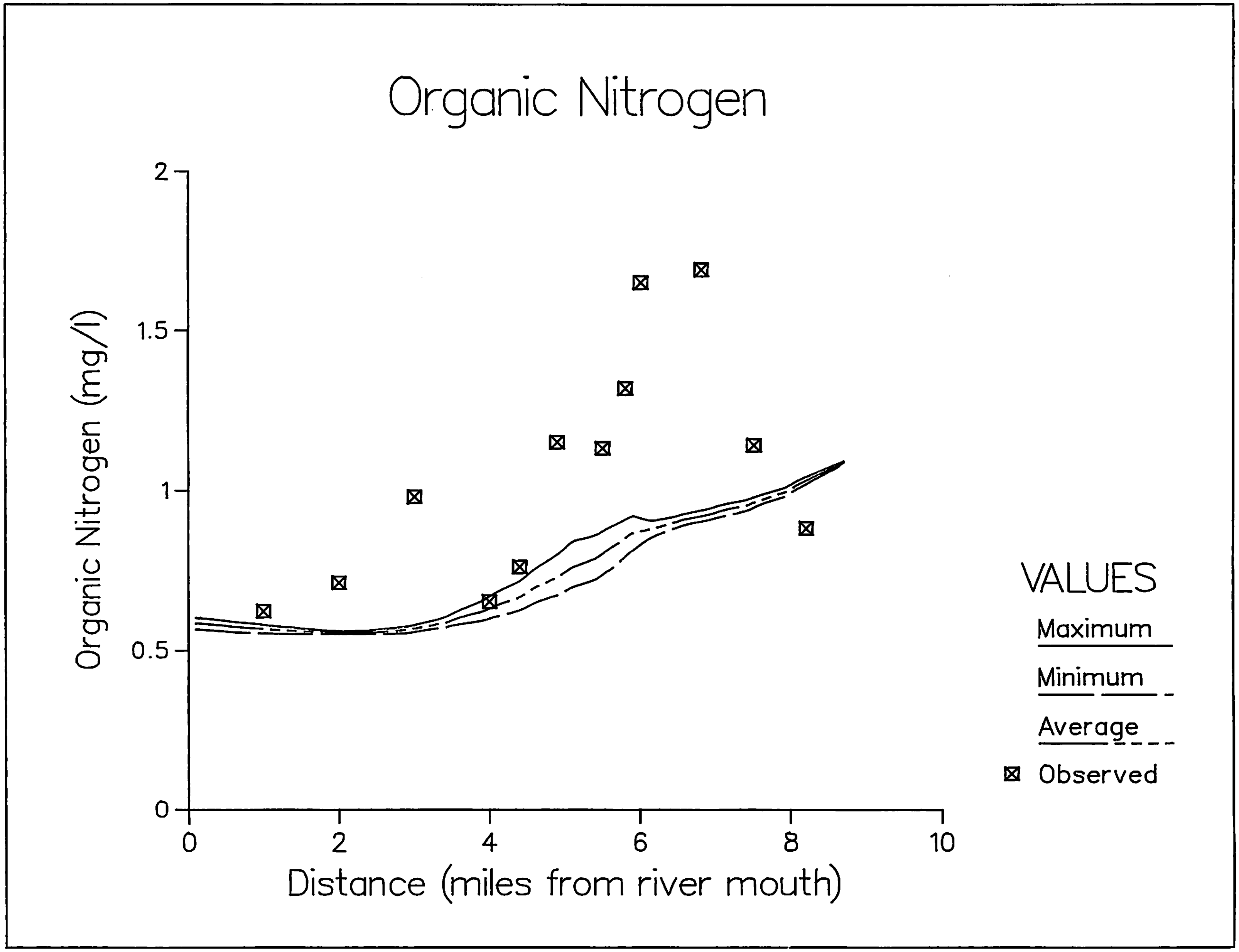


Fig. 10. Calibration of organic nitrogen.

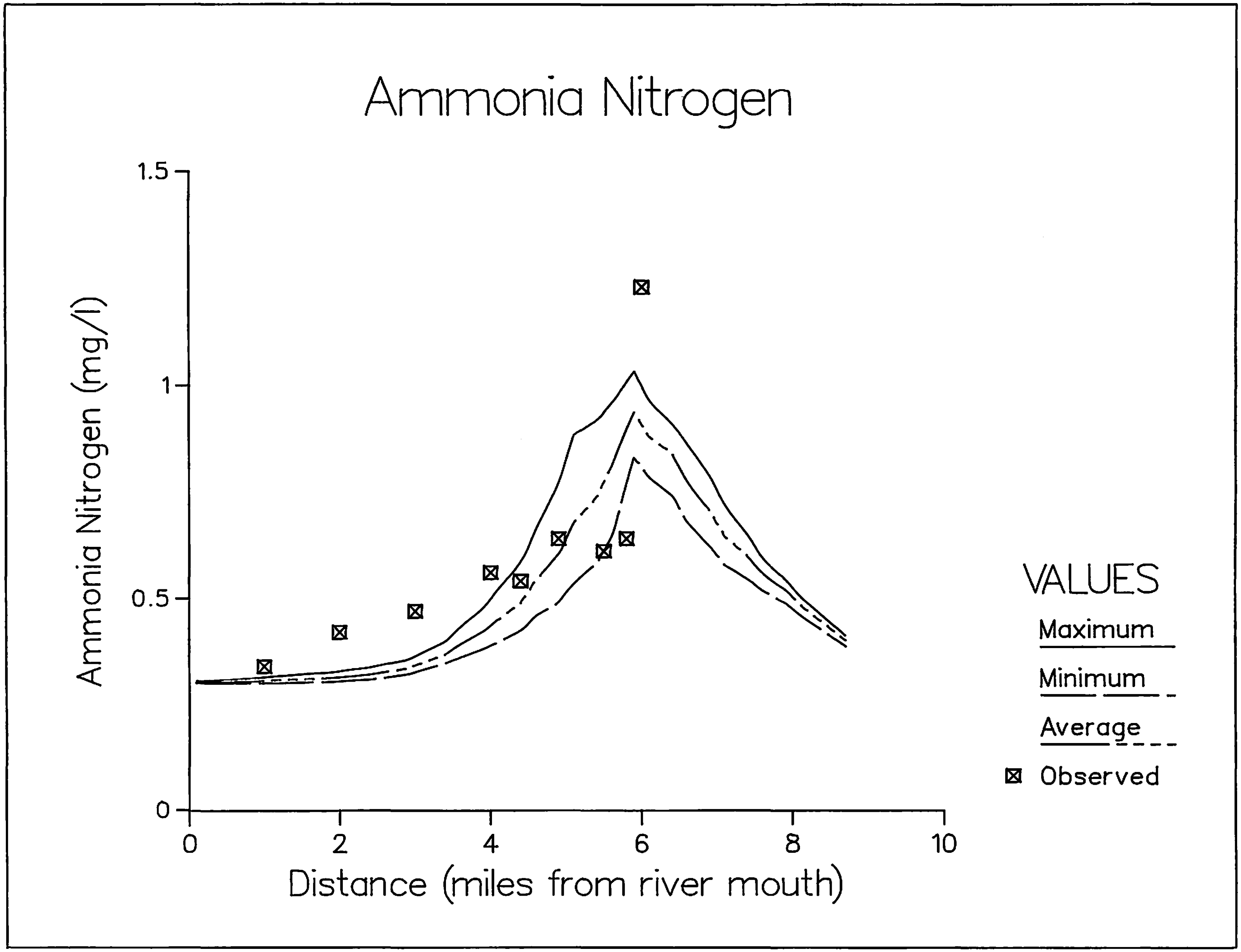


Fig. 11. Calibration of ammonia nitrogen.

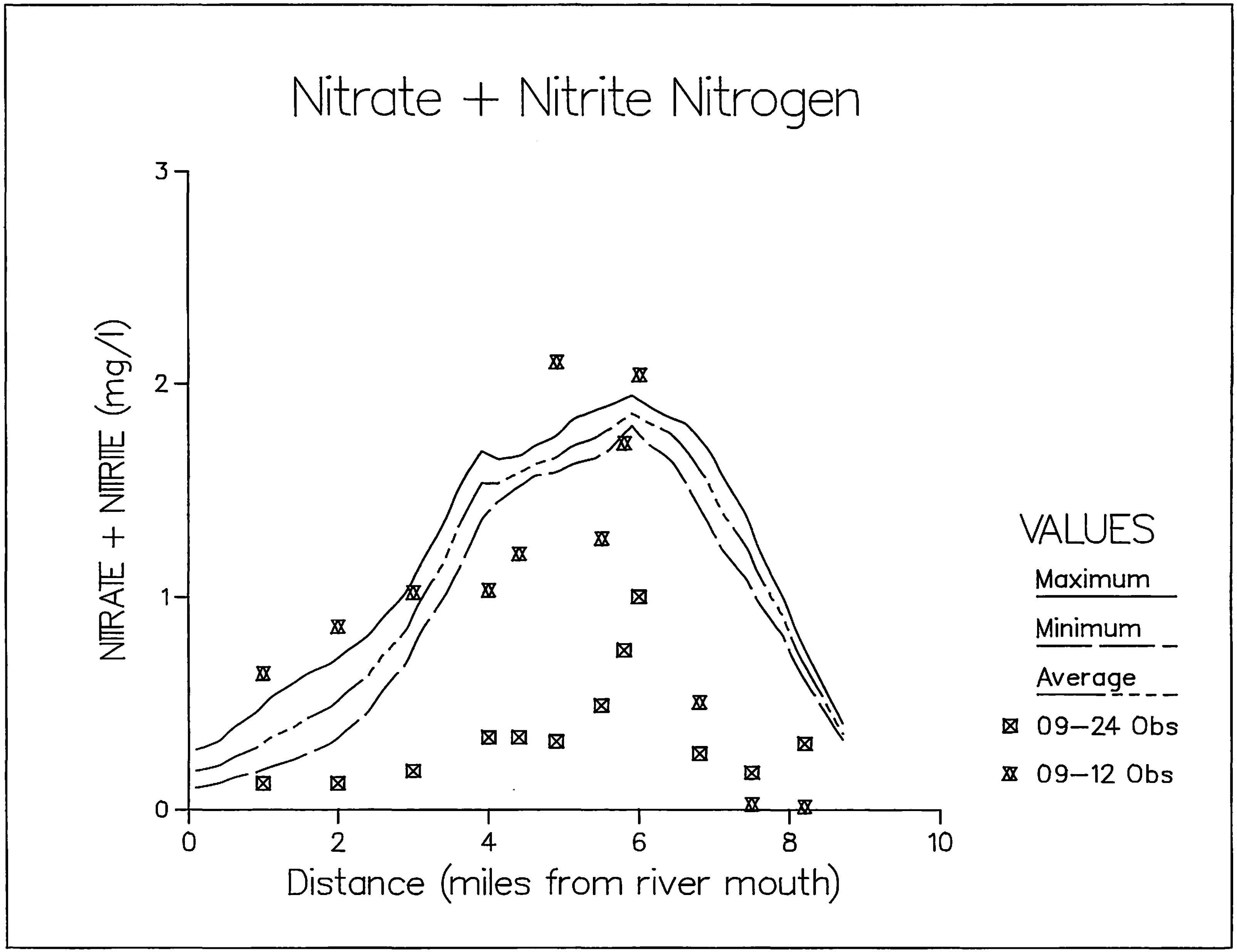


Fig. 12. Calibration of nitrate & nitrite nitrogen.

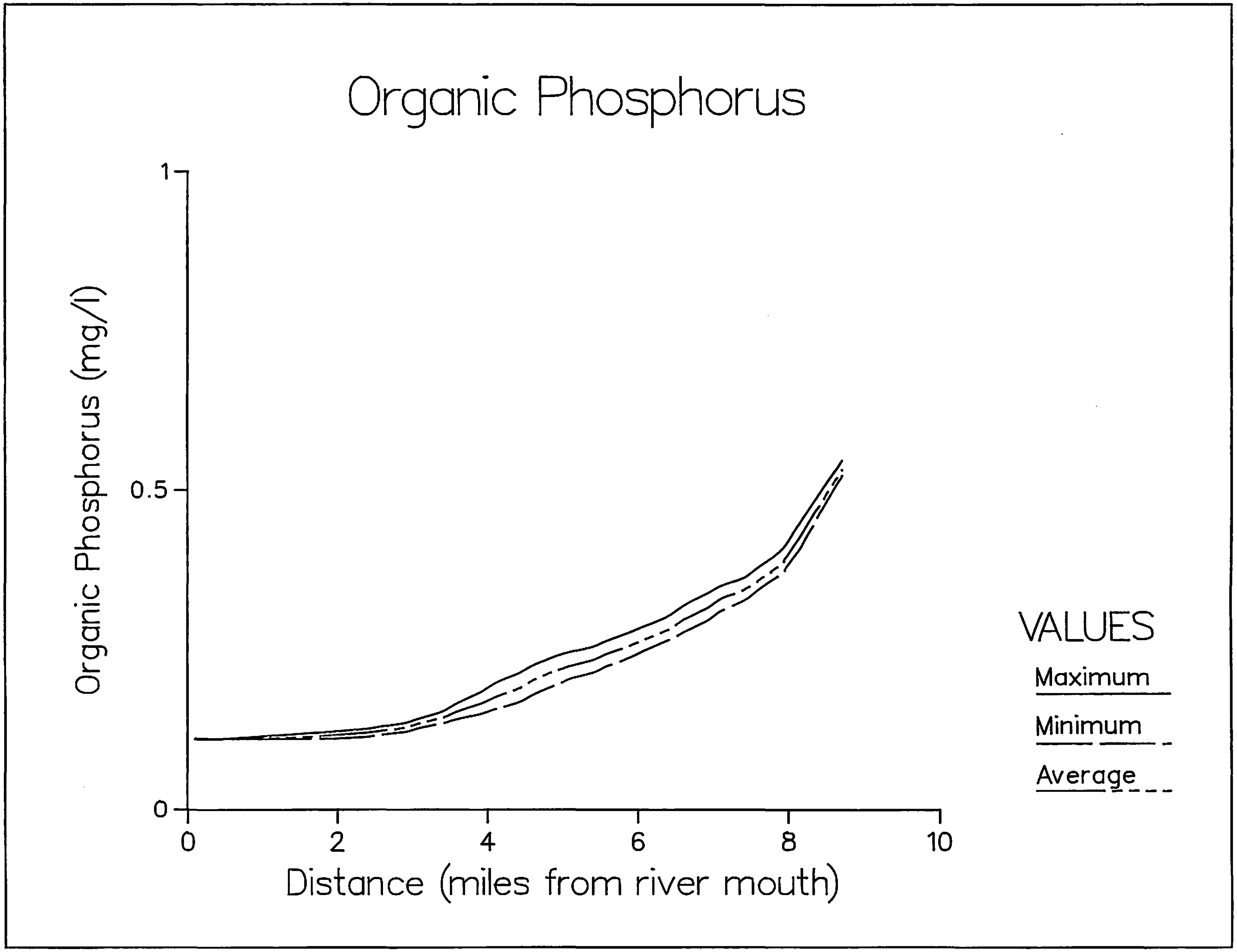


Fig. 13. Model results of organic phosphorus.

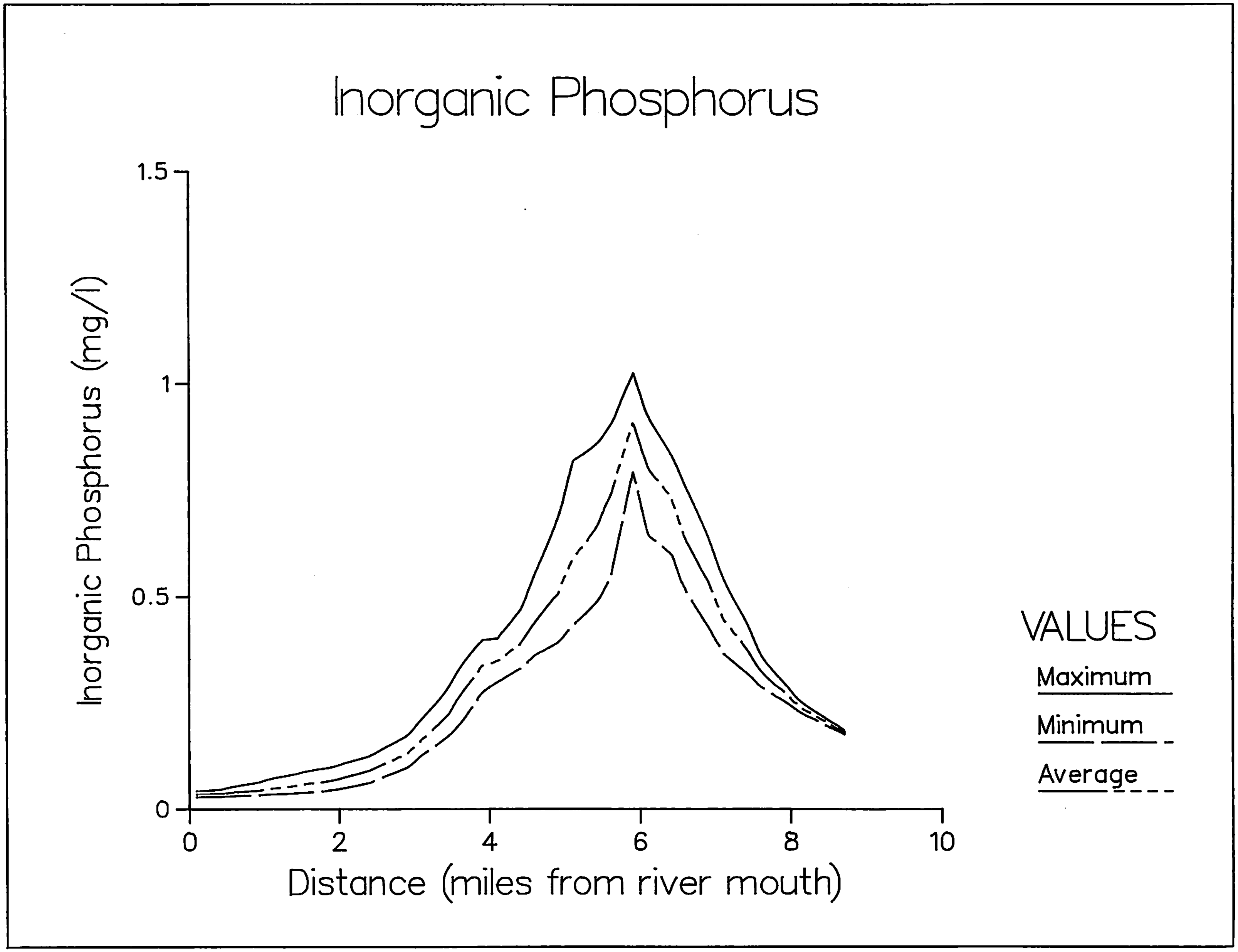
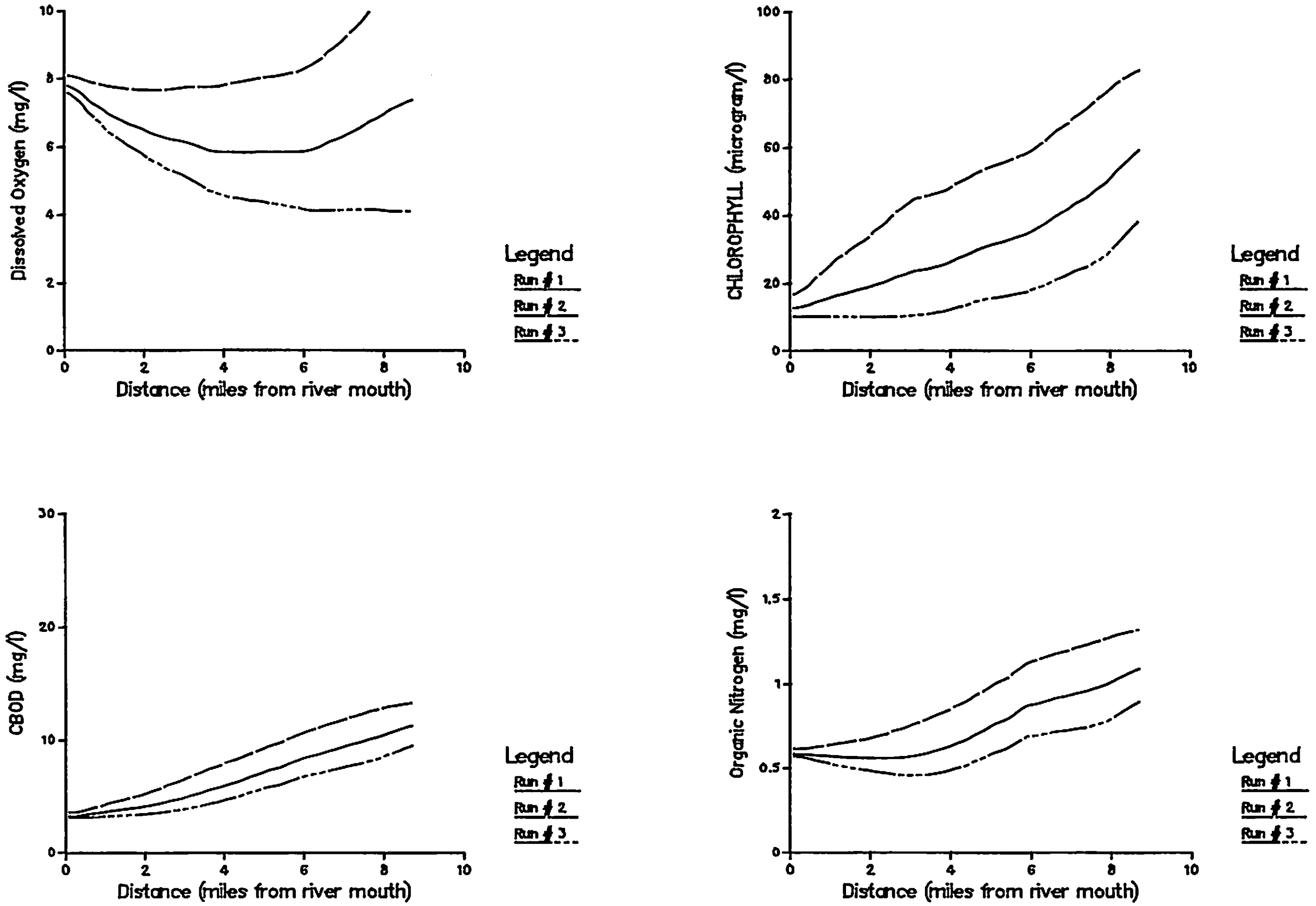


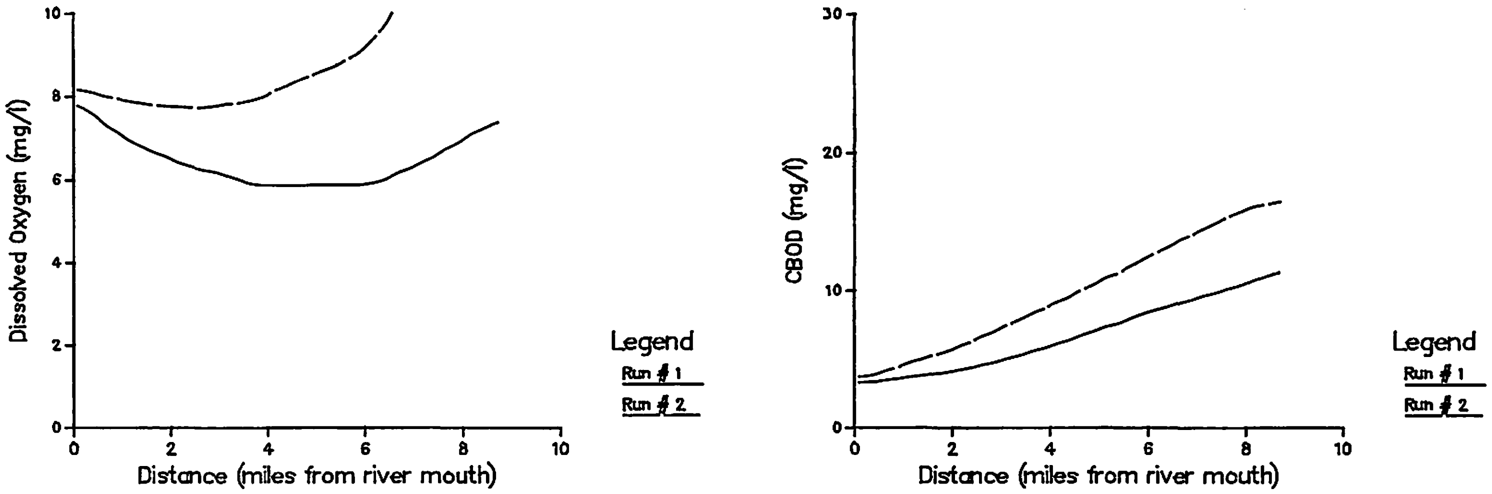
Fig. 14. Model results of inorganic phosphorus.

Fig. 15 SENSITIVITY TO PHYTOPLANKTON GROWTH RATE



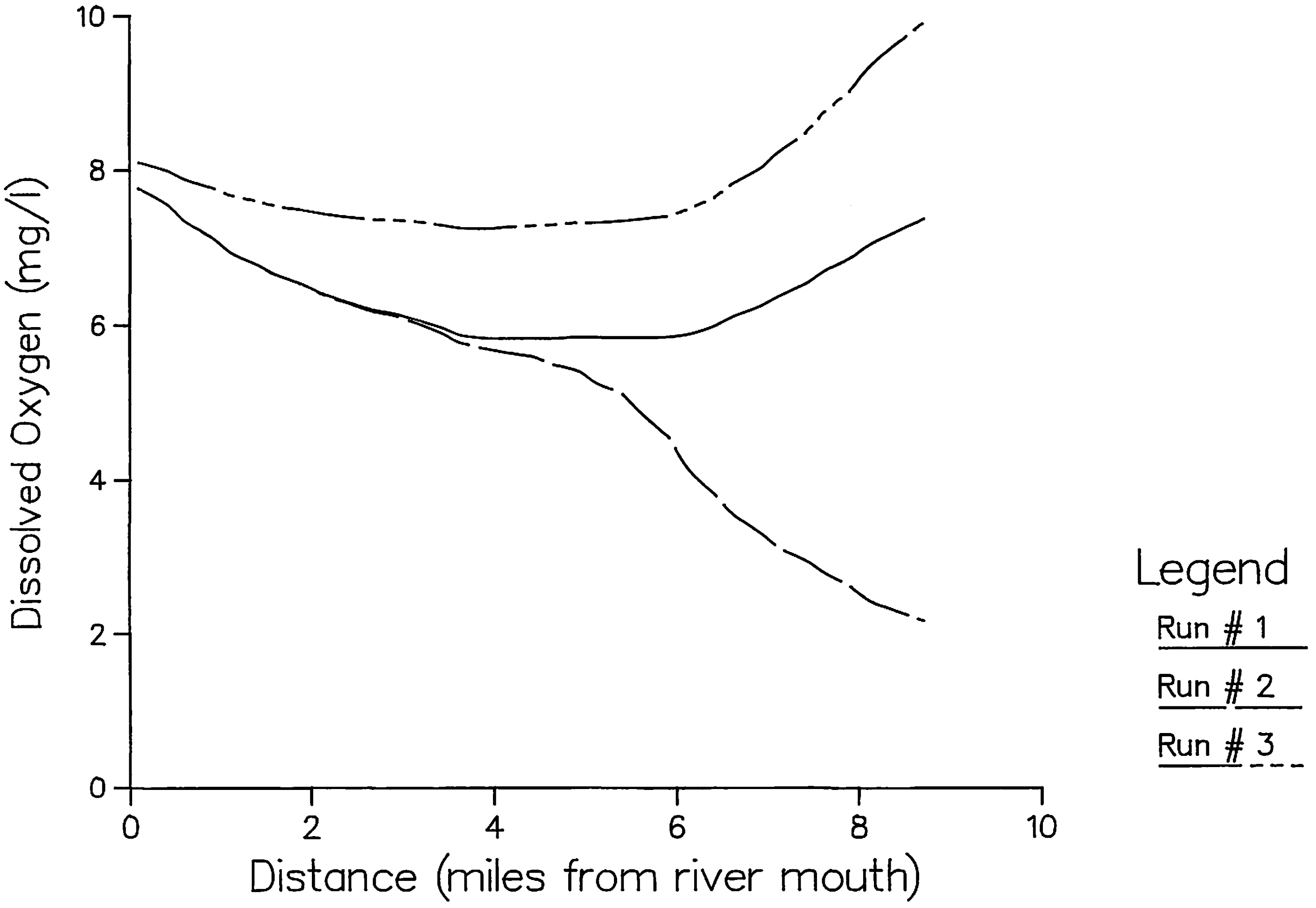
Run # 1 – Calibration growth rate (2.00/day)
Run # 2 – Calibration growth rate plus 20% (2.40/day)
Run # 3 – Calibration growth rate minus 20% (1.60/day)

Fig. 16 SENSITIVITY TO ALGAL CARBON – CHLOROPHYLL RATIO



Run # 1 – Calibration ratio (0.025)
Run # 2 – Twice calibration value (0.50)

Fig. 17 SENSITIVITY TO BENTHIC OXYGEN DEMAND



Note: units are gm oxygen per sq m per day at 20° C

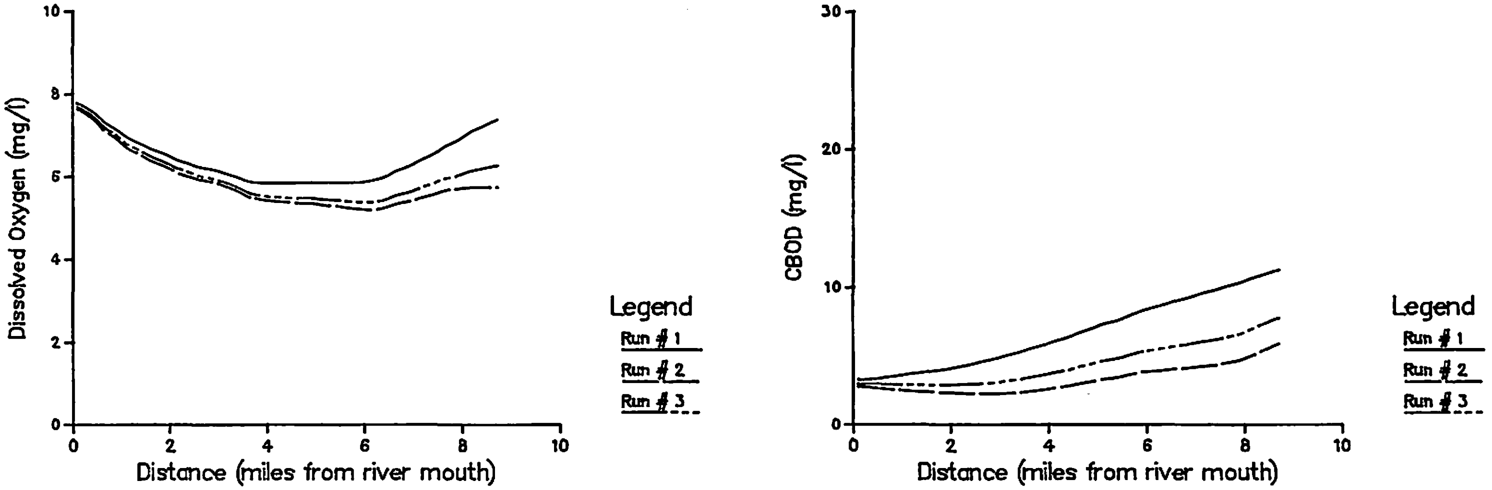
Run # 1 - Calibration values (1.9 throughout)

Run # 2 - 3.8 upriver of 6.0 miles, 1.9 downriver

Run # 3 - 1.0 throughout

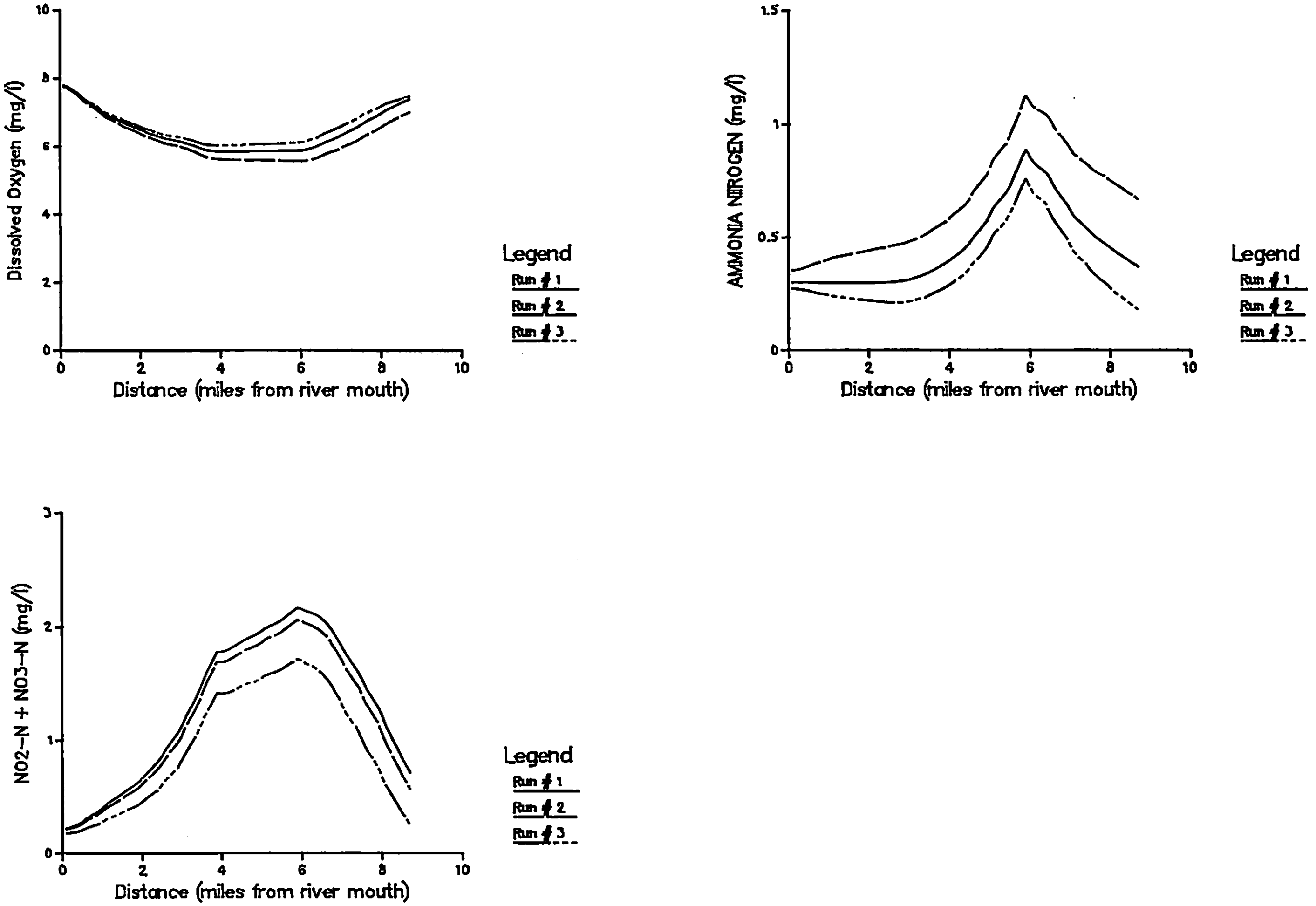
Fig. 18

SENSITIVITY TO CBOD DECAY RATE



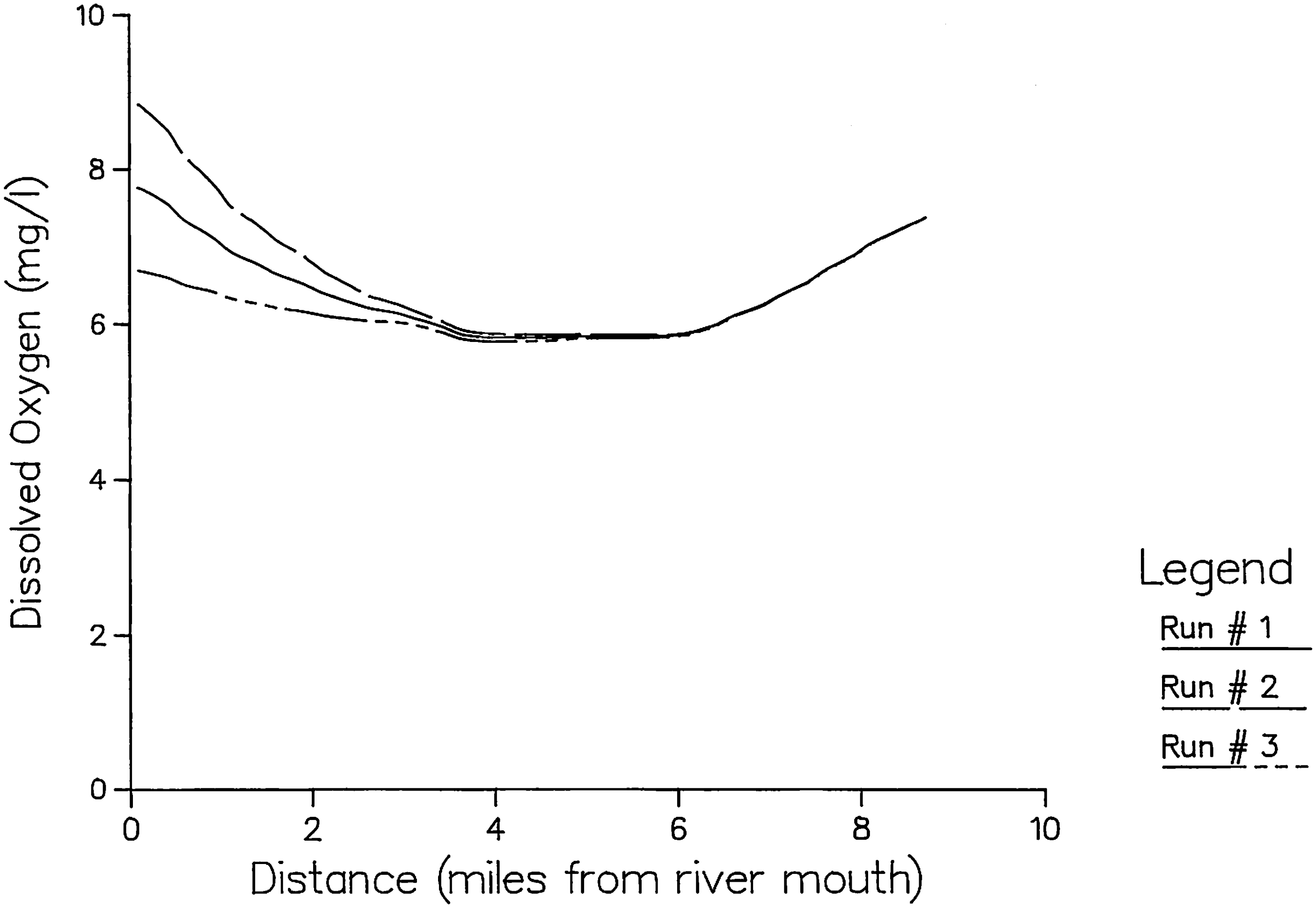
Run # 1 - Calibration value (0.05/day)
Run # 2 - Triple calibration value (0.15/day)
Run # 3 - Double calibration value (0.10/day)

Fig. 19 SENSITIVITY TO AMMONIA NITRIFICATION RATE



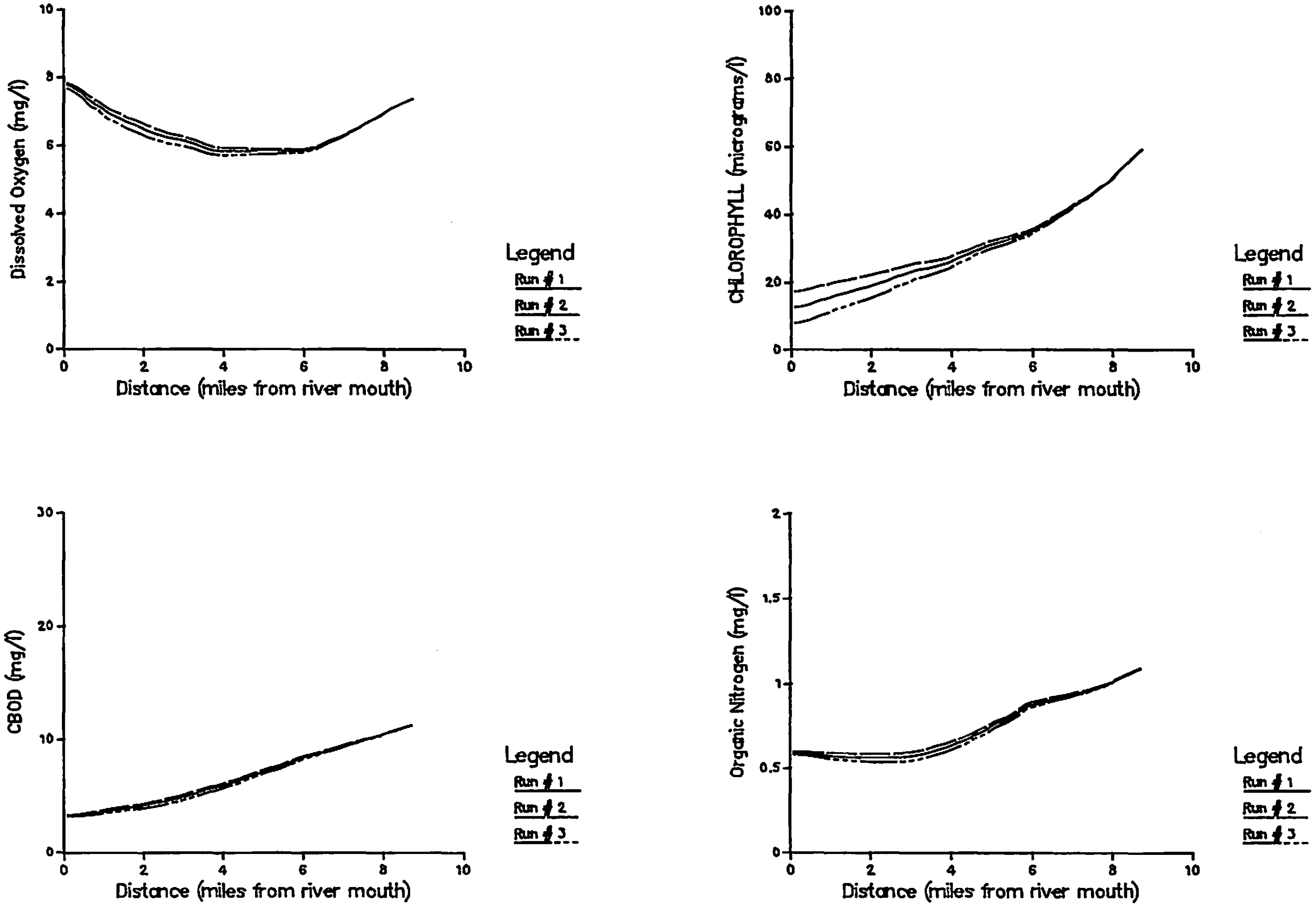
Run # 1 - Calibration value (0.003/day/deg C)
Run # 2 - 333% of calibration value (0.01/day/deg C)
Run # 3 - 33% of calibration value (0.001/day/deg C)

Fig. 20 SENSITIVITY TO DOWNSTREAM B. C. (DO)



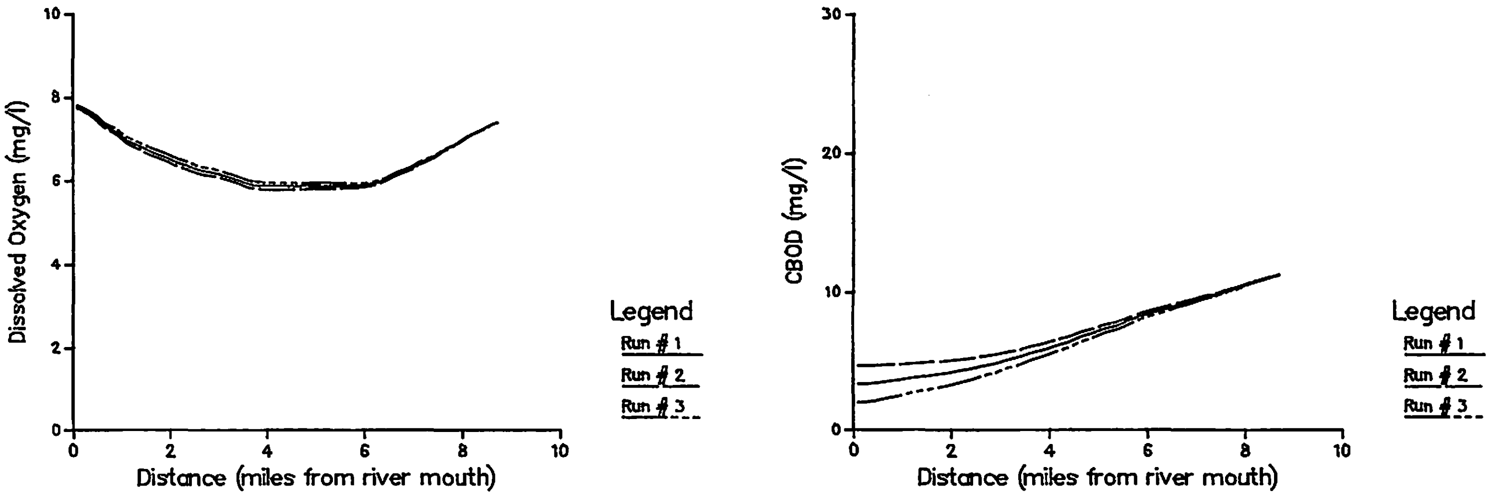
Run # 1 - Calibration value (8.5 mg/l)
Run # 2 - Increase 18% (10.0 mg/l)
Run # 3 - Decrease 18% (7.0 mg/l)

Fig. 21 SENSITIVITY TO DOWNSTREAM B. C. (Ch)



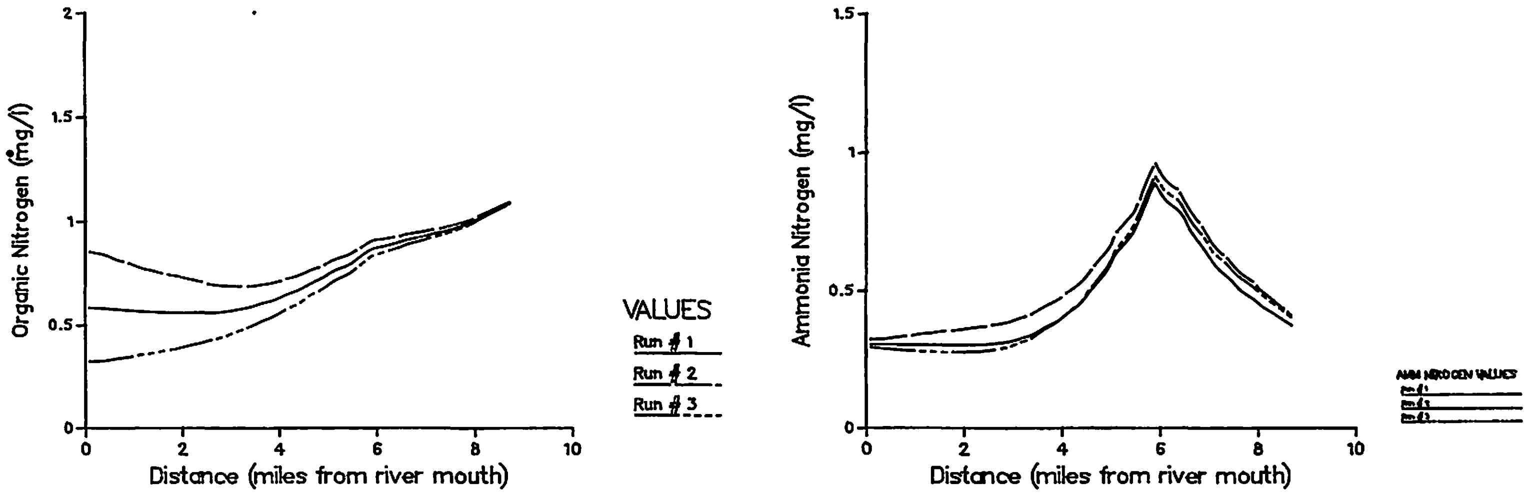
Run # 1 - Calibration value (10.0 micrograms/1)
Run # 2 - Increase 50 % (15.0 micrograms/1)
Run # 3 - Decrease 50 % (5.0 micrograms/1)

Fig. 22 SENSITIVITY TO DOWNSTREAM B. C. (CBOD)



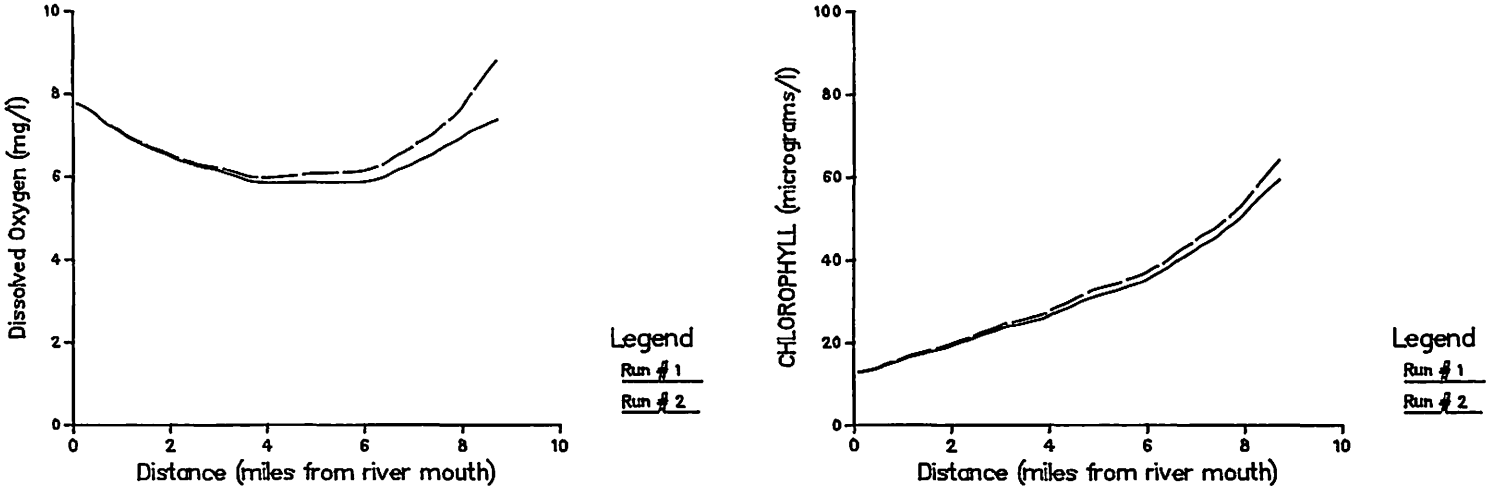
Run # 1 - Calibration value (3.0 mg/1)
Run # 2 - Increase 50% (4.5 mg/1)
Run # 3 - Decrease 50% (1.5 mg/1)

Fig. 23 SENSITIVITY TO DOWNSTREAM B. C. (Organic N)



Run # 1 - Calibration value (0.6 mg/l)
Run # 2 - Increase 50% (0.9 mg/l)
Run # 3 - Decrease 50% (0.3 mg/l)

Fig. 24 SENSITIVITY TO C & DO CONC OF FRESHWATER INFLOW



Run # 1 - Calibration values (Ch = 80 and DO = 6.3 mg/1)
Run # 2 - Increase both values (Ch = 100 and DO = 10.6)

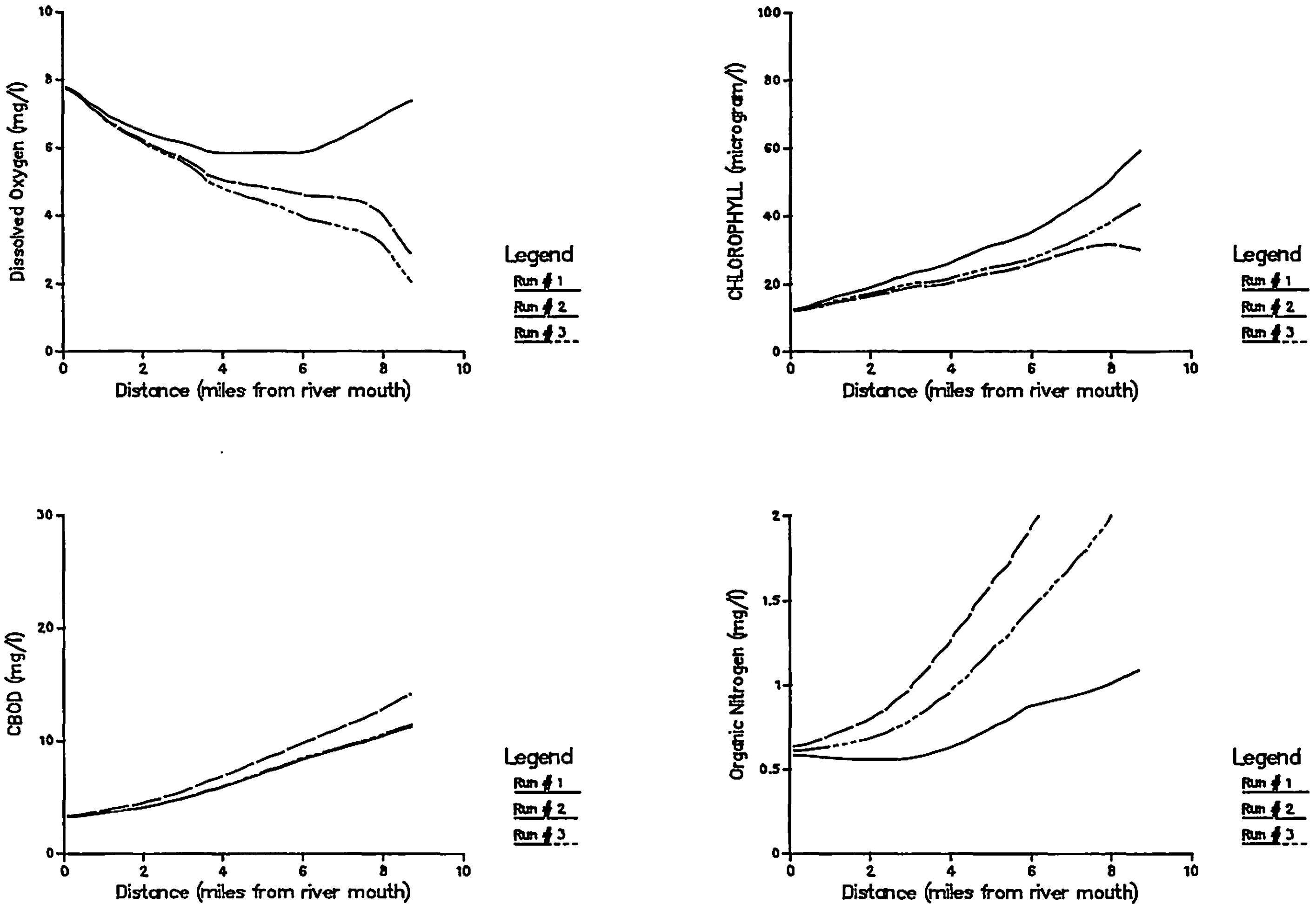


Fig. 25 SENSITIVITY TO NON–POINT SOURCE INPUT

Run # 1 - Calibration run (no non-point source input)
Run # 2 - 26-day run with non-point source at day 21
Run # 3 - 31-day run with non-point source at day 21

Fig. 25 SENSITIVITY TO NON–POINT SOURCE INPUT (Continued)

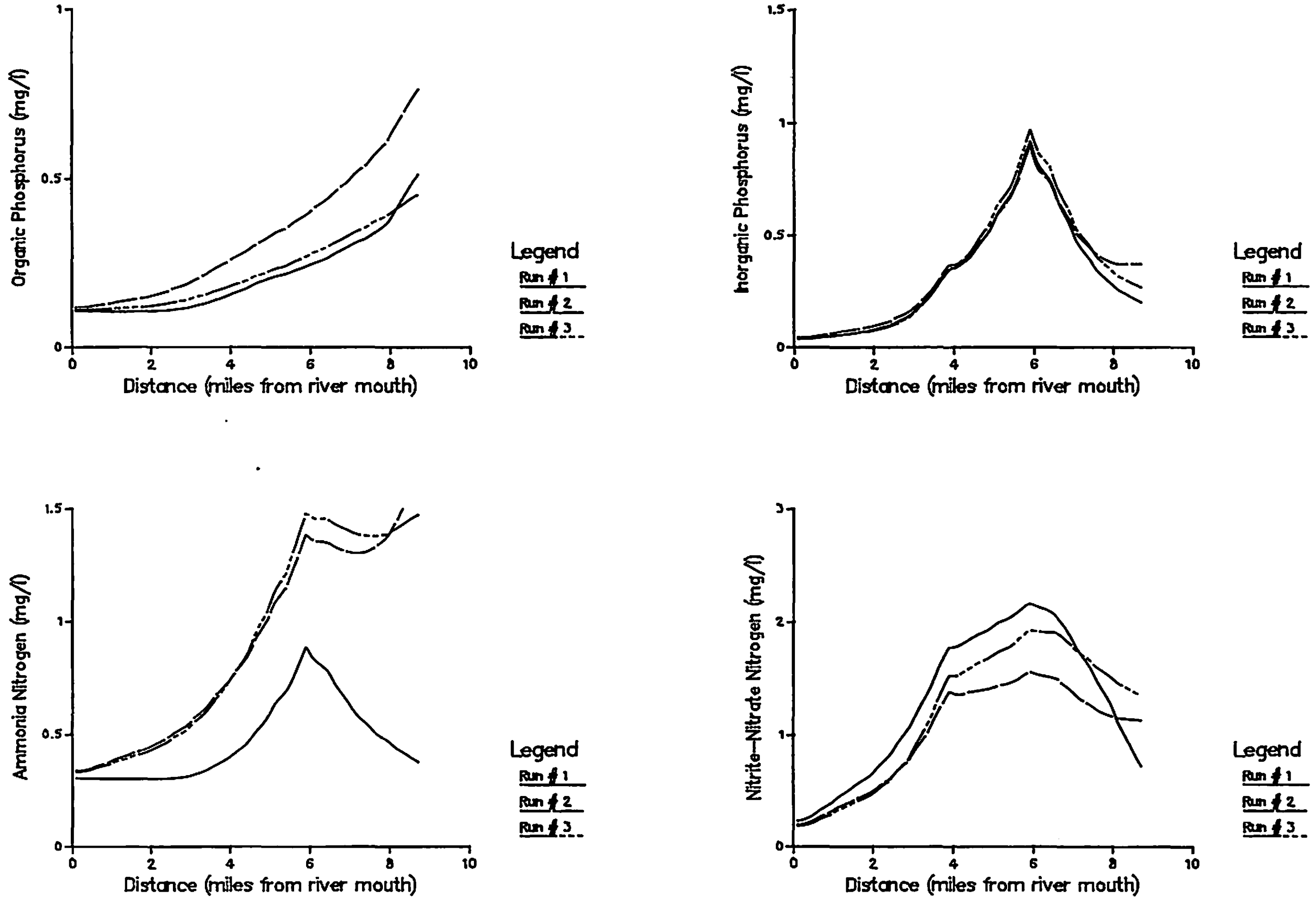
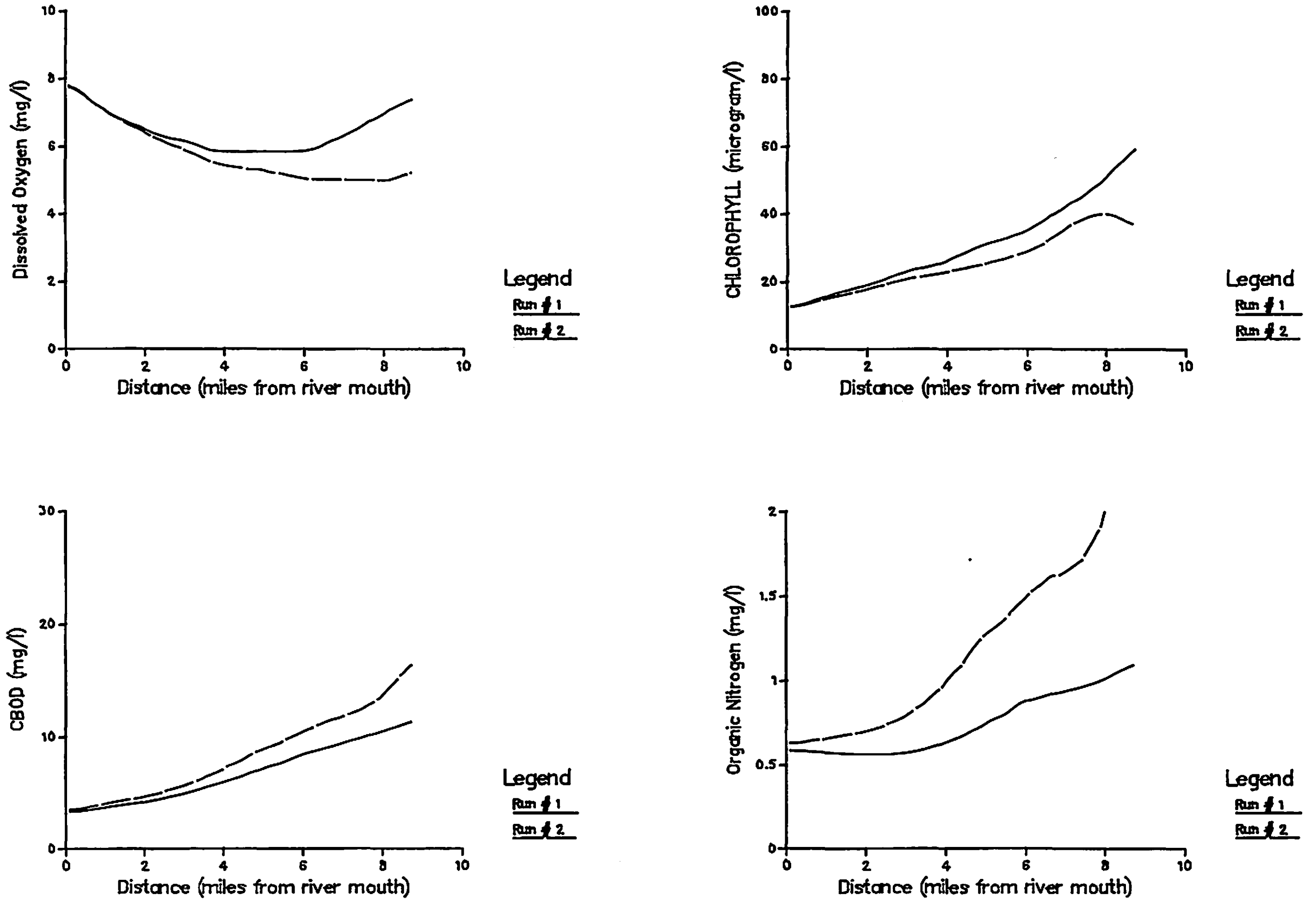


Fig. 26 SENSITIVITY TO AVERAGE NON-POINT SOURCE INPUT



Run # 1 - Calibration run (no non-point source input)

Run # 2 - Constant non-point source input values used based on summer averages

Fig. 26 SENSITIVITY TO AVERAGE NON–POINT SOURCE INPUT (Continued)