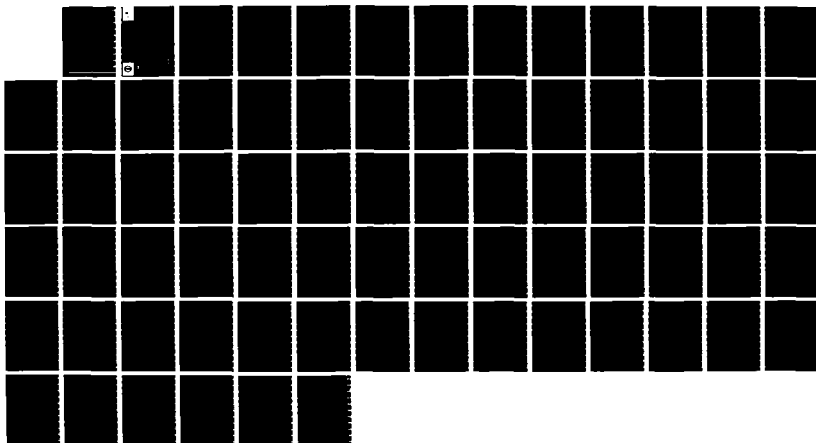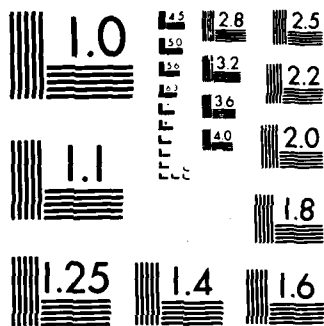AD-A171 871   CALIBRATION OF A WATER QUALITY MODEL FOR LAKE ASHTABULA   1/1
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STATION VICKSBURG MS ENVIR.   J H WLOSINSKI JUN 86

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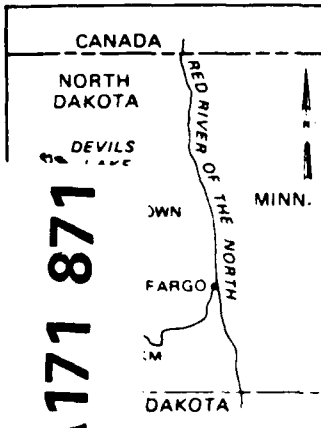# CALIBRATION OF A WATER QUALITY MODEL FOR LAKE ASHTABULA, NORTH DAKOTA
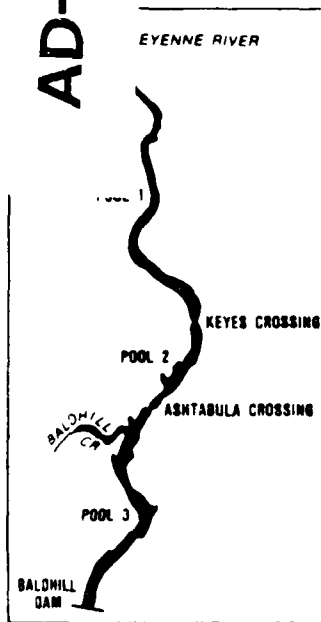
by

Joseph H. Wlosinski

Environmental Laboratory

DEPARTMENT OF THE ARMY
Waterways Experiment Station, Corps of Engineers
PO Box 631, Vicksburg, Mississippi 39180-0631

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US Army Corps
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CANADA

NORTH DAKOTA

DEVILS

RED RIVER OF THE NORTH

MINN.

OWN

FARGO

M

DAKOTA

EYENNE RIVER

POOL 1

KEYES CROSSING

POOL 2

ASHTABULA CROSSING

BALDHILL CR

POOL 3

BALDHILL DAM

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ENVIRONMENTAL LABORATORY

REPORT DOCUMENTATION PAGE

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19 ABSTRACT (Continue on reverse if necessary and identify by block number)

A mathematical model of Lake Ashtabula Reservoir, Valley City, North Dakota, was developed based on the one-dimensional reservoir water quality model CE-QUAL-R1. The major assumption employed in CE-QUAL-R1 is that the reservoir is represented as a vertical series of completely mixed horizontal layers in which longitudinal and lateral variations of constituent concentrations cannot be predicted. Lake Ashtabula, whose pool is long, narrow, and largely confined to the run-of-the-river, exhibits both vertical and longitudinal water quality gradients. The reservoir is constricted at two points along its length, essentially dividing the system into three distinct pools. In order to represent this two-dimensional aspect of the system the model was organized using three CE-QUAL-R1 pools coupled in series in which the simulated outflow constituent quantities for the first and second pools became the inflows for their respective downstream pools. By using this model configuration, it was possible to simulate longitudinal as well as vertical variations of constituent concentrations.

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PREFACE

This report was sponsored by the St. Paul District, US Army Corps of
Engineers, under DA Form 2544, number NCS-IA-85-44-ED-GH dated 28 Jan 85, and
was monitored by Mr. Dennis Holme, St. Paul District. The report describes
the results of calibration simulations of the water quality model CE-QUAL-R1,
representing Lake Ashtabula Reservoir.

The model was calibrated and the report was written by Dr. Joseph
Wlosinski, Water Quality Modeling Group (WQMG), Ecosystem Research and
Simulation Division (ERSD), of the Environmental Laboratory (EL), US Army
Engineer Waterways Experiment Station (WES). Other members of the WQMG who
assisted with the project were Ms. Sandra Berry, Ms. Dorothy Hamlin,
Ms. Dollie Sue Hull, Mr. Issac Jefferson, and Mr. Craig Oldham. The draft
report was reviewed by Dr. Marc Zimmerman, Dr. James Martin, and Ms. Berry of
the WQMG.

The study was conducted under the direct supervision of Mr. Mark Dortch,
Chief, WQMG; and under the general supervision of Mr. Donald Robey, Chief,
ERSD; and Dr. John Harrison, Chief, EL. Director of WES during preparation of
this report was COL Allen F. Grum, USA. Technical Director was Dr. Robert W.
Whalin.

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CONTENTS

PART I: INTRODUCTION

Water quality modeling is one method available to managers to help assess and identify environmental factors which affect water quality conditions. With a correctly calibrated model, it should be possible to evaluate the effects of engineering alternatives on water quality. Lake Ashtabula, North Dakota, has become the subject of such a water quality study by the St. Paul District, US Army Corps of Engineers. Lake Ashtabula is a multiple purpose reservoir located on the Sheyenne River (Figure 1). It is formed by the Baldhill Dam, which is located about 19 km north of Valley City, North Dakota. The reservoir is operated by the US Army Corps of Engineers principally for water supply, flood control and recreation use. Physical characteristics of the reservoir are included in Table 1.

This study grew out of concern over present water quality problems in Lake Ashtabula and possible effects due to planned projects. Planned projects include the US Bureau of Reclamation's Garrison Diversion and the creation of an outlet for Devils Lake by the US Corps of Engineers. Devils Lake, a closed subbasin of the Sheyenne River watershed, contains brackish water. Present water quality problems in Lake Ashtabula include frequent algal blooms and associated periods of oxygen depletion which have significantly reduced the fishery and recreation resource value of the reservoir. Possible strategies to improve water quality at Lake Ashtabula include changing the depth of withdrawal, nutrient input concentrations, surface elevation, or discharge operating plan, or building a small upstream dam to act as a sediment and nutrient trap.

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In 1983 the St. Paul District, using data collected at Lake Ashtabula, evaluated CE-THERM-R1, a one-dimensional reservoir model that simulates temperature, total dissolved solids and suspended solids (Holme,Bakke, and Wlosinski, 1985). CE-THERM-R1 is a sub-model of the larger water quality model, CE-QUAL-R1. In that evaluation, Lake Ashtabula was represented as a series of three pools separated at two reservoir crossings (Figure 1). Each pool was simulated separately, with the inflows to the second and third pools generated by the model during simulation of respective upstream pools. Because the results from that study were satisfactory, the St. Paul District contracted for a similar evaluation of CE-QUAL-R1 using data collected in 1981. In particular, the contract called for:

a. Making the thermal model (CE-THERM-R1), which was developed on the Boeing computer system, operational on the Control Data Corporation Computer system (CDC).

b. Calibrating the CE-QUAL-R1 water quality model and evaluating model performance using statistical methods.

c. Allowing for evaluation of three hypothetical reservoir conditions including a 4-foot pool rise, an upstream sediment trap impoundment and a 30 to 40 percent nutrient load reduction.

d. Making the water quality model (CE-QUAL-R1) operational on the CDC system.

e. Furnishing a report that documents the results.

This report documents the calibration of CE-QUAL-R1 using data collected at Lake Ashtabula, and the conversion of the two models to the CDC computer system.

PART II: THE LAKE ASHTABULA MODEL

CE-QUAL-R1

In CE-QUAL-R1, a reservoir is conceptualized as a vertical series of horizontal layers in which thermal energy and mass are uniformly distributed in each layer. Horizontal layer thicknesses are variable and dependent on the balance of inflowing and outflowing waters. Variable layer thicknesses permit accurate mass balancing and reduce numerical dispersion during periods of large inflow and outflow.

Inflowing waters are distributed vertically based on density differences so that simulations of surface flows, interflows, and underflows are possible. Water density depends on temperature and concentrations of dissolved and suspended solids. Outflowing waters are withdrawn from layers based on density stratification using the selective withdrawal algorithms of Bohan and Grace (1973). Reservoir outflows by port can either be specified, or the user can invoke a subroutine which will choose port flows in order to meet a downstream temperature objective.

The heat budget includes the components of short and long wave radiation, back radiation, reflected solar and atmospheric radiaton, evaporative loss, conductive heat transfer, and gain or loss through inflow and outflow. Vertical transport of thermal energy and mass is achieved through entrainment and turbulent diffusion. Entrainment determines the depth of the upper mixed layer and the onset of stratification. It is calculated from the turbulent kinetic energy influx generated by wind shear and convective mixing using an integral energy approach (Johnson and Ford, 1981). Turbulent diffusion is a

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two-way transport process which incorporates a turbulent or eddy diffusion coefficient that depends on wind speed, magnitude of inflows and outflows, and density stratification.

Forces that directly affect constituent concentrations are temperature, irradiation, wind speed, inflow and outflow rates, and inflowing and outflowing masses. The physical distribution of mass is dependent upon the diffusive and convective processes described above and on settling processes. Biological processes also affect constituent concentrations. Photosynthesis, dark respiration, photorespiration and nonpredatory mortality influence algal and macrophyte mass. Grazing by fish and zooplankton additionally influence algae. Ingestion, egestion, and respiration affect zooplankton and fish growth. Inorganic compounds such as ammonia-nitogen (ammonia), nitrite-nitrogen plus nitrate-nitrogen (nitrite-nitrate), orthophosphate-phosphorus (phosphorus), and silica are consumed and produced as a result of photosynthesis and respiration. Phosphorus and ammonia are adsorbed to solids according to a modified equation for the Langmuir isotherm. Ammonia is also removed by conversion to nitrite-nitrate under aerobic conditions. Nitrite-nitrate is lost through denitrificaton.

Detritus depends on algal and macrophyte mortality, ingestion by fish and zooplankton, zooplankton egestion, and settling. Decomposition of detritus contributes mass to ammonia, phosphorus, and inorganic carbon.

Inflowing and initial concentrations for dissolved organic matter (DOM) are divided into labile and refractory DOM compartments. Photorespiration contributes to labile DOM. Products from DOM decomposition are distributed to inorganic nutrients and refractory DOM.

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Dissolved oxygen concentration is of primary importance to reservoir management. Oxygen is produced by algal and macrophyte photosynthesis. Oxygen demand in CE-QUAL-R1 is simulated by nitrification, decomposition of organic compounds and sediment, respiration, and oxidation of reduced products of anaerobic reactions. Oxygen may also be gained or lost at the air-water interface. Anaerobic and aerobic conditions resulting from changes in oxygen concentration drive many other modeled processes. If the system becomes anaerobic, decomposition of organic material stops, and phosphorus, ammonia, dissolved reduced manganese, iron and sulfide are released from the sediments. Sediments release almost all the anaerobic compounds generated in CE-QUAL-R1: reduction and inflow account for the remainder. Reoxygenation of the system reverses these reactions.

Total dissolved solids (TDS) are simulated to obtain an approximation of ionic strength. Calculations based on the equilibrium reactions of bicarbonate, carbonate, and hydroxyl ions and on ionic strength result in the pH value reported for each layer. This value is then used to calculate the carbon dioxide concentration which contributes to plant growth and diffuses across the air-water interface.

Total alkalinity is simulated in CE-QUAL-R1 to provide an indication of the buffering capacity of the system. Alkalinity is modeled as a conservative substance, being only advected and diffused. Suspended solids influence both the density and light regimes. Suspended solids are subjected to advection, diffusion, and settling. A more detailed description of the final model used in this study is available in the revised CE-QUAL-R1 User's Manual (Environmental Laboratory, 1986).

Modeling Approach

For this application of CE-QUAL-R1, Lake Ashtabula was represented as a series of three pools separated at the two reservoir crossings, Keyes Crossing and Ashtabula Crossing (Figure 1). The reservoir width is reduced from 549 m to 39 m and from 533 m to 50 m by the bridge embankments at the two crossings, respectively. Thus, each crossing was modeled as though it were a dam with an outlet structure, and the one-dimensional assumption was considered applicable to each pool. With this approach, violations of the one-dimensional assumption would not be as severe, and the headwater pool could represent the settling basin. The physical characteristics of the three modeled pools, on the first day of simulations, are given in Table 2. This modeling approach follows from previous work of the St. Paul District (Holme, Bakke, and Wlosinski, 1985).

Model Evaluation

Both graphical and statistical comparisons were made of predicted versus measured values. The statistic used was the Reliability Index (RI) of Leggett and Williams (1981). The RI is scale-variant and does not depend on which one of the values being compared is greater than the other. In the case of perfect prediction, the RI value would be 1.0. If all comparisons differed by a factor or two, the RI value would be 2.0. An RI of 10 signifies that values are an average of one order of magnitude apart. An RI was calculated for each variable for each sampling period over all depths as well as for each variable over depths and sampling periods. Over 300 comparisons were made for each pool. Comparisons were made for temperature, total organic carbon (TOC),

phosphorus, ammonia, total algae, nitrite-nitrate, dissolved oxygen, pH, and TDS. For each calibration simulation, graphical and statistical comparisons were made for all three pools. For each pool, only the data from the deepest station was used for model evaluation. Only one value, for each sampling station for each day, was measured for algae. Because at least two values are needed for calculating the RI, the one measured concentration was arbitrarily used at 0.1 and 1.0 meters.

Data

Most of the data required for this evaluation had already been compiled and were available from the St. Paul District. These data included initial conditions, driving variables (also termed boundary conditions or updates), and calibration data.

Initial conditions and calibration data were taken from data collected on a biweekly basis at 1 meter depth intervals during April through September 1981 (US Geological Survey, 1982). Values for initial conditions for the three pools are included in Appendix A.

Meteorological data were obtained from the National Oceanic and Atmospheric Administration's station at Fargo, North Dakota, 110 kilometers to the east of Lake Ashtabula. Data were averaged over 24 hours, the simulations time step. Discharge, temperature, and constituent concentrations, for inflow to pool 1, were obtained from daily records at the Cooperstown gaging station (US Geological Survey, 1982). Outflow concentrations from pools 1 and 2 were used as inflow values for their respective downstream pools. An additional tributary representing Baldhill Creek was included in pool three. Measured

data for this tributary were determined from the Dazey gaging station (US Geological Survey, 1982).

Coefficients for power curves which describe the physical characteristics of the reservoir were estimated from sedimentation survey data using regression techniques. Correlation coefficients for the stage-area relationship were 0.995, 0.995, and 0.986 for pools 1, 2, and 3, respectively. Coefficients dealing with light penetration and mixing were initially estimated using information supplied in the User's Manual (Environmental Laboratory, 1986), and were calibrated using measured data from pool 1.

During calibration of CE-THERM-R1 by the St. Paul District, initial calculations to establish the pool water levels and flows at the two crossing sites were unsatisfactory (Holme, Bakke, and Wlosinski, 1985). The discrepancies resulted from not including rain falling directly onto the lake surface. Because rainfall was not included in the original version of CE-THERM-R1, the model was modified to allow for rainfall events. Rainfall values were added to the data sets as driving variables. Daily values of rainfall averaged over stations located at Valley City and Cooperstown, North Dakota, were used. Values were obtained from the monthly summaries of climatological data supplied by the National Oceanic and Atmospheric Administration. These same changes were made for the CE-QUAL-R1 simulations. The amount of evaporation during the period of simulation was estimated by using pan evaporation data from the weather station at Carrington, North Dakota, multiplied by a pan coefficient of 0.7 (US Department of Commerce, 1968).

Initial estimates for the biological and chemical coefficients were obtained from the CE-QUAL-R1 Users Manual (Environmental Laboratory, 1986) and from previous modeling studies (Wlosinski and Collins, 1985 a,b). Simulations from all three pools were used for model evaluation. Flux values, which are rates of change between variables, as well as concentration predictions, were taken into account when estimating coefficients for the next calibration simulation. A list of coefficients used in final calibration simulations is provided in Appendix B.

Computers

The initial calibration of CE-THERM-R1 by the St. Paul District used the Boeing Mainstream-EKS interactive time-sharing computer system. Because the Corps of Engineers no longer maintains a contract with this firm, the St. Paul District required that both CE-THERM-R1 and CE-QUAL-R1 for Lake Ashtubula be made operational on the Control Data Corporation (CDC) system. Calibration simulations for CE-QUAL-R1 were made on a VAX 11/750, the in-house computer for the WQMG, after which time the models were translated and tested on the CDC system.

Command Files

Command files were written, tested, and are provided to the District as an aid in using both CE-THERM-R1 and CE-QUAL-R1. Command files help to make the Lake Ashtubula models "user friendly". After reading the command file, the user need only respond to the computer questions to be able to use the models. Seperate command files have been established for CE-THERM-R1

(ASHPRO1) and CE-QUAL-R1 (ASHPROQ). Information concerning use of the command files, data files established, and output files is included as Appendix C.

PART III: RESULTS AND DISCUSSION

Statistical results from the final calibration of the Lake Ashtubula water quality model are presented in Table 3. Graphs, comparing predicted values (solid line) to measured data (x's), are presented for pool 1 (Figure 2), pool 2 (Figure 3), and pool 3 (Figure 4). The average RI, for the nine variables for which the measured data were available, was 1.98, 2.16, and 2.08 for pools one through three, respectively. These values compare favorably with RI values, using the same variables, from other studies. Calibration of CE-QUAL-R1 for DeGray Lake in Arkansas yielded an average value of 2.63 (Wlosinski and Collins, 1985a), and for Eau Galle Reservoir in Wisconsin, 2.27 (Wlosinski and Collins, 1985b). The overall RI for temperature from the thermal model was 1.07, and for total dissolved solids 1.10. The comparable RI values from CE-QUAL-R1 were 1.08 and 1.11, respectively.

All algorithms and coefficients for the Lake Ashtabula Model are the same as described in the CE-QUAL-R1 User's Manual (Environmental Laboratory, 1986), except for the utilization of nitrogen by algae during photosynthesis. Two forms of nitrogen, ammonia and nitrite-nitrate, are modeled. In the original model, the amount of nitrogen utilized from either compartment was based upon the ratio of nitrogen in that compartment compared to total nitrogen. This assumption continually led to poor predictions (RI values above 6.0) for nitrite-nitrate. The algorithm was modified to include a coefficient representing the fraction of total nitrogen, utilized during photosysthesis, which was removed from each of the two nitrogen compartments. This formulation gave better predictions and was retained in the model. The RI for nitrite-nitrate after changes were made ranged from 3.51 to 4.97 for the three

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pools. The nitrogen cycle may not include other processes important at Lake Ashtabula. Peterka (1970) found that 80 percent of the standing crop of algae was due to Aphanizomenon, a Cyanophyte (blue green algae). Blue green algae are able to fix elemental nitrogen for use in photosynthesis, a process which is not included in the water quality model.

Although the overall RI for all variables was considered satisfactory, individual graphs of some variables appear to show that the model does not predict all of the major dynamics measured. For example, predictions of algae in pool 3 represent bloom conditions in late July and early August, whereas very little algae was measured at the deepest station on these dates. In part, this discrepancy is a result of variability within each pool. An example of this variability, representing algae in pool 3, is shown in Figure 5. The solid line represents model predictions, the x´s represent algal concentrations at the deepest station, and the solid circles represent algal concentrations at other stations in pool 3. When data from other stations are considered, the algal predictions in July and August appear more reasonable.

Oxygen is usually considered the most important variable when assessing the overall water quality of a reservoir. Simulation of oxygen was considered satisfactory, because the model correctly predicted slight stratification in pools 1 and 2, and anoxic conditions in pool 3. It appears that the lowest concentrations of oxygen in the hypolimnion of pool 3 occurred immediately after an algal bloom with very little temperature stratification. High winds between the July 28 and August 12 sampling periods were probably responsible for the reoxygenation of hypolimnitic waters. Worst case conditions for

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oxygen would probably occur after an algal bloom accompanied by low wind, heavy cloud cover, and constant or rising water temperatures.

Final predicted flux values also appeared reasonable. Although no measured data were available for comparison with predicted values, a number of fluxes were compared to literature values. The sediment oxygen demand (SOD) for pools 1, 2, and 3 was 0.40, 0.35, and 0.31 grams per square meter per day, respectively. These values are within the range of 46 literature values for lakes and reservoirs as reported by Martin, Effler, and Dobi (1985). Phytoplankton gross production was predicted to be 3.9, 4.0, and 4.7 grams of oxygen per square meter per day. Measured values at Lake Ashtabula during 1966 and 1967 ranged from 2.3 to 18.2 grams of oxygen per square meter per day (Peterka and Reid, 1968).

The percentage of each negative and positive oxygen flux is presented in Table 4. Algal respiration and DOM decay were predicted to be the most important processes affecting oxygen utilization. In pool 1 macrophyte respiration was also a large sink for dissolved oxygen. Since the majority of predicted DOM was created by algae, algal control appears to be necessary in order to increase oxygen concentrations in the hypolimnion. In pool 1, algal photosynthesis was responsible for most of the positive flux of oxygen, whereas, in pools 2 and 3 most of the oxygen is supplied through surface exchange. Controlling algae in pool 1 would not have a negative effect on oxygen concentrations, because exchange of oxygen at the air-water boundary could replace the oxygen not created during photosynthesis.

PART IV: SUMMARY AND CONCLUSIONS

A mathematical model, representing Lake Ashtabula, was developed based on the one-dimensional water quality model, CE-QUAL-R1. The reservoir was represented as three pools, separated at two river crossings. This allowed simulation of both longitudinal and vertical variation in water quality. Graphical and statistical comparisons were made for over 1200 predicted versus observed values which were measured in 1981. Variables included in the evaluation were temperature, TOC, phosphorus, ammonia, total algae, nitrite-nitrate, dissolved oxygen, pH, and TDS.

The average RI for all comparisons was 1.98, 2.16, and 2.08 for pools 1, 2, and 3, respectively. This compared favorably with RI values from other reservoir studies. Predicted flux values also appeared to be reasonable.

Both CE-QUAL-R1, and the thermal model representing Lake Ashtabula (CE-THERM-R1), now reside on the St. Paul District account of the CDC computer system. Command files for both models were created to allow District personnel to easily use the models.

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Table 1

Description of Baldhill Dam and Lake Ashtabula Reservoir

Baldhill Dam

Type	Compacted earth fill
Length	502.9 meters
Crest	Elevation 389.7 meters msl
Top Width	6.0 meters
Maximum Height	18.6 meters
Freeboard above Project Pool	3.8 meters

Reservoir

Contributing Drainage Area	4950 km^2
Elevation	385.9 meters msl
Storage	84,626,000 m^3
Area	21,449,000 m^2
Average Depth	3.9 m
Length	43.4 km
Maximum Width	1.0 km
Length of Shoreline	125.5 km
Mean Annual Flow (Sheyenne River and Baldhill Creek)	105,635,000 m^3
Average Residence Time	292.4 days

Table 2

Physical Characteristics of the Three Modeled Pools

	Pool 1 (Upstream)	Pool 2 (Middle)	Pool 3 (Downstream)
Storage	$11,817,000 \ m^3$	$15,523,000 \ m^3$	$62,174,000 \ m^3$
Area	$5,220,000 \ m^2$	$4,200,000 \ m^2$	$9,720,000 \ m^2$
Length	6.7 km	7.6 km	19.1 km
Maximum width	0.8 km	1.0 km	1.0 km
Mean depth	2.3 m	3.7 m	6.4 m
Mean annual flow (Sheyenne River)	$92,053,00 \ m^3$	$92,053,000 \ m^3$	$105,635,000 \ m^3$
Average residence time	47 days	62 days	215 days

Table 3

Reliability Index Values for the Three Pools of the
Lake Ashtabula Water Quality Model

Variable	Pool 1	Pool 2	Pool 3
Temperature	1.06	1.09	1.10
TOC	1.40	1.58	1.63
Phosphorus	2.53	3.16	2.22
Ammonia	2.15	2.05	1.89
Algae	3.80	3.27	4.20
Nitrite-Nitrate	3.51	4.97	4.24
Dissolved Oxygen	1.18	1.20	1.31
pH	1.04	1.02	1.03
TDS	1.11	1.11	1.10
Average	1.98	2.16	2.08

Table 4

Percentages of Negative and Positive Oxygen
Flux for Different Processes

Negative Oxygen Flux	Pool 1	Pool 2	Pool 3
algal respiration	29.5	37.9	44.0
ammonia decay	3.2	7.6	8.0
detritus decay	1.0	1.5	.7
sediment decay	7.2	6.1	5.0
zooplankton respiration	1.3	2.5	1.0
anaerobic oxidation	.2	.1	.2
fish respiration	1.6	1.2	1.0
labile DOM decay	15.1	15.6	14.6
outflow	4.3	6.7	2.1
refractory DOM decay	8.3	17.5	19.3
macrophyte respiration	28.3	3.3	4.0

Positive Oxygen Flux			
algal photosynthesis	50.2	38.1	39.4
inflow	2.5	3.8	1.4
surface exchange	12.7	54.9	55.5
macrophyte photosynthesis	34.6	3.2	3.7
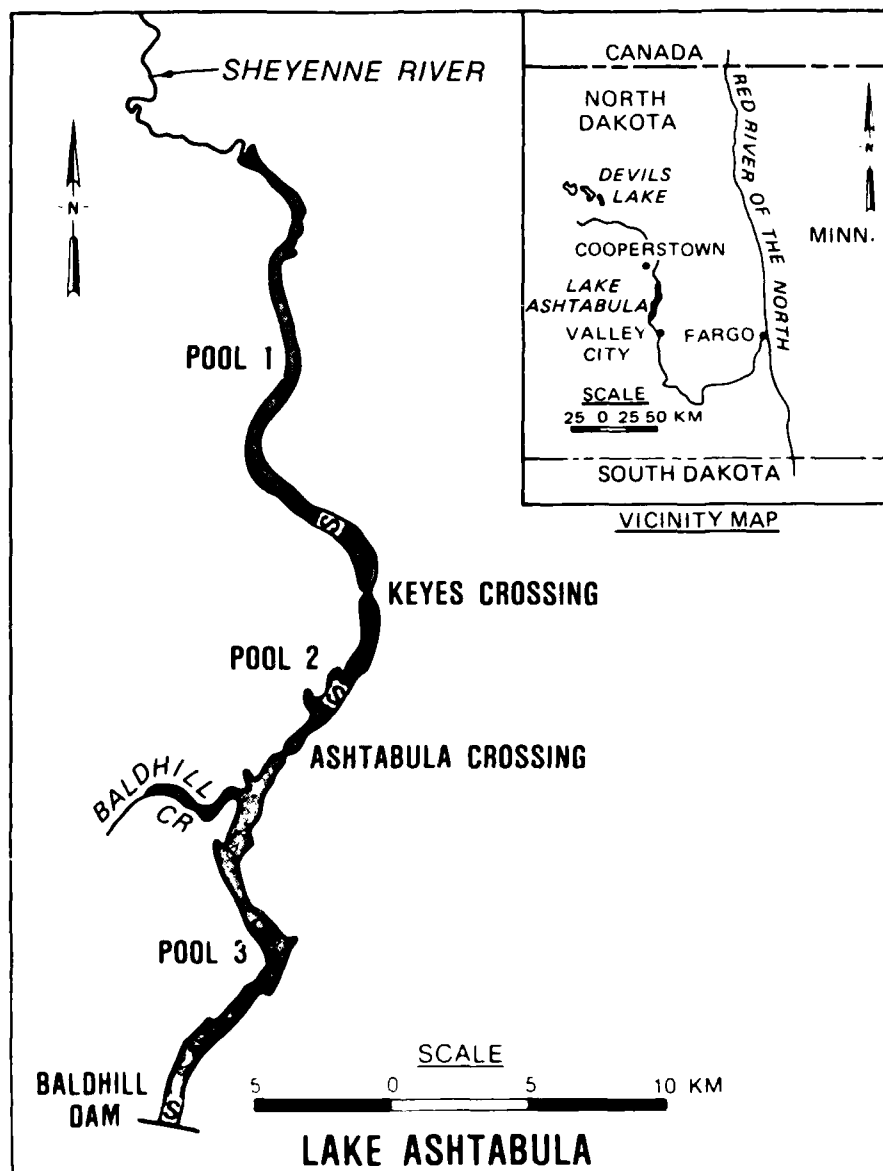
LAKE ASHTABULA

SHEYENNE RIVER

POOL 1

KEYES CROSSING

POOL 2

ASHTABULA CROSSING

BALDHILL CR

POOL 3

BALDHILL DAM

SCALE
5   0   5   10 KM

VICINITY MAP

CANADA

NORTH DAKOTA

DEVILS LAKE

COOPERSTOWN

LAKE ASHTABULA

VALLEY CITY

FARGO

MINN.

RED RIVER OF THE NORTH

SCALE
25 0 25 50 KM

SOUTH DAKOTA

Figure 2. Predicted (solid line) versus measured (x's) values for Pool 1.

Figure 2 (continued)

Figure 2 (continued)

Figure 2 (continued)

Figure 2 (continued)

Figure 2 (continued)

Figure 2 (continued)

Figure 2 (continued)

Figure 2 (concluded)
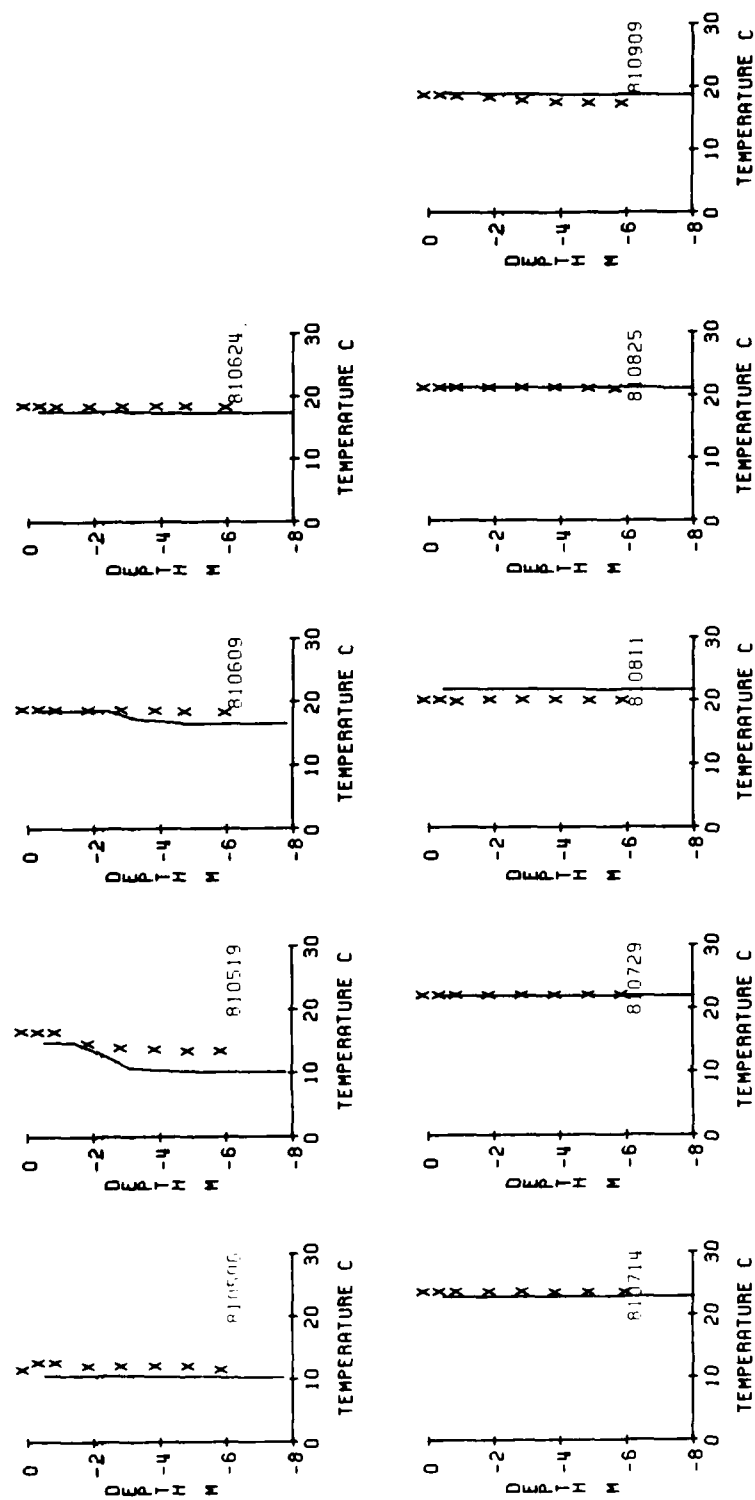
Figure 3. Predicted (solid line) versus measured (x's) values for Pool 2.
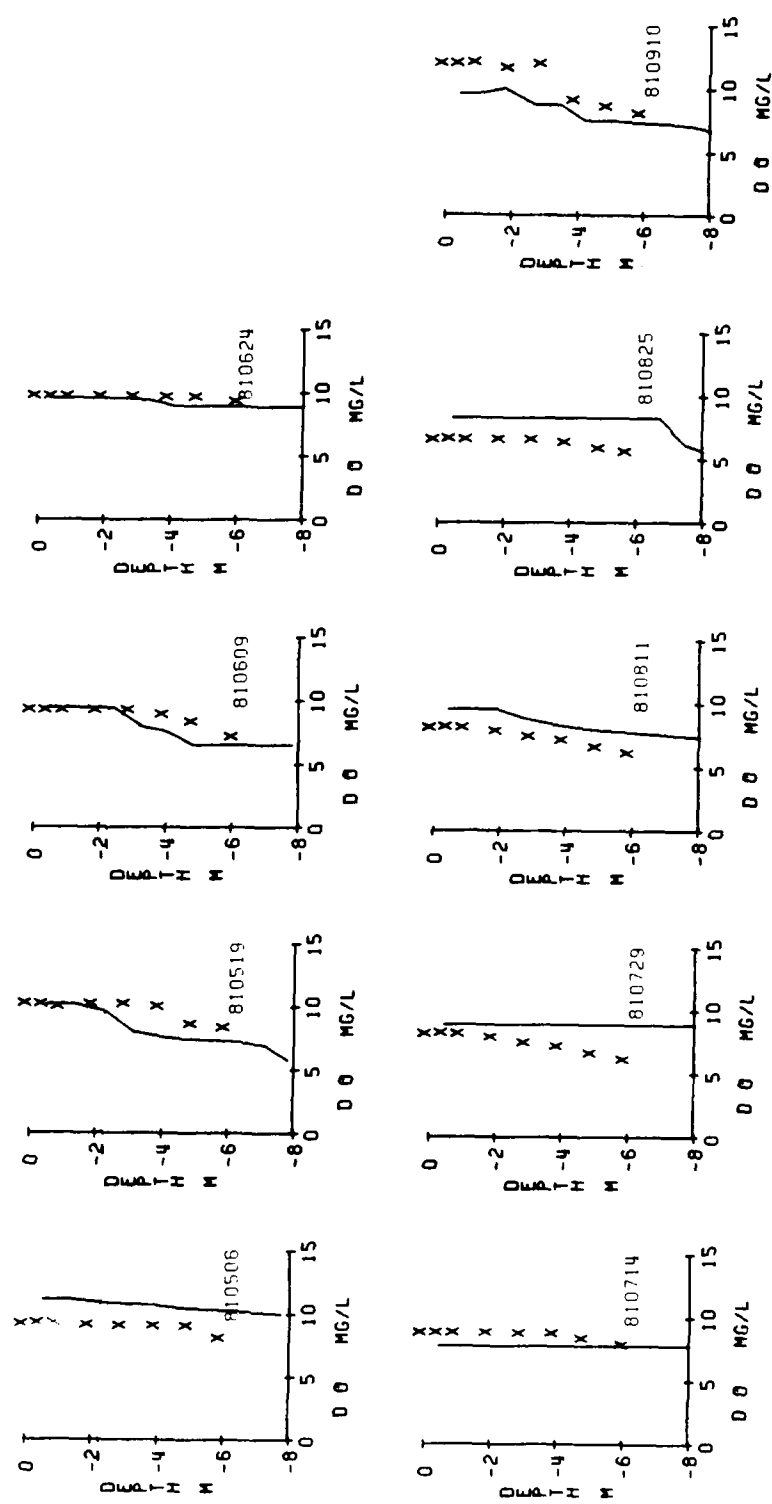
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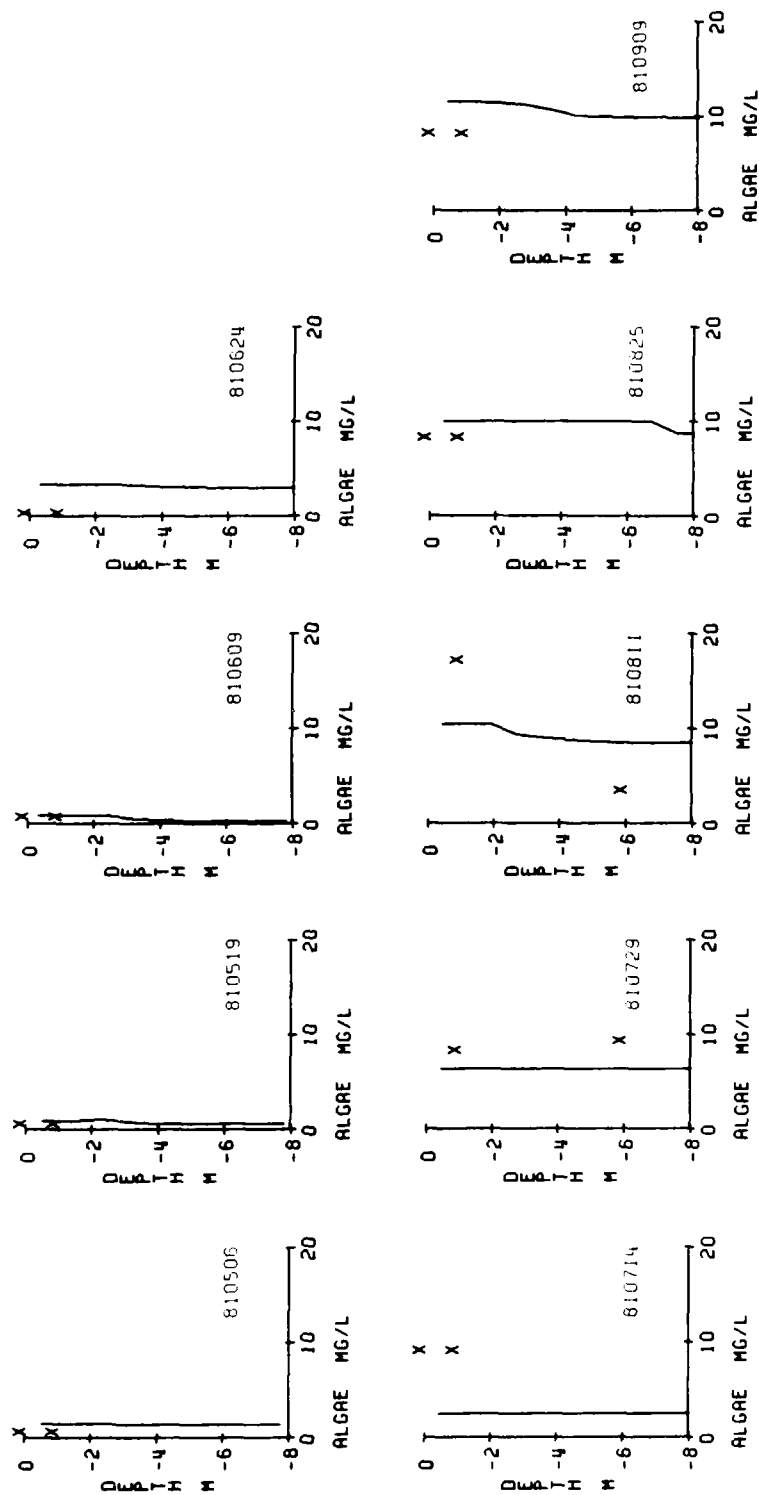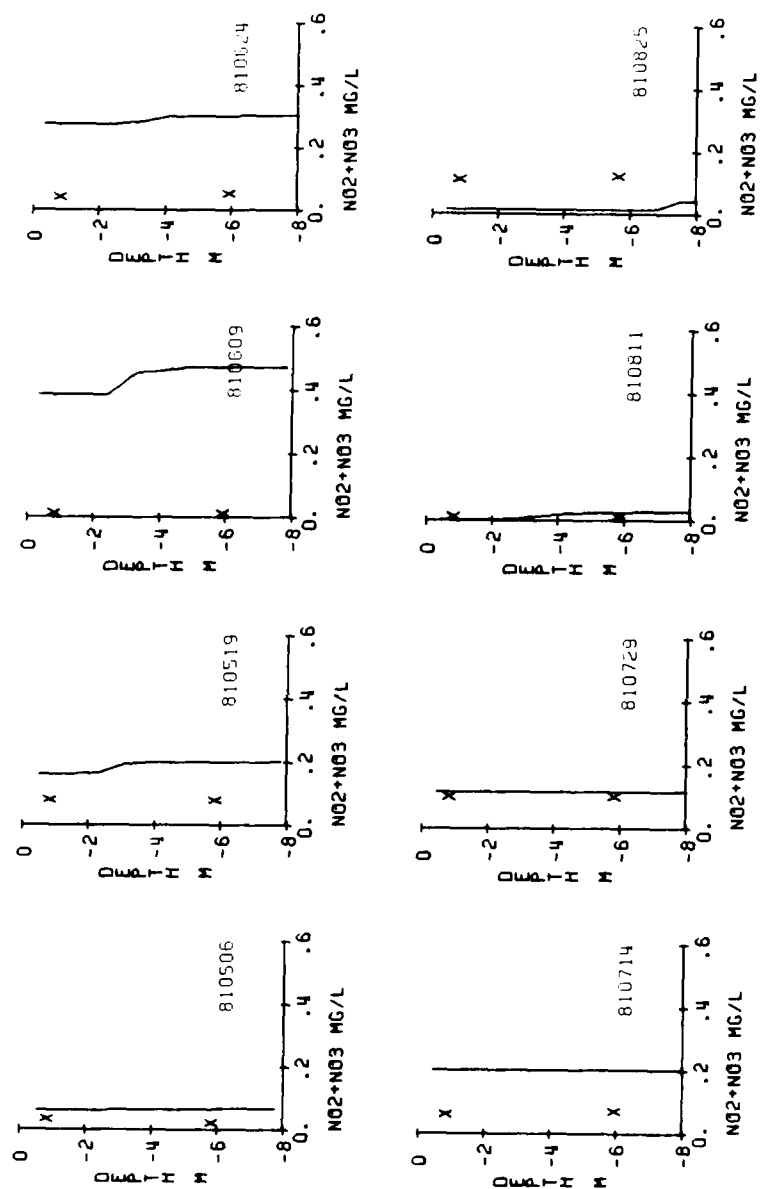
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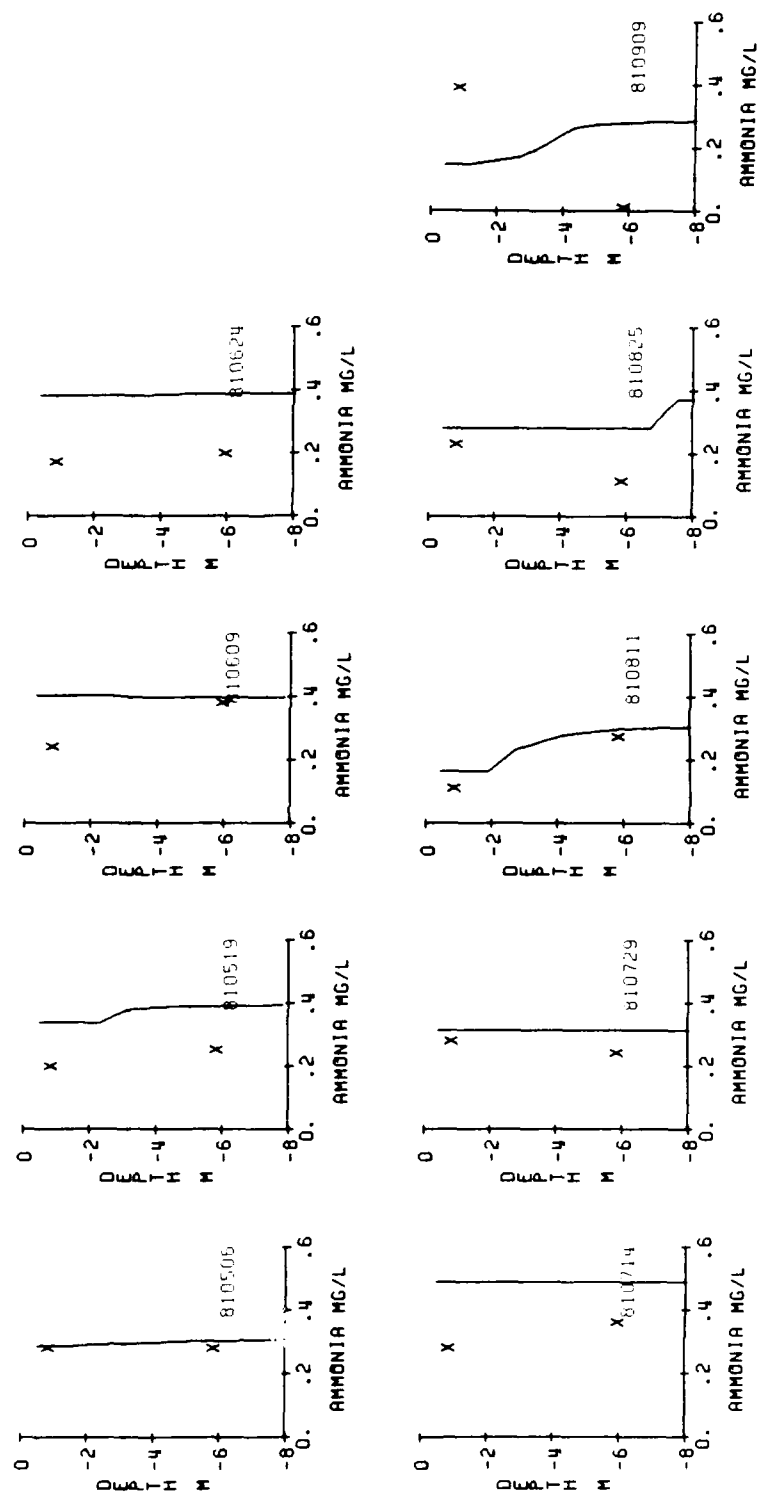
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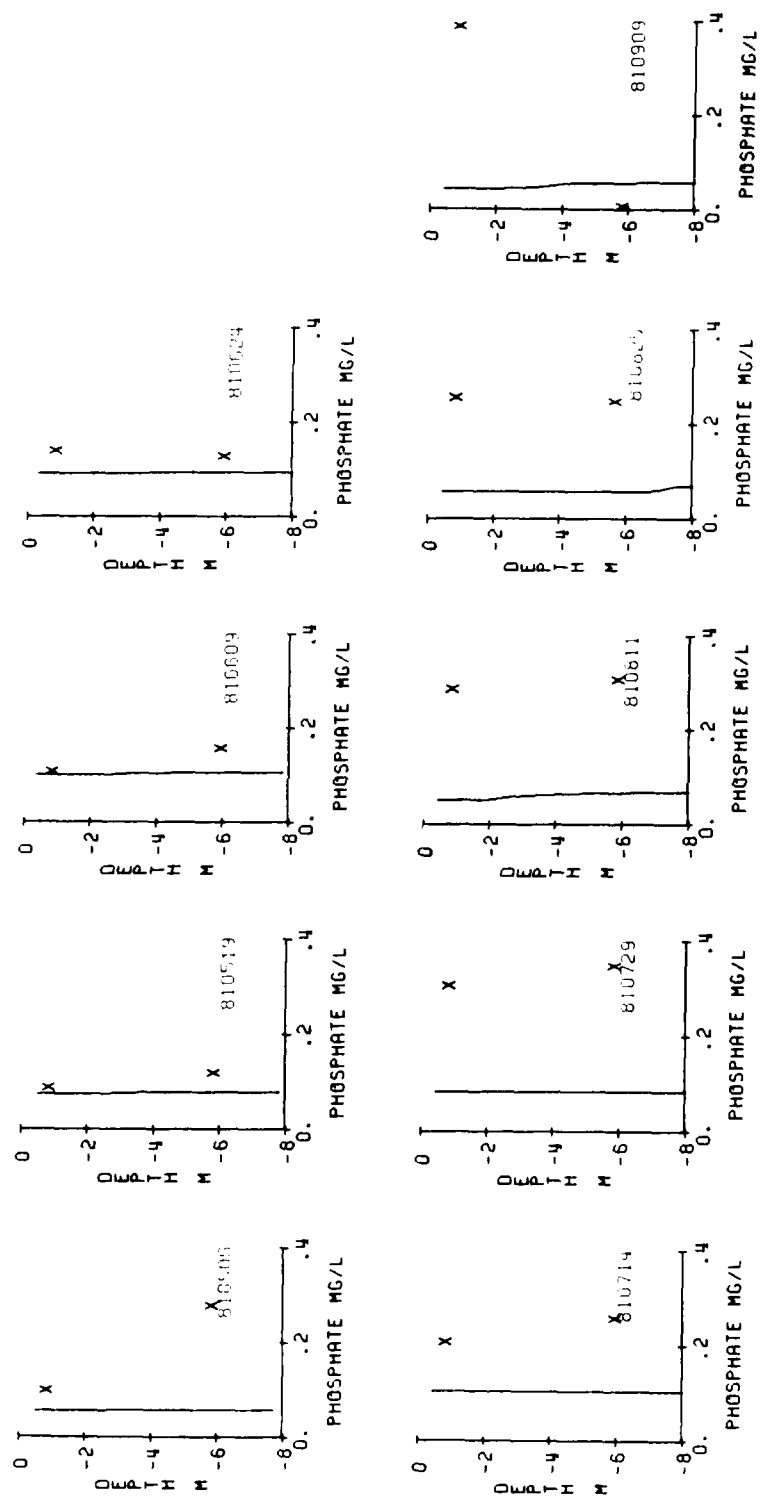
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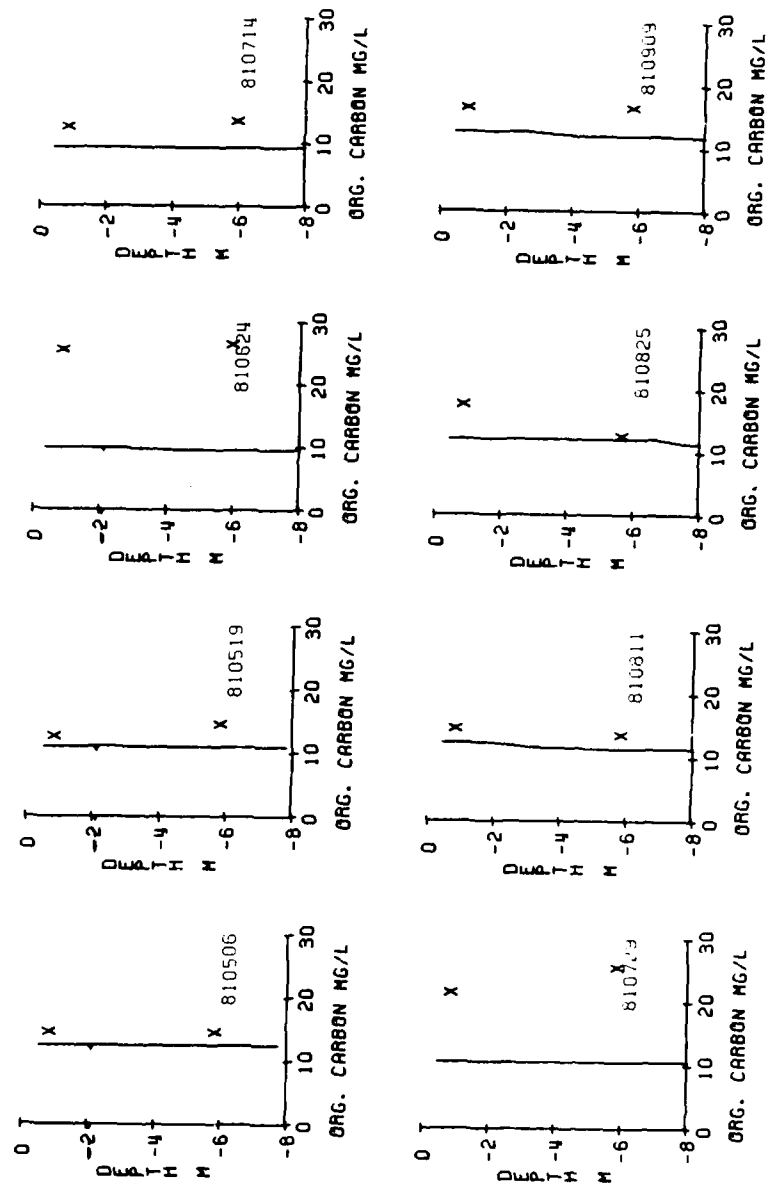
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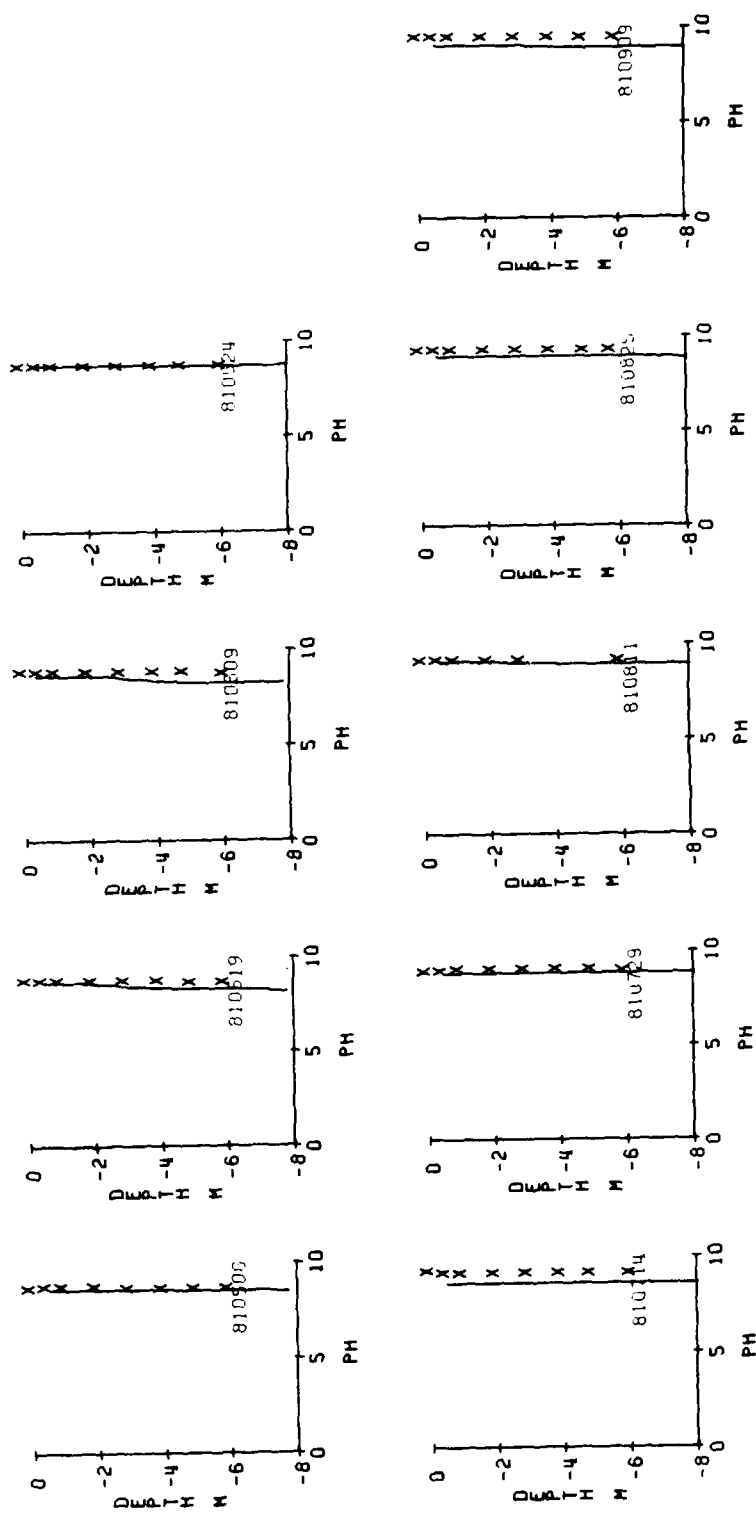
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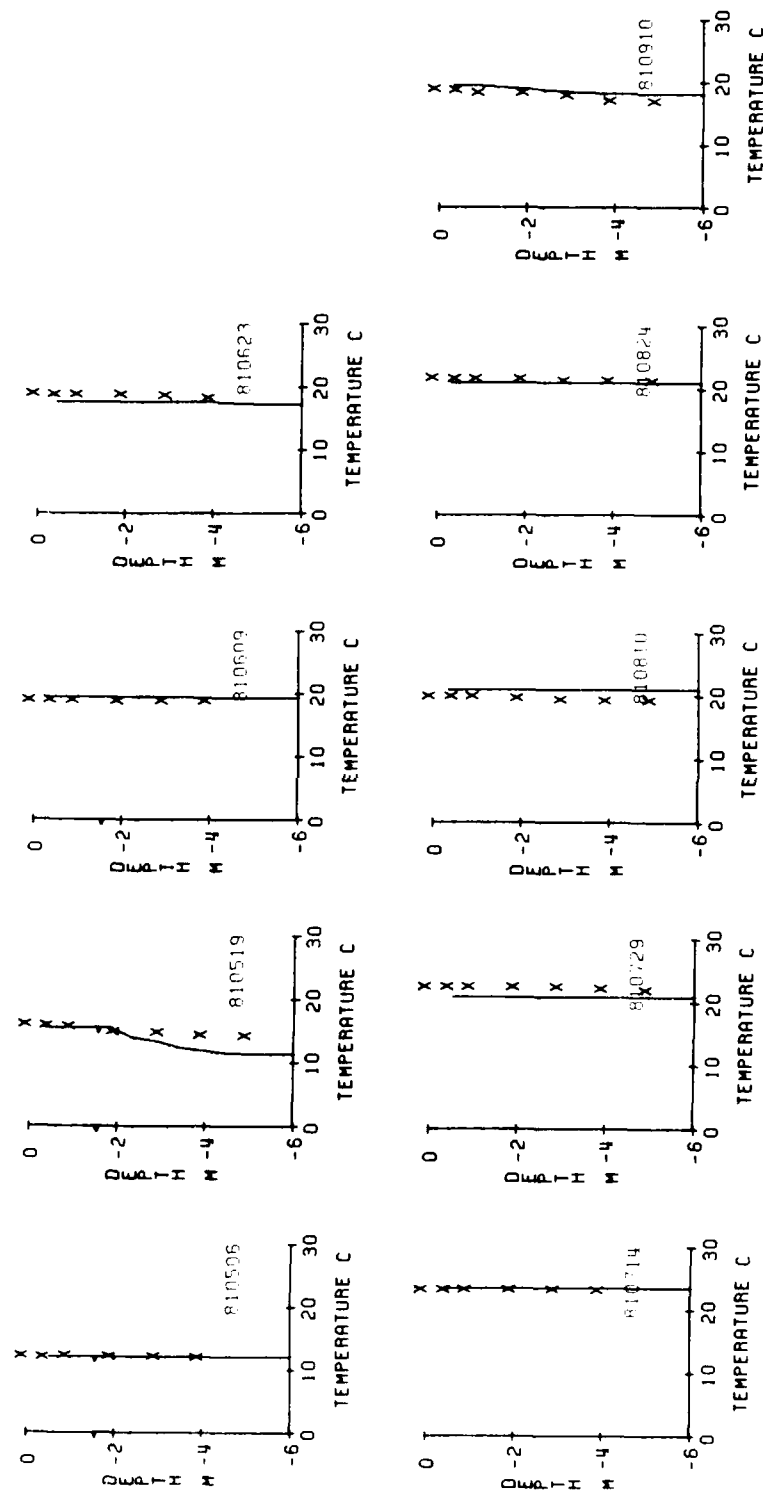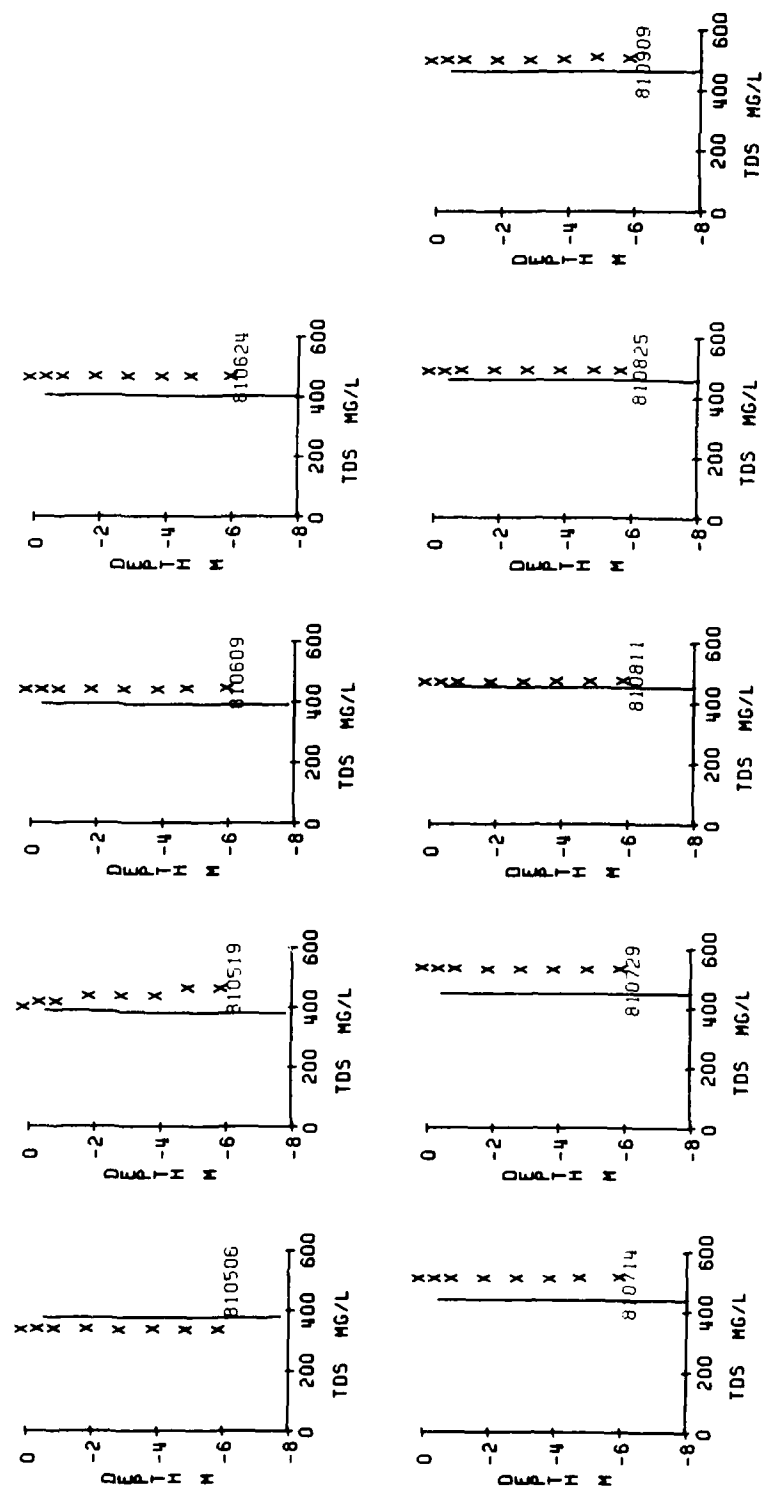
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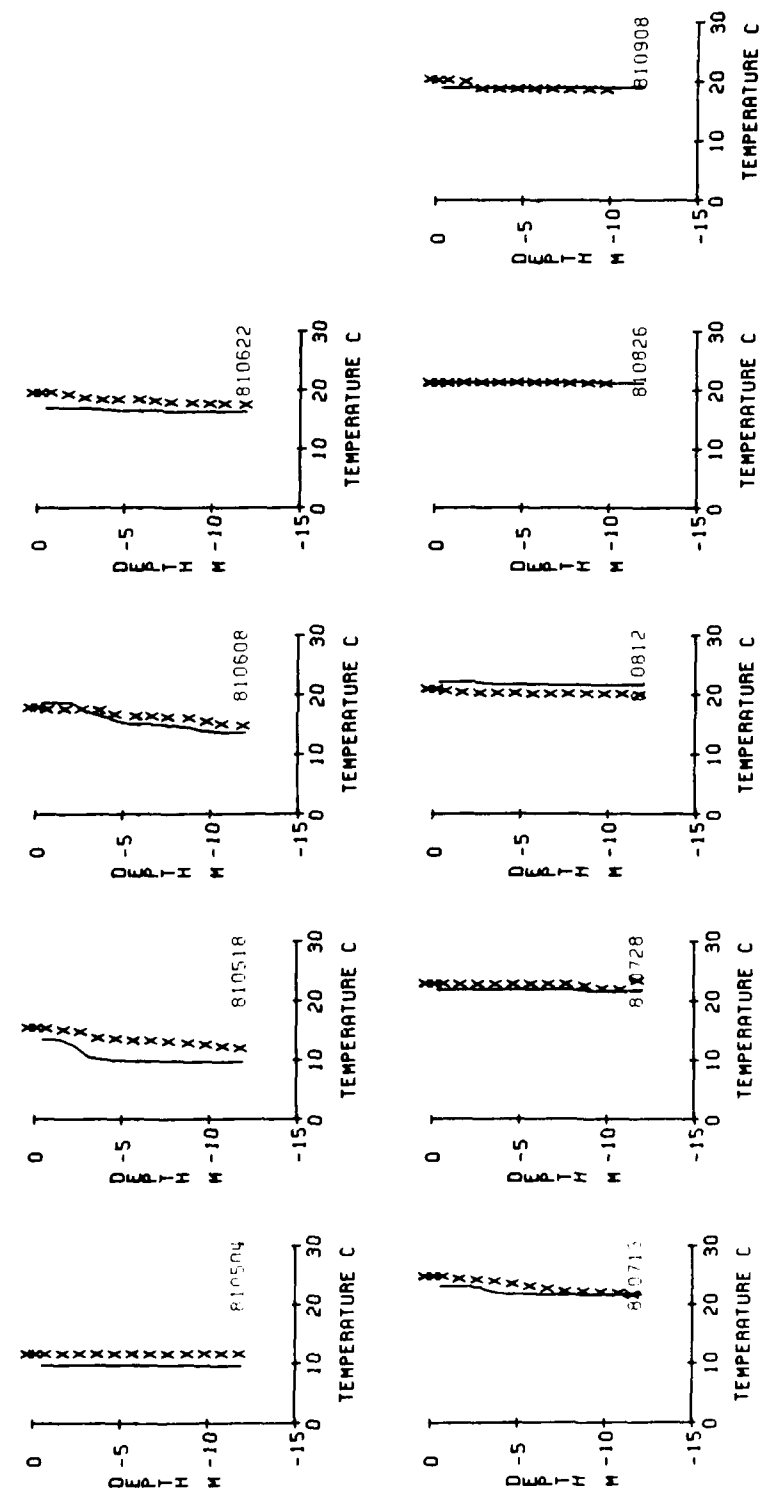
Figure 4. Predicted (solid line) versus measured (x's) values for Pool 3.
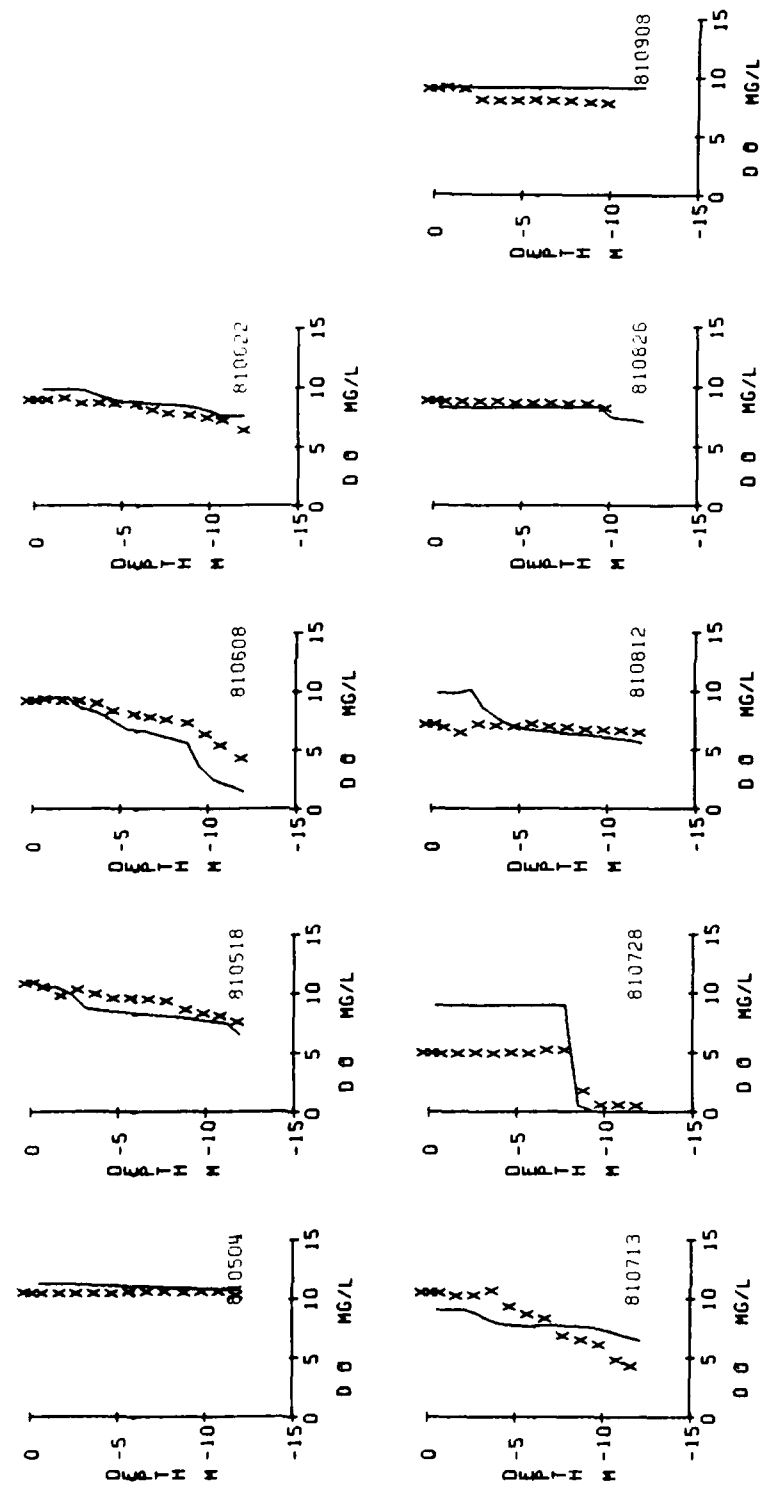
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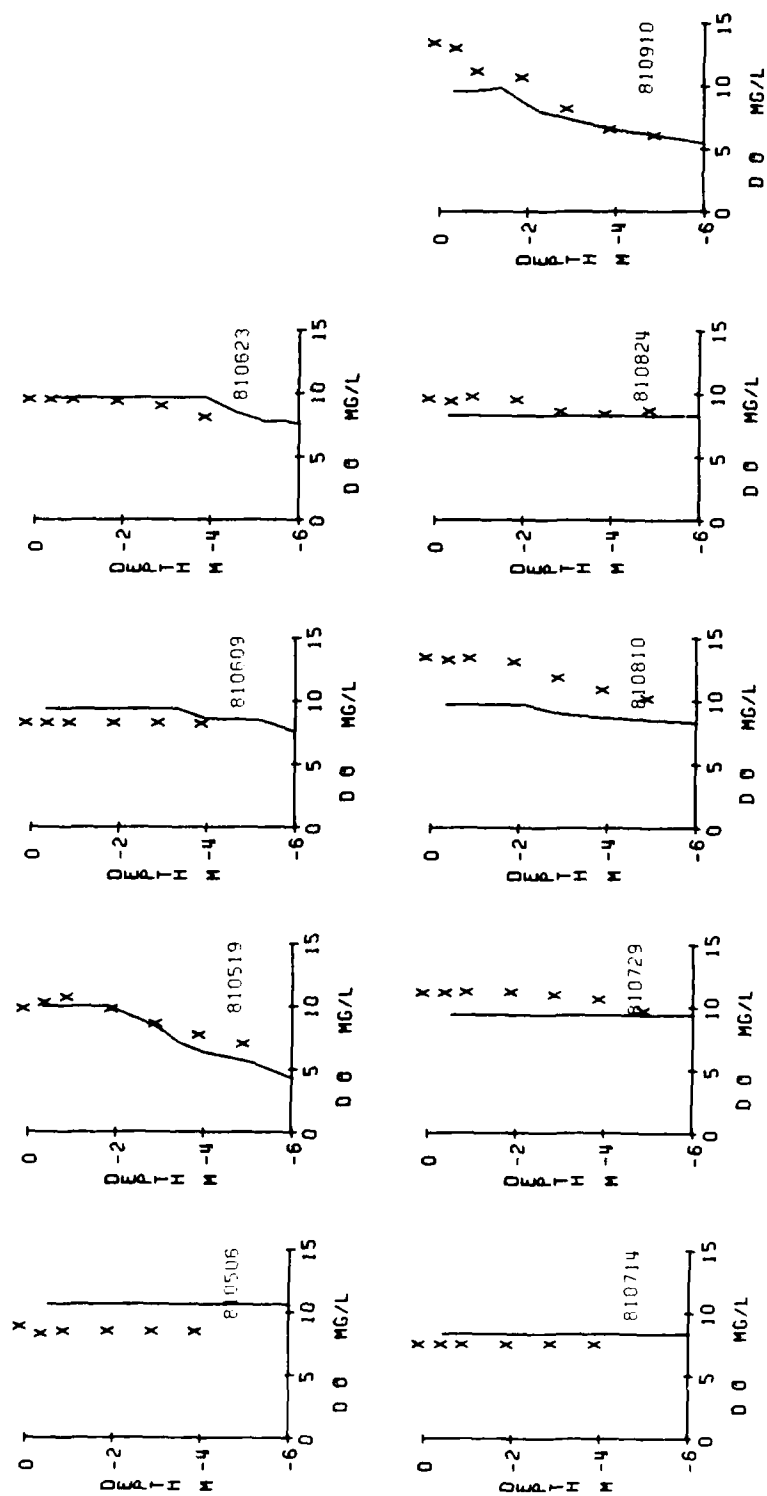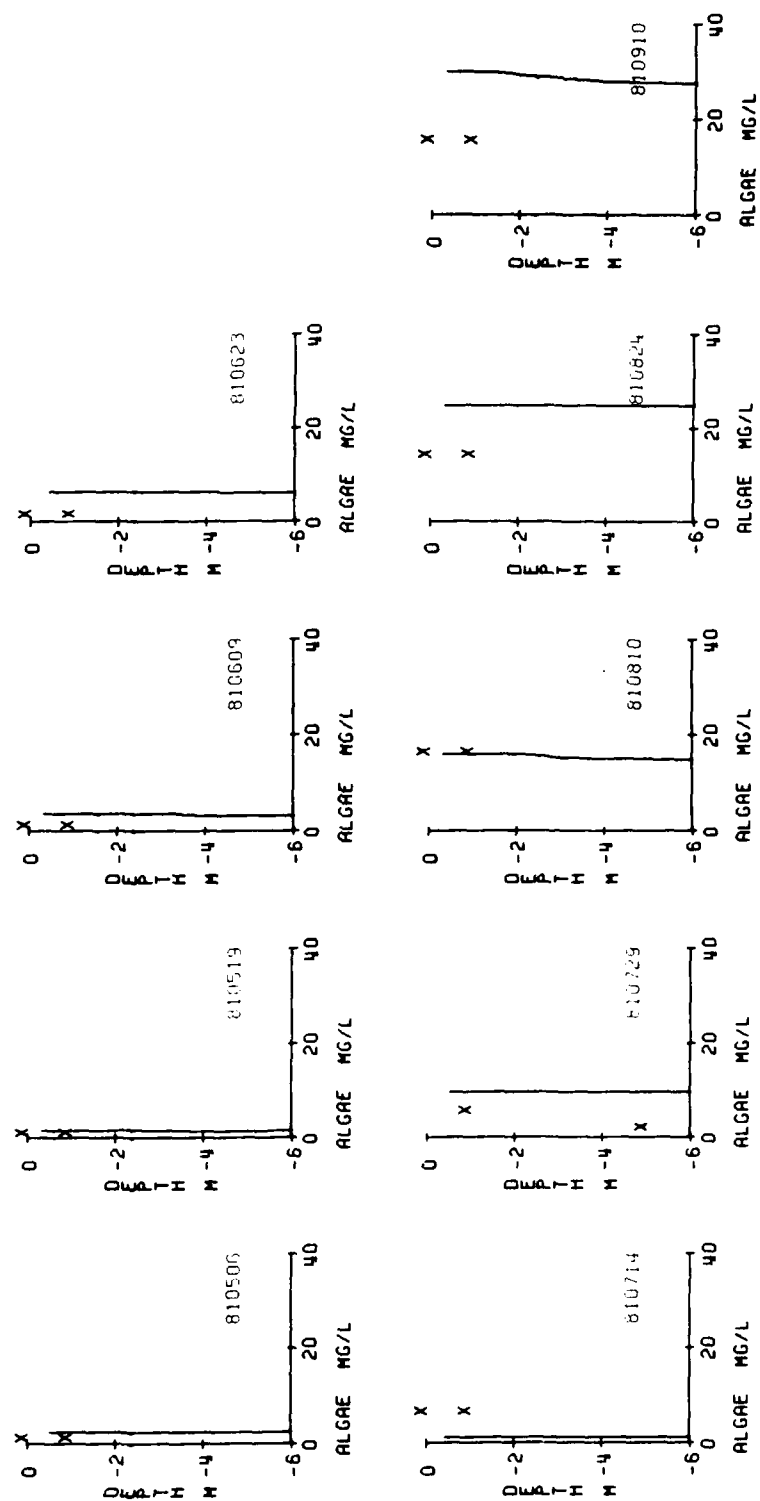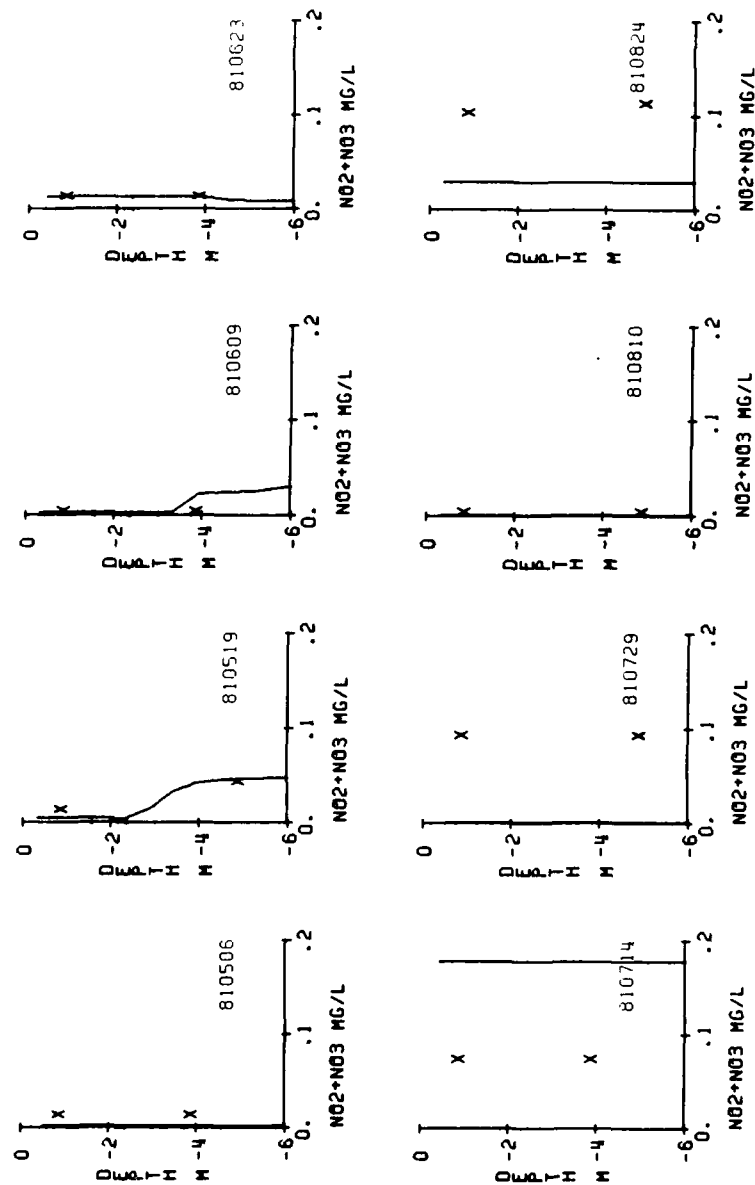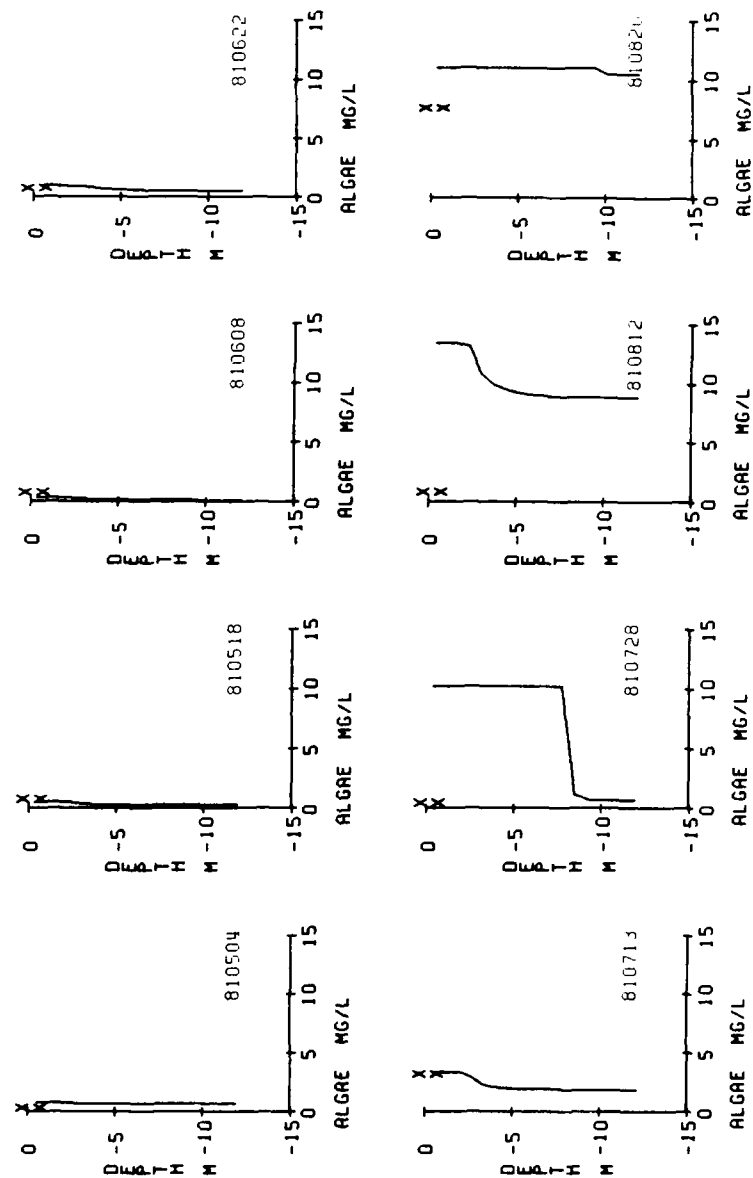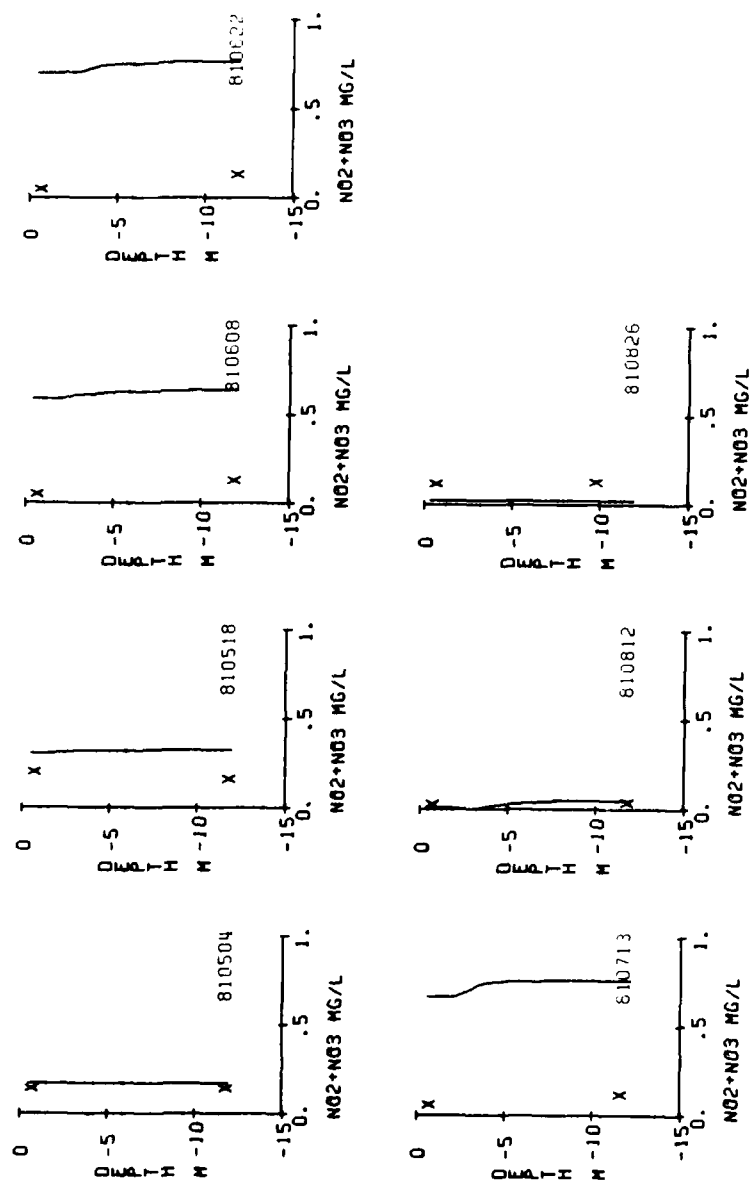
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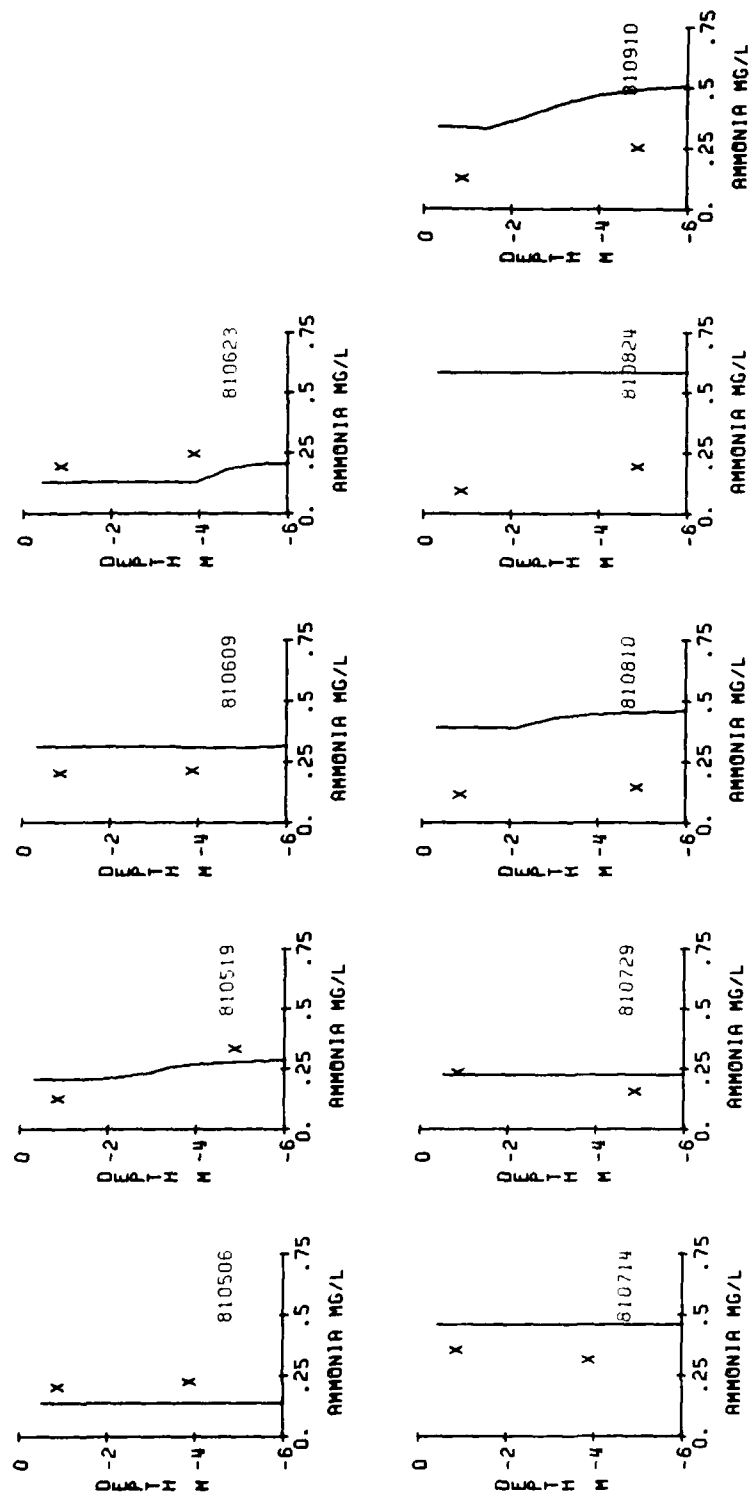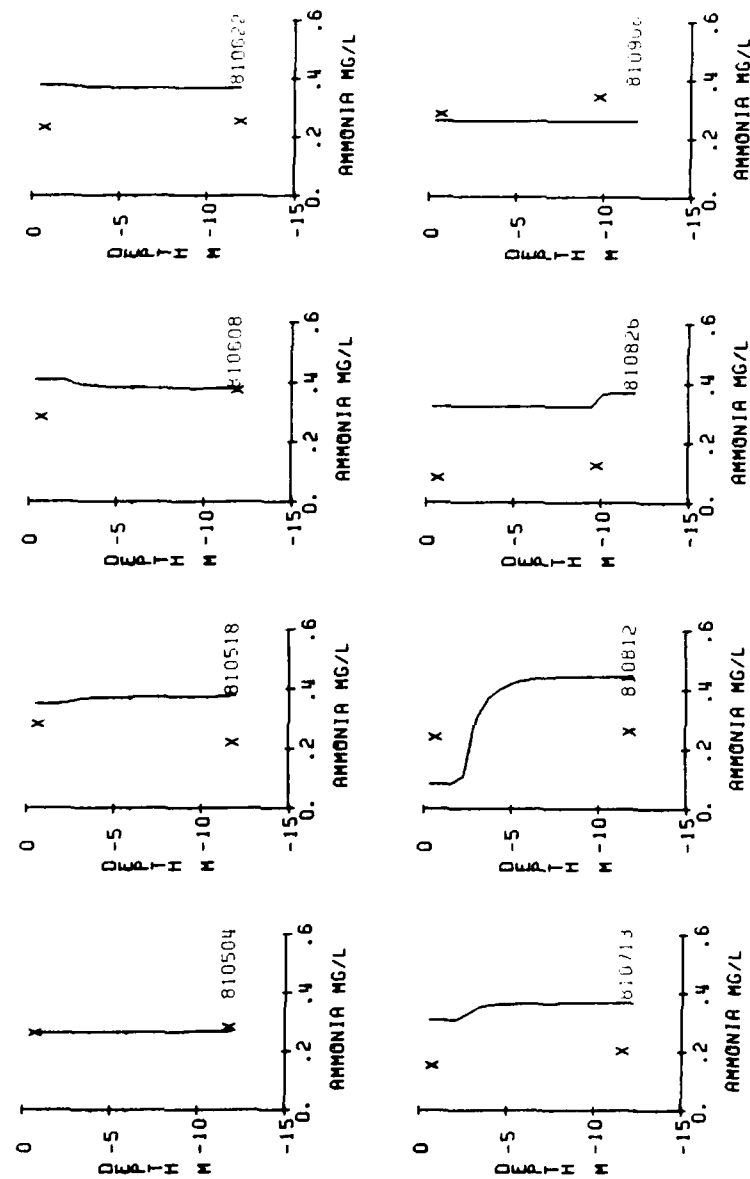
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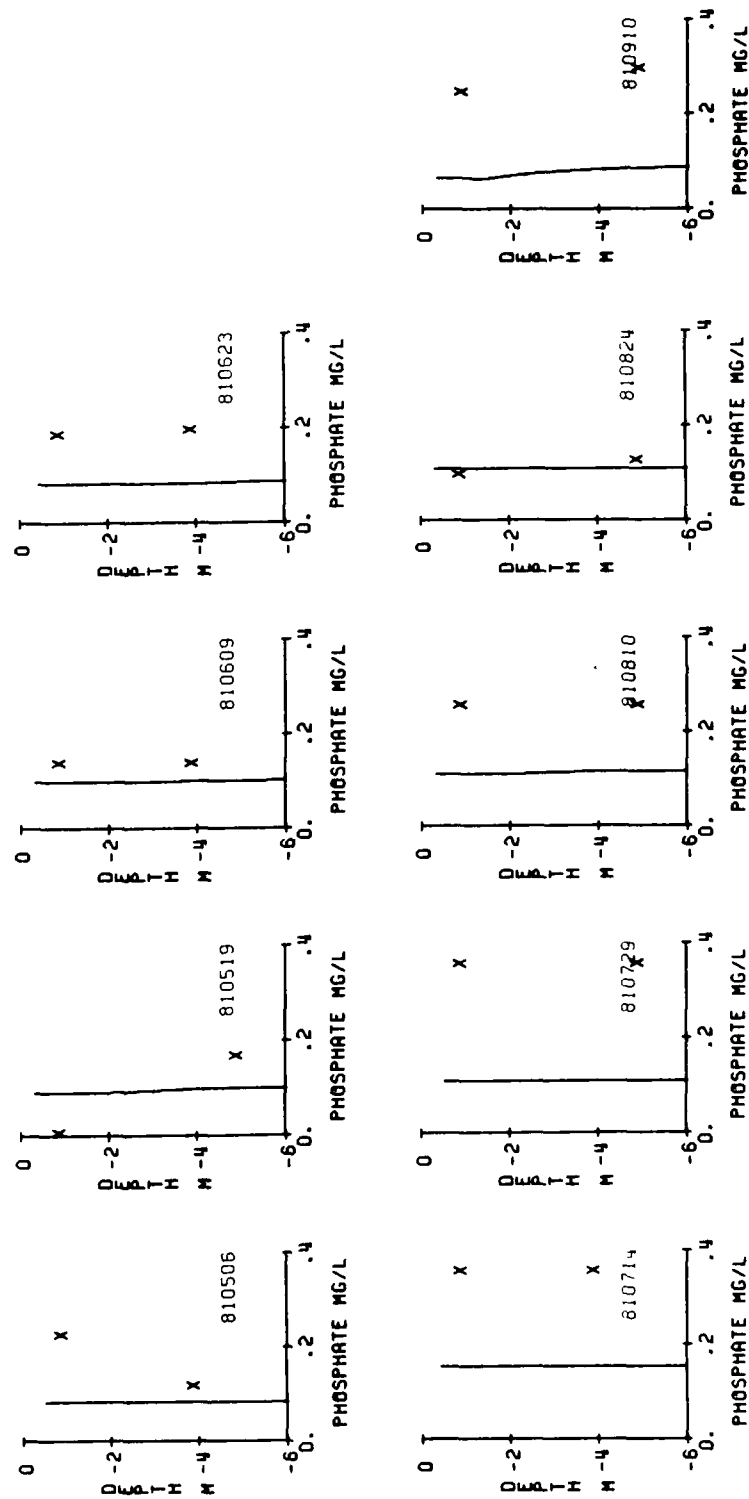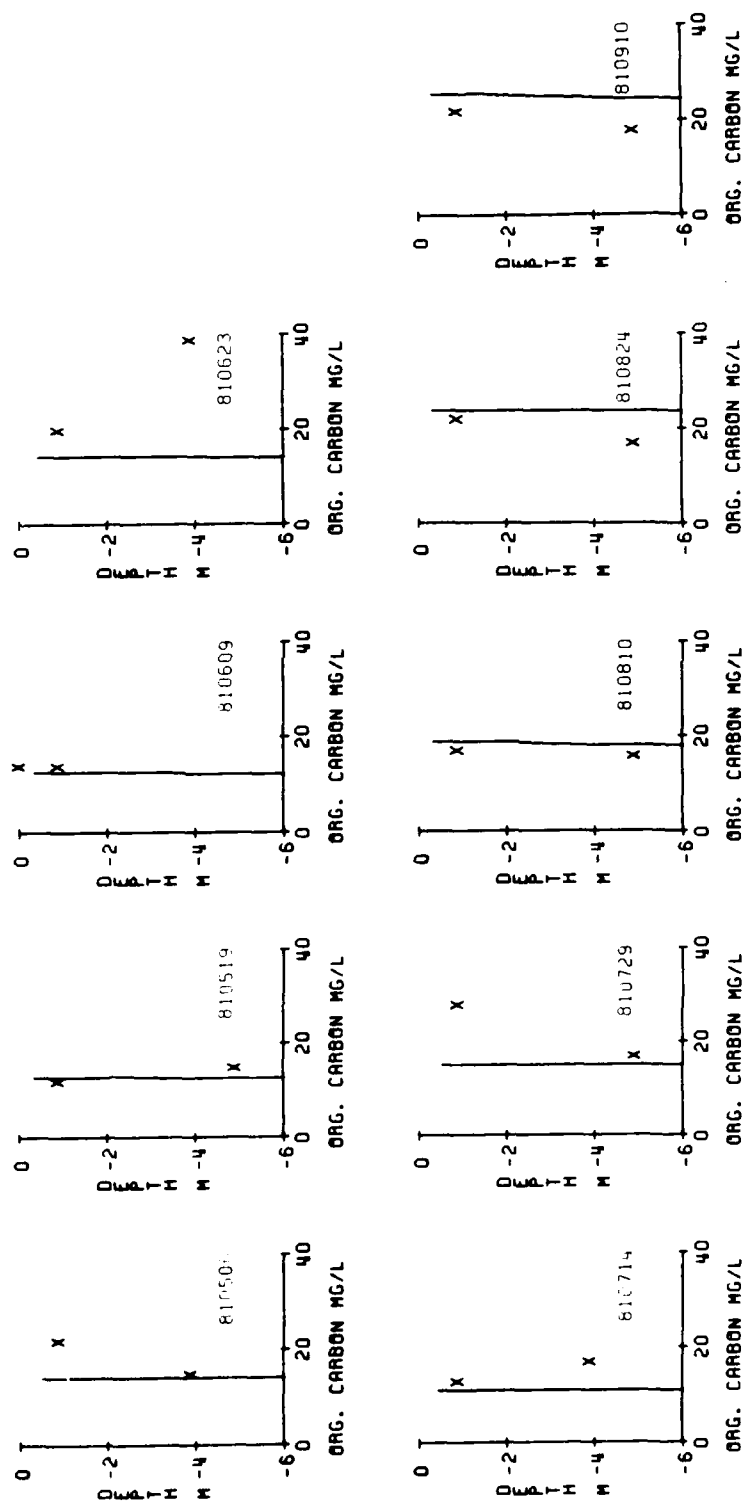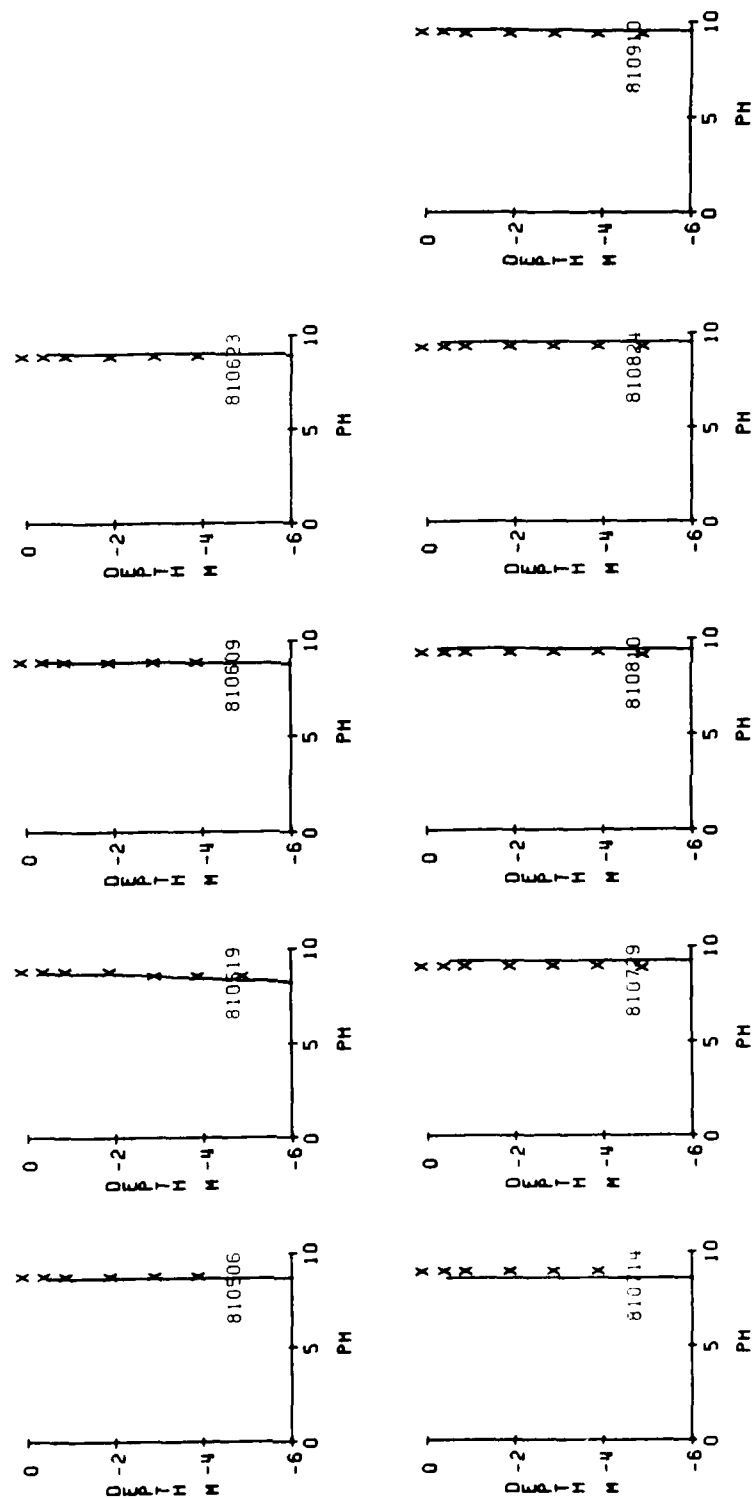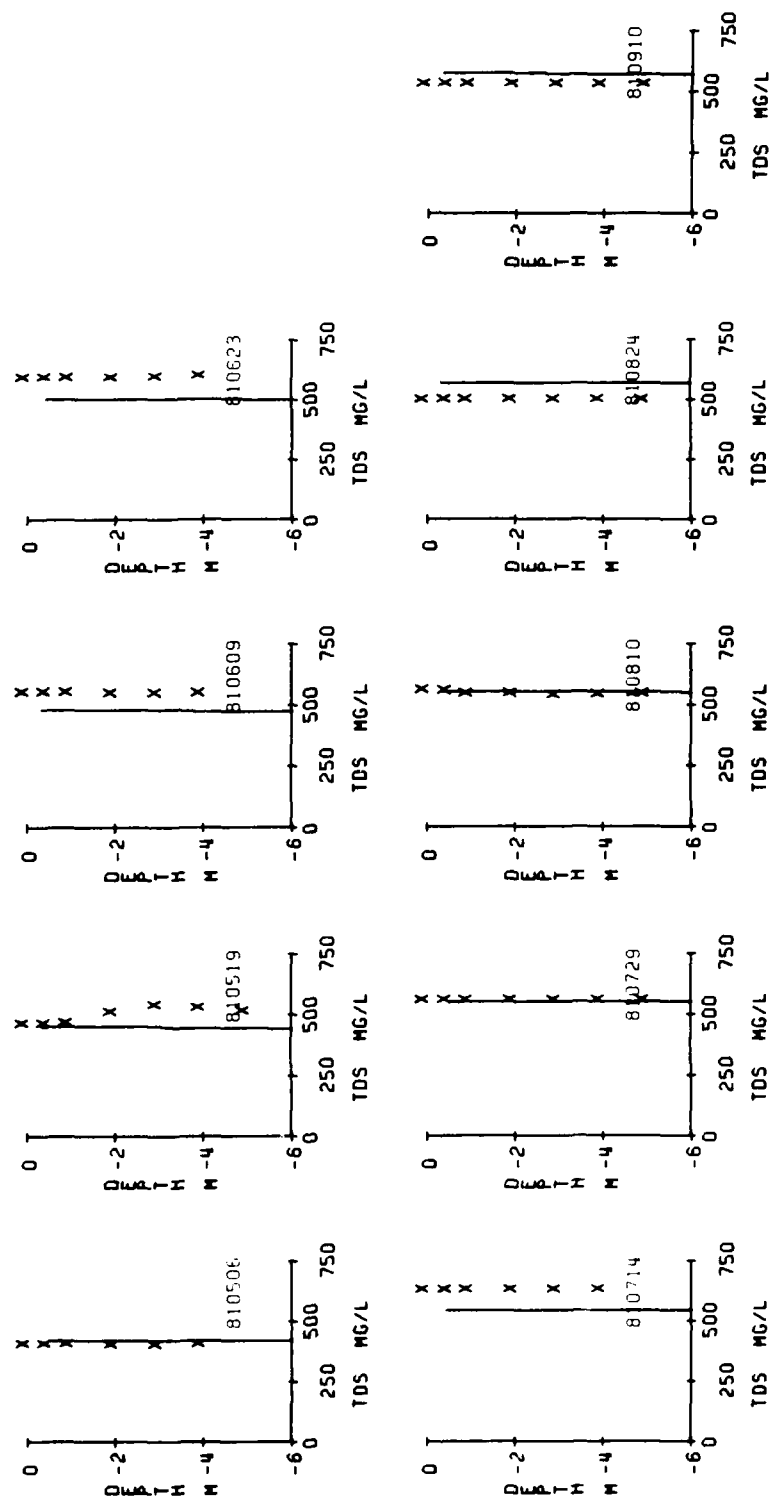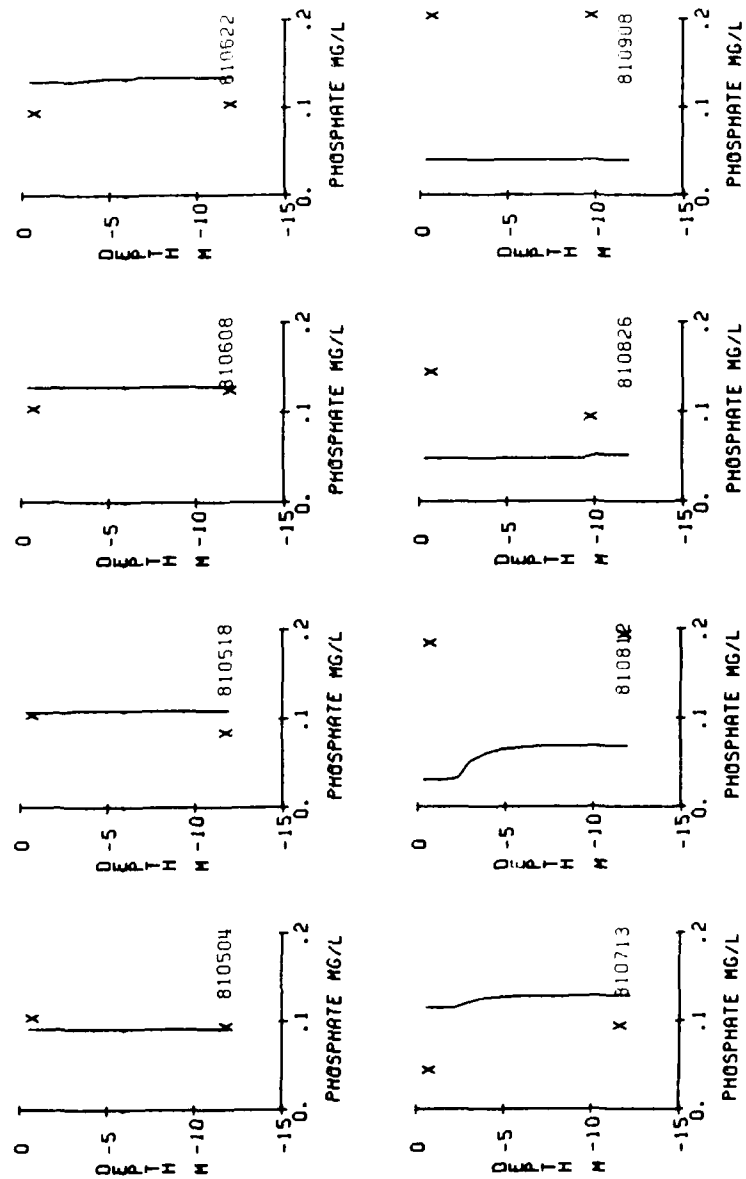Figure 4 (continued)
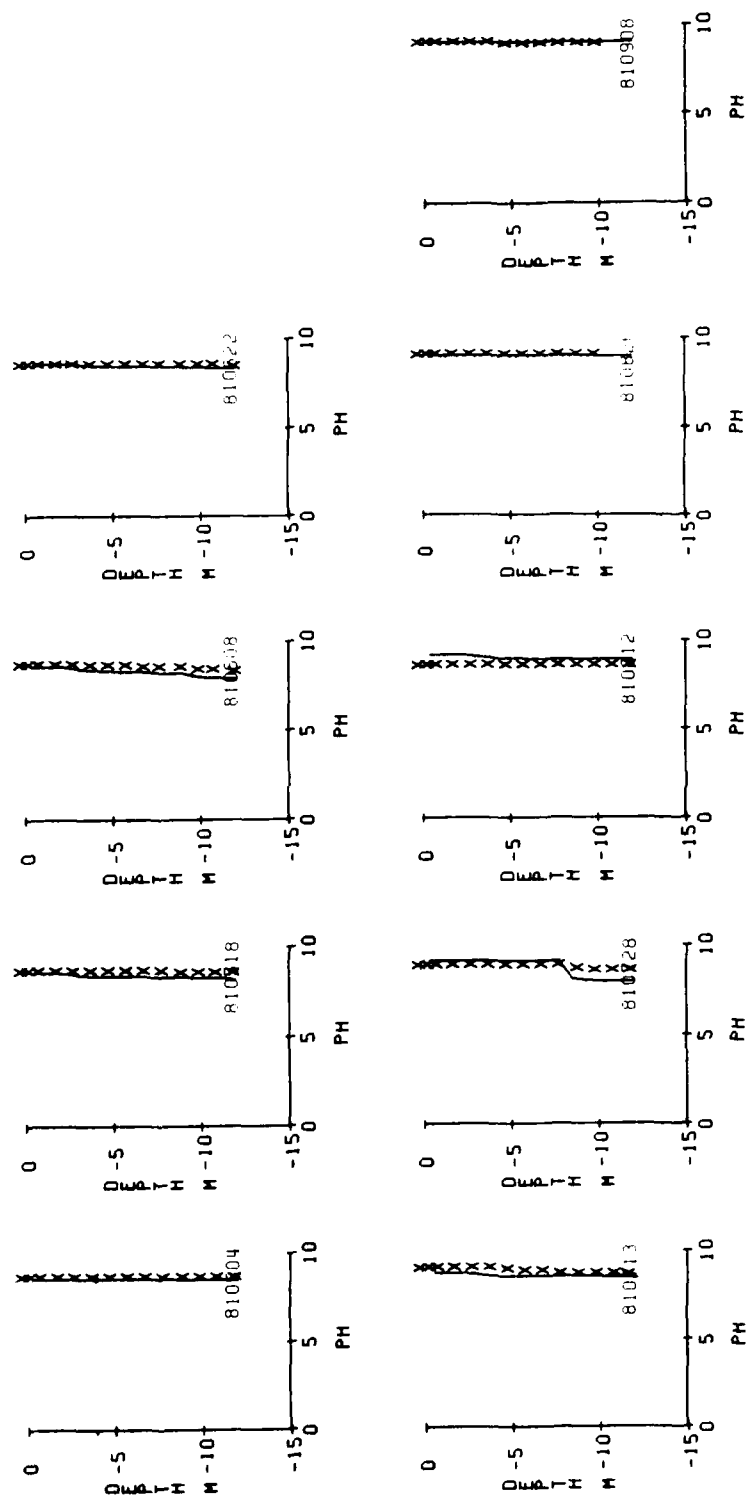
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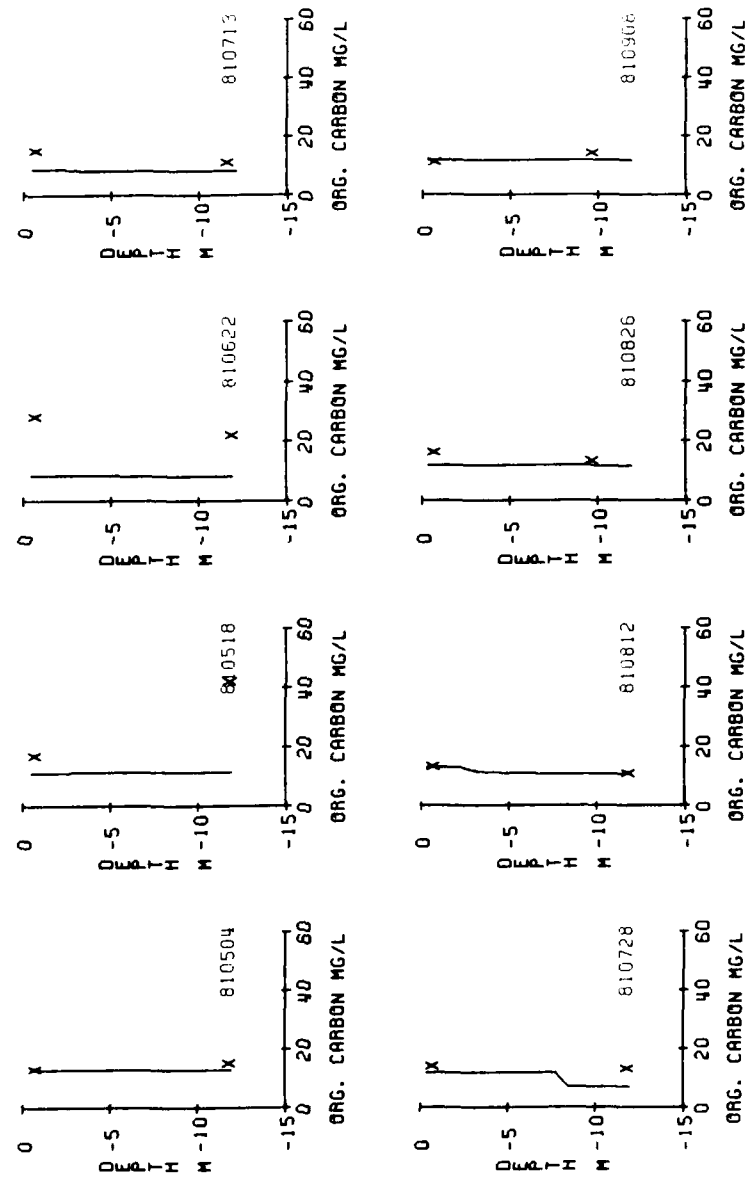
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Figure 4 (continued)
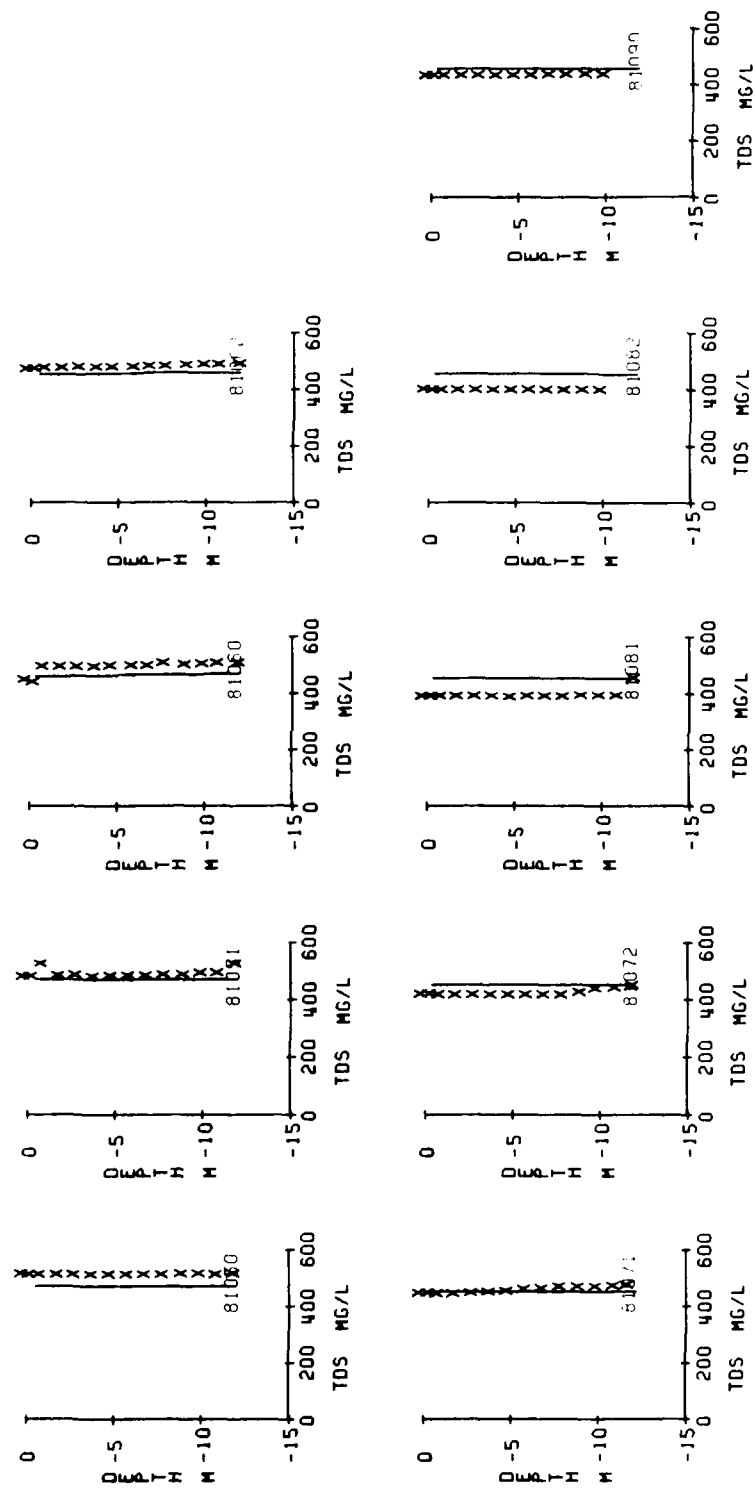
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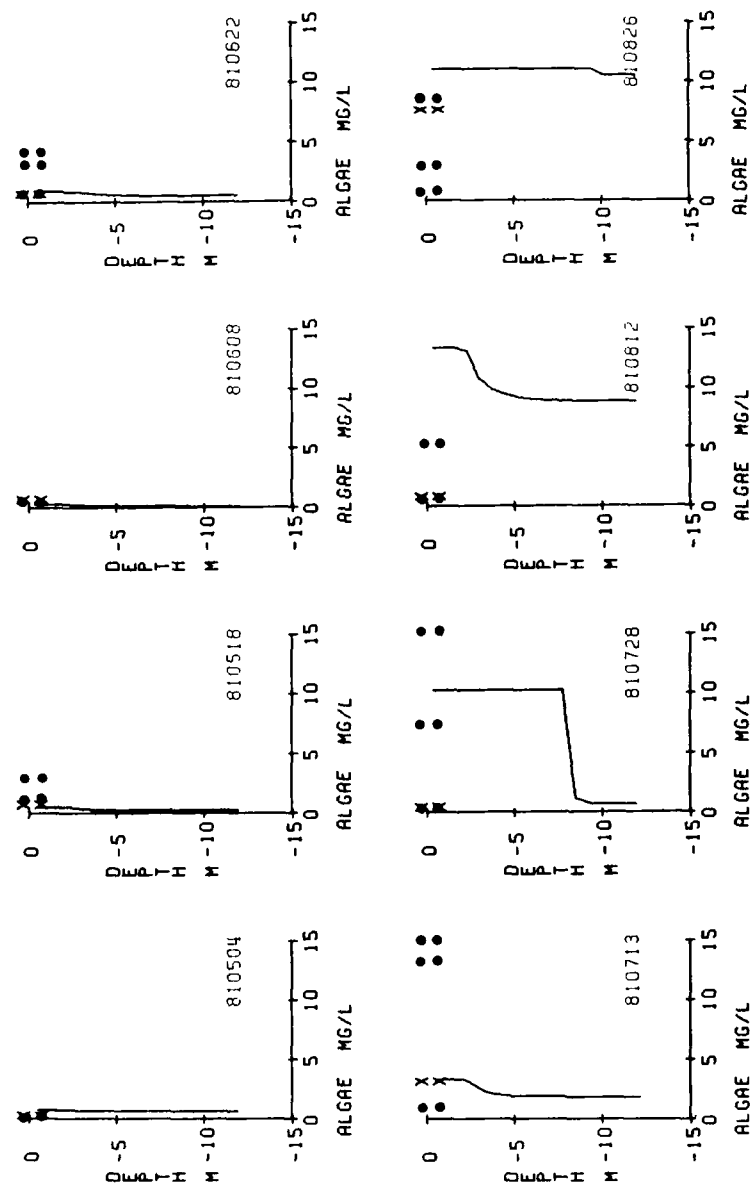
Figure 5. Predicted concentrations of algae (solid line) versus measured values from the deepest station (x's) and the other stations (solid circles) in Pool 3.

APPENDIX A: INITIAL VALUES OF STATE VARIABLES
FOR LAKE ASHTABULA SIMULATIONS

Variables	Units	Pool 1		Pool 2		Pool 3	
		Bottom	Surface	Bottom	Surface	Bottom	Surface
Temperature	deg. C	8.5	8.5	7.0	7.0	7.0	7.1
Oxygen	mg/l	11.1	11.4	9.1	9.2	11.1	11.1
Algae (1)	mg/l	.09	.09	.09	.09	.04	.04
Algae (2)	mg/l	.4	.4	.25	.25	.1	.1
Algae (3)	mg/l	3.9	3.9	2.5	2.5	1.0	1.0
Zooplankton	mg/l	.3	.3	.3	.3	.3	.3
Ammonia-N	mg/l	.140	.08	.14	.14	.11	.09
NO2-N + NO3-N	mg/l	.008	.01	.001	.01	.14	.12
PO4-P	mg/l	.070	.080	.05	.02	.09	.07
Detritus	mg/l	1.5	1.5	1.5	1.5	1.5	1.5
Sediment	g/m^2	101.1	101.1	101.1	101.1	101.1	101.1
Alkalinity	mg/l	337.	337.	337.	337.	337.	337.
Total Dissolved Solids	mg/l	403.	401.	361.	388.	481.	477.
Suspended Solids	mg/l	20.	30.	20.	30.	20.	30.
Labile Organics	mg/l	14.3	14.3	13.	14.	12.	16.
Refractory Organics	mg/l	14.3	14.3	13.	14.	12.	16.
pH		8.7	8.6	8.8	8.8	8.9	8.7
Particulate Manganese	mg/l	0.0	0.0	0.0	0.0	0.0	0.0

Variables	Units	Pool 1		Pool 2		Pool 3	
		Bottom	Surface	Bottom	Surface	Bottom	Surface
Sediment Manganese	mg/l	600.	600.	600.	600.	600.	600.
Dissolved Manganese	mg/l	0.0	0.0	0.0	0.0	0.0	0.0
Particulate Iron	mg/l	0.0	0.0	0.0	0.0	0.0	0.0
Sediment Iron	mg/l	12000.	12000.	12000.	12000.	12000.	12000.
Dissolved Iron	mg/l	0.0	0.0	0.0	0.0	0.0	0.0
Iron Sulfide- Sediment	mg/l	0.0	0.0	0.0	0.0	0.0	0.0
Iron Sulfide- Water	mg/l	0.0	0.0	0.0	0.0	0.0	0.0
Sulfate	mg/l	40.0	40.0	40.0	40.0	40.0	40.0
Sediment Sulfur	mg/l	200.	200.	200.	200.	200.	200.
Sulfide	mg/l	0.0	0.0	0.0	0.0	0.0	0.0
Sediment P	mg/l	400.	400.	400.	400.	400.	400.
Sediment N	mg/l	2000.	2000.	2000.	2000.	2000.	2000.
Dissolved Silica	mg/l	1.0	1.0	1.0	1.0	1.0	1.0

APPENDIX B: COEFFICIENTS FOR THE LAKE ASHTUBULA MODELS

DESCRIPTION	Model Acronym	Units	Values Pool 1	Pool 2	Pool 3
*DL = dimensionless					
PHYSICAL					
Number of outlets ports	NOUTS	DL	2	2	2
Number of tributaries	NTRIBS	DL	1	1	2
Reservoir Latitude	XLAT	decimal degrees	47.2	47.2	47.2
Reservoir Longitude	XLON	decimal degrees	98.1	98.1	98.1
Reservoir length	RLEN	m	8000.	12964.	32186.
Minimum layer thickness	SDZMIN	m	.4	.4	.4
Maximum layer thickness	SDZMAX	m	1.0	1.0	1.0
Area coefficient	ACOEF(1)	DL	310200.	2170000.	2065800.
Area coefficient	ACOEF(2)	DL	1.6624	.3304	.6484
Width coefficient	WCOEF(1)	DL	218.2	166.5	261.6
Width coefficient	WCOEF(2)	DL	.535	.490	.317
Port 1					
Elevation	ELOUT(1)	m	6.0	7.3	8.5
Vertical dimension	PVDIM(1)	m	2.0	2.0	1.5
Horizontal dimension	PHDIM(1)	m	25.	25.	36.6

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
Port 2					
Elevation	ELOUT(2)	m	1.5	1.5	2.9
Vertical dimension	PVDIM(2)	m	2.	2.0	.61
Horizontal dimension	PHDIM(2)	m	10.	10.	1.1
Physical coefficients					
Turbidity factor	TURB	DL	2.5	2.5	2.5
Wind coefficient	AA	m/(mb-sec)	1.2E-9	1.2E-9	1.2E-9
Wind coefficient	BB	1/mb	1.10E-9	1.10E-9	1.10E-9
Sheltering coefficient	SHELCF	DL	.96	.96	.96
Penetrative convection fraction	PEFRAC	DL	.00	.00	.00
Wind mixing coefficient	CDIFW	DL	.000003	.000003	.000003
Advection mixing coefficient	CDIFF	DL	.000006	.000006	.000006
Critical density for inflow	CDENS	g/1	.5	.5	.5
Extinction coefficient					
For water	EXCO	1/m	.35	.35	.35
For inorganic solids	EXTINS	1/m*mg/1	.11	.11	.11
For organic solids	EXTINP	1/m*mg/1	.11	.11	.11
Surface radiation fraction	SURFRAC	DL	.35	.35	.35

Description	Model Acronym	Units	Values Pool 1	Pool 2	Pool 3
Reaeration coefficient - oxygen	DMO2	m^2/sec	1.04E-8	1.04E-8	1.04E-8
Reaeration coefficient - CO2	DMCO2	m^2/sec	1.63E-9	1.63E-9	1.63E-9
Fraction of dead algae to detritus	ALDIGO	DL	.25	.25	.25

Organics

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Carbon fraction of dry weight	BIOC	DL	.46	.46	.46
Nitrogen fraction of dry weight	BION	DL	.09	.09	.09
Phosphorus fraction of dry weight	BIOP	DL	.0080	.0080	.0080

Phytoplankton

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Gross production rate	TPMAX(1)	1/day	1.0	1.0	1.0
	TPMAX(2)	1/day	.8	.8	.8
	TPMAX(3)	1/day	.6	.6	.6
Settling rate	TSETL(1)	m/day	.01	.01	.01
	TSETL(2)	m/day	.15	.15	.15
	TSETL(3)	m/day	.20	.20	.20

Half-saturation

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Phosphorus	PS2PO4(1)	mg/1	.04	.06	.05
	PS2PO4(2)	mg/1	.06	.06	.06
	PS2PO4(3)	mg/1	.05	.05	.05

Description	Model Acronym	Units	Values Pool 1	Pool 2	Pool 3
Nitrogen	PS2N(1)	mg/l	.30	.30	.30
	PS2N(2)	mg/l	.08	.08	.08
	PS2N(3)	mg/l	.10	.10	.10
Carbon	PS2CO2(1)	mg/l	.05	.05	.05
	PS2CO2(2)	mg/l	.10	.10	.10
	PS2CO2(3)	mg/l	.10	.10	.10
Light saturation level	PISAT(1)	$kcal/m^2/hr$	80.	45.	30.
	PISAT(2)	$kcal/m^2/hr$	80.	45.	30.
	PISAT(3)	$kcal/m^2/hr$	80.	45.	30.
Maximum excretion rate	TPEXCR(1)	1/day	.03	.03	.03
	TPEXCR(2)	1/day	.03	.03	.03
	TPEXCR(3)	1/day	.03	.03	.03
Maximum mortality rate	TPMORT(1)	1/day	.03	.03	.03
	TPMORT(2)	1/day	.03	.03	.03
	TPMORT(3)	1/day	.03	.03	.03
Maximum respiration rate	TPRESP(1)	1/day	.085	.085	.085
	TPRESP(2)	1/day	.070	.070	.070
	TPRESP(3)	1/day	.055	.055	.055

Temperature multipliers

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Low threshold	ALG1T1	deg.C	16.	16.	16.
	ALG2T1	deg.C	6.	6.	6.
	ALG3T1	deg.C	2.	2.	2.
Low optimum	ALG1T2	deg.C	22.	22.	22.
	ALG2T2	deg.C	16.	16.	16.
	ALG3T2	deg.C	8.	8.	8.
High optimum	ALG1T3	deg.C	26.	26.	26.
	ALG2T3	deg.C	18.	18.	18.
	ALG3T3	deg.C	10.	10.	10.
High threshold	ALG1T4	deg.C	32.	32.	32.
	ALG2T4	deg.C	24.	24.	24.
	ALG3T4	deg.C	16.	16.	16.

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
Low minimum	ALG1K1	DL	.1	.1	.1
	ALG2K1	DL	.1	.1	.1
	ALG3K1	DL	.1	.1	.1
High minimum	ALG1K4	DL	.1	.1	.1
	ALG2K4	DL	.1	.1	.1
	ALG3K4	DL	.1	.1	.1
Nitrogen fraction from ammonia	FRACN4(1)	DL	.6	.6	.6
for algae growth	FRACN4(2)	DL	.2	.2	.2
	FRACN4(3)	DL	.8	.8	.8

Macrophytes

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Maximum production rate	TPLMAX	1/day	.5	.5	.5
Maximum dark respiration rate	TMRESP	1/day	.2	.2	.2
Maximum excretion rate	TMEXCR	1/day	.1	.1	.1
Maximum nonpredatory rate	TMMORT	1/day	.05	.05	.05
Dead plants to dissolved organics	PLDIGO1	DL	.5	.5	.5
Dead plants to detritus	PLDIGO2	DL	.4	.4	.4
Dead plants to sediment	PLDIGO3	DL	.1	.1	.1
Temperature difference for mortality	TMPMAC	deg.C	1.5	1.5	1.5

Description	Model Acronym	Units	Values Pool 1	Pool 2	Pool 3
Self shading coefficient	EXTINM	$(1/m)\times(mg/1)$	.04	.04	.04
Carbon half-saturation	PLIMC	mg/1	.05	.05	.05
Nitrogen half-saturation	PLIMN	mg/1	.01	.01	.01
Phosphorus half-saturation	PLIMP	mg/1	.006	.006	.006
Plant density	PLDENS	g/m^3	10.	10.	10.
Light saturation	PLITE	$kcal/m^2/hr$	20.	20.	20.
Nutrient fraction from sediments	PLFRAC	DL	.5	.5	.5
Maximum depth for plant growth	PLNTDEP	m	2.5	2.5	2.5

Temperature multipliers

Low threshold	PLTT1	deg.C	2.	2.	2.
Low optimum	PLTT2	deg.C	20.	20.	20.
High optimum	PLTT3	deg.C	28.	28.	28.
High threshold	PLTT4	deg.C	38.	38.	38.
Low minimum	PLTK1	DL	.1	.1	.1
High minimum	PLTK4	DL	.1	.1	.1

Zooplankton

Maximum ingestion	TZMAX	1/day	.65	.65	.65
Maximum mortality	TZMORT	1/day	.02	.02	.02

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
Ingestion efficiency	ZEFFIC	DL	.35	.35	.35
Food preference					
For algae 1	PREF(1)	DL	.1	.1	.1
For algae 2	PREF(2)	DL	.3	.3	.3
For algae 3	PREF(3)	DL	.3	.3	.3
For detritus	PREF(4)	DL	.3	.3	.3
Respiration rate	TZRESP	1/day	.10	.10	.10
Feeding threshold	ZOOMIN	mg/l	.05	.05	.05
Food Half-saturation	ZS2P	mg/l	.6	.6	.6
Temperature multipliers					
Low threshold	ZOOT1	deg.C	2.	2.	2.
Low optimum	ZOOT2	deg.C	12.	12.	12.
High optimum	ZOOT3	deg.C	25.	25.	25.
High threshold	ZOOT4	deg.C	35.	35.	35.
Low minimum	ZOOK1	DL	.1	.1	.1
High minimum	ZOOK4	DL	.1	.1	.1

Fish

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
Maximum Ingestion	TFMAX	1/day	.03	.03	.03
Food Half-saturation	FS2FSH	mg/l	2.	2.	2.

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3

Food preference

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
For benthos and sediment	FPSED	DL	.01	.01	.01
For alga 1	FPALG(1)	DL	.12	.12	.12
For alga 2	FPALG(2)	DL	.12	.12	.12
For alga 3	FPALG(3)	DL	.12	.12	.12
For zooplankton	FPZOO	DL	.51	.51	.51
For detritus	FPDET	DL	.12	.12	.12
Ingestion efficiency	FEFFIC	DL	.80	.80	.80
Maximum mortality	TFMORT	1/day	.001	.001	.001
Maximum respiration	TFRESP	1/day	.004	.004	.004

Temperature multipliers

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Low threshold	FSH1T1	deg.C	1.	1.	1.
Low optimum	FSH1T2	deg.C	20.	20.	20.
High optimum	FSH1T3	deg.C	28.	28.	28.
High threshold	FSH1T4	deg.C	34.	34.	34.
Low minimum	FSH1K1	DL	.1	.1	.1
High minimum	FSH1K4	DL	.1	.1	.1

Decomposition

Description	Model Acronym	Units	Pool 1	Pool 2	Pool 3
Labile DOM	TDOMDK	1/day	.04	.04	.04
Ammonia	TNH3DK	1/day	.05	.05	.05

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
Detritus	TDETDK	1/day	.02	.02	.02
Coliforms	TCOLDK	1/day	1.4	1.4	1.4
Sediment	TSEDDK	1/day	.008	.008	.008
Refractory DOM	TRFRDK	1/day	.005	.005	.005
Labile to refractory organics	TDOMRF	1/day	.01	.01	.01
Nitrite-Nitrate denitrification	TNO3DK	1/day	.01	.01	.01
Temperature multipliers					
DOM low threshold	DOMT1	deg.C	0.	0.	0.
DOM optimum	DOMT2	deg.C	28.	28.	28.
DOM low minimum	DOMK1	DL	.1	.1	.1
NH3 low threshold	NH3T1	deg.C	0.	0.	0.
NH3 optimum	NH3T2	deg.C	20.	20.	20.
NH3 low minumum	NH3K1	DL	.1	.1	.1
NO3 low threshold	NO3T1	deg.C	0.	0.	0.
NO3 optimum	NO3T2	deg.C	28.	28.	28.
NO3 low minimum	NO3K1	DL	.1	.1	.1

Detritus

Description	Model Acronym	Units	Values		
Detrital settling velocity	TDSETL	m/day	.2	.2	.2

Description	Model Acronym	Units	Values Pool 1	Pool 2	Pool 3
Temperature multiplier					
Lower threshold	DETT1	deg.C	1.	1.	1.
Optimum temperature for decomposition	DETT2	deg.C	30.	30.	30.
Low minimum	DETK1	DL	.1	.1	.1
Chemical					
Solids settling	TSSETL	m/day	.10	.10	.10
PO4 adsorption	ADSRBP	1/m	3.0	3.0	3.0
Nitrogen adsorption	ADSRBN	1/m	40.	40.	40.
PO4 adsorption	ADMAXP	g/g	.001	.001	.001
Nitrogen maximum adsorption	ADMAXN	g/g	.003	.003	.003
Stoichiometry					
Oxygen – ammonia	O2NH3	DL	4.57	4.57	4.57
Oxygen – detritus decay	O2DET	DL	1.4	1.4	1.4
Oxygen – respiration	O2RESP	DL	1.1	1.1	1.1
Oxygen – photosynthesis	O2FAC	DL	1.4	1.4	1.4
Oxygen – dissolved organics	O2DOM	DL	1.4	1.4	1.4
Oxygen – reduced manganese	O2MN2	DL	.15	.15	.15

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
oxygen – reduced iron	O2FE2	DL	.14	.14	.14
Oxygen – sulfide	O2S2	DL	2.0	2.0	2.0
Anaerobics					
Dissolved oxygen concentration	OXYLIM	mg/l	.5	.5	.5
Sediment thickness	SEDTHK	cm	5.	5.	5.
Manganese settling	TMN4ST	m/day	.05	.05	.05
Manganese reduction rate	TMN4RE	1/day	.02	.02	.02
Manganese release rate	TMNREL	g/m /day	.10	.10	.10
Manganese oxidation rate	TMN2OX	1/day	0.	0.	0.
Particulate iron settling	TFE3ST	m/day	.05	.05	.05
Iron reduction rate	TFE3RE	1/day	.03	.03	.03
Iron release rate	TFEREL	g/m/day	.10	.10	.10
Iron oxidation rate	TFE2OX	1/day	0.	0.	0.
Sediment iron sulfide oxidation	TFESAD	1/day	.90	.90	.90
Iron sulfide settling	TFESST	m/day	.50	.50	.50
Iron sulfide oxidation	TFESBD	1/day	.5	.5	.5
Sulfate reduction	TSO4RE	1/day	.0010	.0010	.0010
Sulfur release rate	TSREL	g/m/day	.000012	.000012	.000012

Description	Model Acronym	Units	Values		
			Pool 1	Pool 2	Pool 3
Sulfide oxidation	TS2OXI	1/day	.30	.30	.30
Sulfide to iron sulfide reduction	TS2DK	1/day	0.	0.	0.
Orthophosphate sediment	TXP4RE	g/m/day	.001	.001	.001
Ammonia sediment release	TCNREL	g/m/day	.01	.01	.01

APPENDIX C: COMMAND, SOURCE, OBJECT, INPUT, AND OUTPUT FILES
FOR THE LAKE ASHTABULA MODELS

Both the Lake Ashtabula thermal model(CE-THERM-R1) and water quality model
(CE-QUAL-R1) reside on the St. Paul District's account of the CDC computer
system. After establishing communication the user should type

BEGIN,,ASHPRO1

to invoke the command file for the thermal model. The first six characters
of the command file are letters and the last character is a number. For
the water quality model type

BEGIN,,ASHPROQ

where all characters are letters.

Both models then ask the user to respond to a series of questions. A typical
terminal session is included below, where the small letters are printed by the
computer and the capitals are typed by the user.

BEGIN,,ASHPROQ

  enter 1,2, or 3 for pool to be simulated? 1

  enter outflow (yes or no) for outflow prediction? YES

  enter statanal (yes or no) for statistical analysis? YES

enter graphics (yes or no) for graphics? YES

enter priority p2,p3,p4, or p6? P4

graphics files being prepared.

after this run is complete, type:

        begin,,ashgrph

* * * * * * * * w a r n i n g * * * * * * * *

* graphics can be executed from a tektronics *

* 4014 or equivalent only.   *

* * * * * * * * w a r n i n g * * * * * * * *

08.32.20. submit complete.   jobname is ai3zqrh

A yes answer to the second question causes the model to replace inflow
concentrations for the next pool with the predicted outflow concentrations
from the pool that was simulated. The second question is asked only when
pool 1 or 2 is simulated. For statistical analysis or graphics, answer
YES to the proper question. Priority P2 is low, or overnight, priority,
and P6 is used for immediate turnaround. P4 represents normal daily
turnaround.

A number of files are associated with the Lake Ashtabula models. Besides
the thermal (CE-THERM-R1) and water quality (CE-QUAL-R1) programs, five other
programs are included in the modeling package. GRAFORM is a data manipula-
tion program, GRAF8 is the graphics program, STSTIC contains the statistical

package, and QSPASH and TSPASH update the inflowing concentrations for the downstream pool for the water quality and thermal models, respectively.

The FORTRAN programs, or source files, the object files, and command files to compile the programs are listed in Table C1. The only files needed to run either model are the object files. The other files can be written to tape to lower the cost of file storage.

Input data files are also needed, and have been created, for the two models. Before the user invokes the command file, he or she should edit the input files. Input files which are stored on the St. Paul CDC computer account are listed in Table C2.

A list of the output files created by the model are included in Table C3. A number of these files are quite large. The user should write the files to tape or delete them in order to save storage costs.

TABLE C1

Source, Object, and Command Files for the Lake Ashtabula Models

Program Name	Source File	Object File	Command File
CE-THERM-R1	ASHXCQT	CQT5OBJ	SFCQT
CE-QUAL-R1	ASHXCQR	CQR5OBJ	SFCQR
GRAFORM	GRAFORM	GRFOBJ	SFGFORM
GRAF8	ASHGRF8	GRF8OBJ	SFGRF8
STSTIC	STSTIC	STOBJ	
QSPASH	QSPASH	QSPOBJ	SFQSP
TSPASH	TSPASH	TSPOBJ	

TABLE C2

A List of Input Files for the Lake Ashtabula Models

File Name	Used in Program	Used for Pool	Model
ASHTP1	CE-THERM-R1	1	thermal
ASHTP2	CE-THERM-R1	2	thermal
ASHTP3	CE-THERM-R1	3	thermal
ASHQP1	CE-QUAL-R1	1	water quality
ASHQP2	CE-QUAL-R1	2	water quality
ASHQP3	CE-QUAL-R1	3	water quality
GRP1	GRAFORM	1	thermal
GRP2	GRAFORM	2	thermal
GRP3	GRAFORM	3	thermal
GQP1	GRAFORM	1	water quality
GQP2	GRAFORM	2	water quality
GQP3	GRAFORM	3	water quality
G8TP1	GRAF8	1	thermal
G8TP2	GRAF8	2	thermal
G8TP3	GRAF8	3	thermal
G8QP1	GRAF8	1	water quality
G8QP2	GRAF8	2	water quality
G8QP3	GRAF8	3	water quality
VASHP1	GRAF8 and STSTIC	1	both
VASHP2	GRAF8 and STSTIC	2	both
VASHP3	GRAF8 and STSTIC	3	both
STSWT	STSTIC	1,2,3	thermal
STSWQ	STSTIC	1,2,3	water quality

TABLE C3

A List of the Output Files for the Lake Ashtabula Models

File Name	From Program	From Pool	Model
PLTWC	CE-THERM-R1	1,2,3	thermal
PLTIN	CE-THERM-R1	1,2	thermal
PLTOUT	CE-THERM-R1	1,2,3	thermal
OFILE	CE-THERM-R1	1,2,3	thermal
PLTIN1	CE-THERM-R1	3	thermal
PLTIN2	CE-THERM-R1	3	thermal
PLQWC	CE-QUAL-R1	1,2,3	water quality
PLQIN	CE-QUAL-R1	1,2	water quality
PLQOUT	CE-QUAL-R1	1,2,3	water quality
QFILE	CE-QUAL-R1	1,2,3	water quality
WCFLOW	CE-QUAL-R1	1,2	water quality
PLQIN1	CE-QUAL-R1	3	water quality
PLQIN2	CE-QUAL-R1	3	water quality
GRAOTP	GRAFORM	1,2,3	both
STST	STSTIC	1,2,3	both
TAPE16	GRAF8	1,2,3	both

END

10-86

DTIC