APPLICATION OF WASP5 FOR WATER QUALITY MODELING OF BACK BAY OF BILOXI

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INTRODUCTION AND PURPOSE

The development of hydrodynamic and water quality models for Back Bay of Biloxi was initiated in response to an increasing need for a comprehensive water quality model that will facilitate decision-making in the overall management activities of the Bay estuarine system, including assessment of existing water quality, estimation of waste assimilative capacity under various conditions and seasonal variations, and analysis of the effect of waste discharge into the Bay. The Water Quality Analysis Simulation Program-5 (WASP5) was chosen for application to Back Bay of Biloxi (Ambrose et al. 1993). This model is capable of interpreting and predicting water quality responses to natural phenomena and man-made pollution. Due to the nutrient enrichment and eutrophication problems in the Back Bay of Biloxi, intermediate eutrophication kinetics, which is complexity level 5 in EUTRO5 is utilized. WASP5 system consists of three stand-alone computer programs, DYNHYD5, EUTRO5, and TOXI5 that can be run in conjunction or separately. The hydrodynamics program, DYNHYD5, simulates the movement of water; while the water quality program, EUTRO5, simulates the movement and interaction of pollutants within the water.

The study area is located along the Mississippi Gulf Coast and is adjacent to Jackson and Hancock Counties (Figure 1). Also included in the study area are the metropolitan areas of Biloxi, Gulfport, Ocean Springs, and D'Iberville.

The initial model calibration was accomplished utilizing historical data collected during the periods of July 28-August 2, 1972, and June 14-16, 1977 (Shindala et al. 1996). Final model calibration was performed utilizing a set of field data acquired on the Back Bay of Biloxi, during September 12-21, 1994. Model verification was conducted against another set of field data taken in the Bay, during April 25-May 2, 1995. This paper presents the details of the implementation of the water quality modeling framework together with results of the water quality calibration/verification effort. Details of the hydrodynamic calibration effort are discussed in the Completion Report (Shindala et al. 1996) and reference (Zitta et al. 1999).

WATER QUALITY MODEL COMPUTATIONAL METHODOLOGY

The WASP5 modeling framework consists of several components, one of which (EUTRO5) was specifically designed for the assessment of processes impacting eutrophication and dissolved oxygen dynamics. EUTRO5 is a dynamic compartment modeling program for aquatic systems, including both the water column and the underlying benthos. The time-varying processes of advection, dispersion, point and non-point mass loading, and boundary exchange are represented in the basic program. The hydrodynamic model that supplies dynamic or tidally averaged circulation information to the EUTRO5 water quality model is DYNHYD5. Theoretical basis and underlying equations incorporated in DYNHYD5 can be found in the WASP5 User's Manual (Ambrose et al. 1993) and reference (Zitta et al. 1999). The hydrodynamic model is a pseudo two-dimensional model that simulates water movement due to tides, winds, and tributary inflows.

The underlying framework of the analysis, used in water quality modeling, is based on the principle of conservation of mass. The mass balance equation around an infinitesimally small fluid volume is (Ambrose et al. 1993):

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(U_x C) - \frac{\partial}{\partial y}(U_y C) - \frac{\partial}{\partial z}(U_z C) + \frac{\partial}{\partial x}(E_x \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(E_y \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z}(E_z \frac{\partial C}{\partial z}) + S_L + S_B + S_K \quad (1)$$

where C is concentration of the water quality constituent (mg/l); t is time (days); U_x, U_y, and U_z are longitudinal, lateral, and vertical advective velocities, respectively (m/day); E_x , E_y , and E_z are longitudinal, lateral, and vertical advective diffusion coefficients (m^2/day); S_L is direct and diffuse loading rate (g/m^3-day); S_B is boundary loading rate (including upstream, downstream, benthic, and atmospheric (g/m^3-day); S_K is total kinetic transformation rate; positive is source, negative is sink (g/m^3-day).

Equation (1) can also be written as a general mass-balance equation of a non-conservative substance, dissolved or suspended in flowing fluids, and may be expressed as (Park et al. 1996):

$$\frac{\partial C}{\partial t} = (physical\ transport) + (kinetic\ processes) \qquad (2)$$

where C = concentration and t = time. The time scale in equation (2) can be intra- or inter-tidal. The term (physical transport) is presumed to be identical for all water quality state variables. The physical transport moves materials spatially and can be in zero-, one-, two- or three-dimensional spatial scale. The term (kinetic processes) is different for different water quality state variables and may involve interactions among state variables. The complexity arising from the kinetic processes is largely dependent on one's objectives: the number of model state variables and kinetic processes that are represented in the model. EUTRO5 can be operated at various levels of complexity to simulate some or all of the related variables and interactions. Due to the nutrient enrichment and eutrophication problems in the Back Bay of Biloxi, intermediate eutrophication kinetics, which is complexity level 5 in EUTRO5 is used.

A great deal of complexity and difficulty may be avoided if the physical transport and the kinetic processes in equations (1) and (2) are decoupled. The decoupling method has been employed in WASP5. The solution scheme involved two-step computation, in which substances are physically transported and then followed by the application of kinetic processes.

Equation (1) is the general WASP5 mass balance equation and represents three major classes of water quality processes, namely: transport, loading, and transformation. It is solved for each state variable. To this general equation, the EUTRO5 subroutines add specific transformation processes to customize the general mass balance for the eight state variables in the water column and benthos. The water quality parameters can be considered as four interacting systems: phytoplankton kinetics, the phosphorus cycle, the nitrogen cycle, and the dissolved oxygen balance.

Five state variables modeled in EUTRO5 for dissolved oxygen balance are: phytoplankton carbon, ammonia, nitrate, carbonaceous biochemical oxygen demand, and dissolved oxygen. In the application of the model to the Back Bay of Biloxi, sediment layers are not incorporated. In EUTRO5, flow-induced reaeration is based on the Covar (1976) method, and wind-induced reaeration is determined by O' Connor (1983).

Three phosphorus variables modeled in EUTRO5 are: phytoplankton phosphorus, organic phosphorus, and inorganic (orthophosphate) phosphorus. Four nitrogen variables modeled in EUTRO5 are: phytoplankton nitrogen, organic nitrogen, ammonia nitrogen, and nitrate nitrogen.

SEGMENTATION OF BACK BAY OF BILOXI

Segmentation of the Back Bay of Biloxi established for the hydrodynamic and water quality models is illustrated in Figure 1. The segmentation scheme used for both models does not include vertical resolution. Although there are indications of vertical variations in transport, the data reviewed to date does not include sufficient information to either establish the boundaries or to estimate exchanges between vertical layers. Finally, benthic layers are not incorporated in this effort due to the unavailability of data needed to simulate eutrophication with benthos. Thus, the model application will be for a two-dimensional vertically mixed system for the bay and one-dimensional vertically mixed system for the tributaries. Overall, the Back Bay of Biloxi was divided into 641 segments, including twenty eight (28) model boundaries. Thirteen downstream boundary segments are required at Mississippi Sound and fifteen upstream segments are required at major river tributaries (Brickyard Bayou, Bernard Bayou, Turkey Creek, Biloxi River, Fritz Creek, Tchoutacabouffa River, Old Fort Bayou, Keegan Bayou, St. Martin Bayou, Bayou Poito, Heron Bayou, Davis Bayou, Simmons Bayou, and two segments boundaries for Mississippi Power Co-Watson Steam).

MODEL INPUT PARAMETERS

Input parameters to the water quality model EUTRO5 include environmental, transport, boundaries, and transformations. All of the parameters incorporated in the model were either temporal or spatial variables or both. Since available data were not sufficient to define many of the variables mentioned above on an hourly basis, they were approximated by a series of piecewise linear functions. The piecewise linear functions or approximations used in this model consist of a series of variables and break points usually at high slack, low slack time interval, or daily interval dependent on the type of the variable and availability of data.

Environmental Parameters

Environmental parameters in EUTRO5 define the basic identity, including the segmentation, and the simulation control. In particular the environmental input parameters include, type of simulation, number of segments, number of systems, time step option, advection factor, and segment volumes. In the model network, eight state variables of Ammonia Nitrogen (NH3), Nitrate Nitrogen (NO3), Inorganic Phosphorus

(PO4), Phytoplankton Carbon (CHL), Carbonaceous Biochemical Oxygen Demand (CBOD), Dissolved Oxygen (DO), Organic Nitrogen (ON), and Organic Phosphorus (OP) are simulated in the 641 segments. In the water quality model advection factor v = 0 is specified to modify the finite difference approximation of $\partial c/\partial x$ used in the advection term by EUTRO5. This will result in the most stable solution (Ambrose et al. 1993). Initial volumes for each segment are specified by using the segment surface area and depth. However, the volumes and time step specified in these environmental parameters will be reset by the hydrodynamic file.

Transport Parameters

This group of parameters defines the advective and dispersive transport of simulated model variables. Input parameters include advective flows, dispersion coefficients, cross-sectional areas, and characteristic lengths. The hydrodynamic results file (*.HYD) contains averaged hydrodynamic variables for use in EUTRO5 simulations. This includes basic network and inflow information; junction volumes (m^3), flows (m^3/sec), depths (m), and velocities (m/sec); and channel flows (m^3/sec). Flow continuity is automatically maintained.

The number of exchange fields between segments is 894. The cross-sectional areas are specified for each dispersion coefficient, reflecting the area through which mixing occurs. The characteristic mixing lengths are also specified for each dispersion coefficient, reflecting the characteristic length over which mixing occurs.

Boundary Conditions

This group of parameters includes: A) boundary concentrations, B) waste loads, and C) initial conditions.

A) Boundary Concentrations. Boundary concentrations are specified for twenty-eight (28) model boundary segments at thirteen upstream boundaries, two Mississippi Power Co-Watson Steam boundaries, and thirteen downstream (seaward) boundary junctions with Mississippi Sound. Constant concentrations are specified for each water quality constituent at each boundary. Freshwater inflow studies made during the two surveys were used as the main source of model upstream boundary concentrations. The downstream boundary concentrations at Back Bay of Biloxi were extrapolated from transect station 1.

B) Waste Loads. The waste source survey conducted by Mississippi DEQ during the period July-September 1994 was used in both calibration and verification phases. Industrial, municipal, and domestic waste sources were considered. However, non-point source loads from urban and agricultural runoff, precipitation, and atmospheric deposition of pollutants were not incorporated into the model. A constant waste load with time is inputted at the nearest segment.

C) Initial Conditions. Initial conditions include initial concentrations, as well as solids transport field for each solid and the dissolved fraction in each segment. For dynamic simulations where the transient concentration response is desired, initial concentrations are inputted closely reflecting the measured values at the beginning of the simulation. Longitudinal linear interpolation was made between available sampling stations (Figure 2) for determining the initial concentrations throughout the water quality segments.

Transformation Parameters

This group of parameters includes spatially variable parameters, constants, and kinetic time functions for the eight water quality state variables being simulated herein. Spatially variable parameters such as water temperature, sediment oxygen demand, salinity, extinction coefficient, specific temperature correction coefficient for sediment oxygen demand, and segment specific reaeration rate are inputted for each segment. Specified values of constants as shown in Table 1 apply over the entire network throughout the simulation.

WATER QUALITY MODEL CALIBRATION AND VERIFICATION

Initial calibration of the water quality model (EUTRO5) for the Back Bay of Biloxi was accomplished utilizing historical data (USEPA 1973; USGS 1978). Results of this initial calibration effort are discussed in the Supplement to Completion Report (Shindala et al. 1996). The results of simulation utilizing the September 12-21, 1994, and April 25-May 2, 1995, intensive survey data were considered as the final calibration and verification efforts, respectively.

The final calibration is a set of consistent model coefficients (Table 1) that are reasonable and are capable of reproducing the observed data for all state variables with the exception of exogenous variables such as flow, temperature, solar radiation, and extinction coefficients. The method employed in determining the values for the model coefficients was essentially one of trial and error. The starting point was a set of rate constants and parameter values that were used in the initial calibration (Shindala et al. 1996). Model constants that were used in previous modeling studies were also consulted (Ambrose et al. 1993; Bowie et al. 1985).

Database

General field data jointly collected by USEPA and Mississippi DEQ (Mississippi Department of Environmental Quality) during the two study periods (September 12-21, 1994, and April 25-May 2, 1995) were used to calibrate and verify the water quality model, respectively. Since the chlorophyll-a data collected in the study periods were limited, averaged measurements of chlorophyll-a from NASA imagery studies (Eleuterius et al. 1993) collected in October and April-May 1972 were used to supplement the calibration and verification data, respectively, for the Bay modeling.

The locations of the water quality sampling stations for the September 12-24, 1994 and April 25-May 2, 1995 surveys are shown in Figure 2. In the surveys, a large number of physical, chemical, and bacteriological parameters were collected from several selected sampling stations as shown in the figure. Several types of waste sources (municipal, industrial, domestic, and federal) were surveyed during July-September 1994 study. Waste sources that were discharging into the Bay during April 25-May 2, 1995, were considered to be the same as September 12-24, 1994. The air temperature measurements were made at Spoil Island Meteorological Station and Mississippi Power Company Meteorological Station by Mississippi DEQ.

Calibration and Verification Results of Water Quality Model

During the calibration and verification phases, several dispersion coefficients were used to test the sensitivity of the model to variations in the dispersion coefficient. However, results of simulations using several dispersion coefficients revealed the insensitivity of EUTRO5 to changes in the dispersion coefficients. The model reproduces the observed salinity data very well under different conditions, at dispersion coefficient of 1 m^2/sec. A reasonably good fit of the salinity as shown in Completion Report (Shindala et al. 1996) and in Figures 3 and 4 (Zitta et al. 1999) clearly indicates that the model reproduces the principal transport mechanisms of the estuary.

Specified values of constants as shown in Table 1 apply over the entire network throughout the simulation and were used in the study. A sample of spatial and/or temporal profiles of observed versus model computed water quality parameters for calibration and verification phases is presented in Figure 3 and 4, respectively. For dissolved oxygen, the computed values at the Bay and tributaries generally fell within the range of observed data. For CBODU, nitrogen and phosphorus compounds, the computed values generally reproduces the observed data within its ranges very well. Examination of the profiles clearly shows that EUTRO5, in general, reproduces most of the observed water quality data but does not compute every data point.

CONCLUSION

A two-dimensional vertically mixed system and real-time model consisting of linked hydrodynamic and water quality models was developed. Results of simulations using several dispersion coefficients revealed the insensitivity of EUTRO5 to changes in the dispersion coefficients. Comparisons of the computed and observed data were made qualitatively by using spatial and temporal comparisons. The response of model prediction calculations is consistent with trends of the observed data ranges, but not with absolute values in all cases. The model, in general, can accurately predict the concentration of water quality constituents in the range of observed data taken.

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Table 1: EUTRO5 Model Constants for Back Bay of Biloxi

Description	ISC	Name	Units	Typical Value/Range	Back Bay of Biloxi
Nitrification Rate @ 20 °C	11	K12C	Day^{-1}	0.09[1] 0.02-0.2[2]	0.05 0.025*
Temperature Coefficient for Nitrification	12	K12T	-	1.08[1] 1.02-1.08[2]	1.08
Half – saturation Constant for Nitrification-Oxygen Limitation	13	KNIT	Mg O_2/L	2.0[1]	0.5 2.0*
Denitrification Rate @ 20 °C	21	K20C	Day^{-1}	0.09[1] 0.0-1.0[2]	0.1
Temperature Coefficient for Denitrification	22	K20T	-	1.045[1] 1.02-1.09[2]	1.045
Half – Saturation Constant for Denitrification-Oxygen Limitation	23	KNO3	Mg O_2/L	0.1[1]	0.1
CBOD Deoxygenation rate @ 20° C	71	KDC	Day^{-1}	0.21,0.16[1] 0.02-5.6[2]	0.05
Temperature Coefficient for Carbonaceous Deoxygenation	72	KDT	-	1.047[1] 1.02-1.15[2]	1.047 1.045*
Half - Saturation Constant for Deoxygenation	75	KBOD	Mg O_2/L	0.5[1]	0.5
Mineralization rate of Dissolved Organic Nitrogen	91	K71C	Day^{-1}	0.075[1] 0.02-0.075[2]	0.1 0.075*
Temperature Coefficient for ON Mineralization	92	K71T	-	1.08[2]	1.08
Mineralization Rate of Dissolved Organic Phosphorus	100	K83C	Day^{-1}	0.22[1] 0.22[2]	0.22 0.2*
Temperature Coefficient for OP Mineralization	101	K83T	-	1.08[1,2]	1.08
Half Saturation Constant for Phytoplankton Limitation of Phosphorus	59	KMPHY	-	1.0	
Saturation Growth Rate @ 20 °C	41	K1C	Day^{-1}	2.0[1] 0.2-8[2]	1.5
Temperature Coefficient for Growth	42	K1T	-	1.068[1]	1.068
Fraction of Dead and Respired (FON) Phytoplankton Nitrogen Recycled to Organic Nitrogen	95	FON	-	0.5[1]	0.5
Fraction of Dead and Respired (FOP) Phytoplankton Phosphorus Recycled to Organic Phosphorus	104	FOP	-	1.0[1]	0.5 1.0*
Carbon/Chlorophyll Ratio	46	CCHL	mg C/mg Chla	21-45[1] 10-112[2]	50.0 30.0*
Saturation Light Intensity	47	IS1	Ly/day	200-350[2]	300
Nitrogen Half – Saturation Constant for Growth	48	KMNG1	Mg N/L	25[1] 1.5 - 400[2]	25 50*
Phosphorus Half - Saturation Constant for Growth	49	KMPG1	µg PO_4-P/L	1[1] 0.5-30[2]	1
Endogeneous Respiration rate @ 20°C	50	K1RC	Day^{-1}	0.125[1] 0.02-0.6[2]	0.15 0.1*
Temperature Coefficient for Respiration	51	K1RT	-	1.045[1]	1.045
Non - Predatory Death Rate	52	K1D	Day^{-1}	0.02[1] 0.005-0.172[2]	0.05 0.08*
Grazing Rate on Phytoplankton Per Unit Zooplankton Population	53	K1G	L/cell-day	0.0[1]	0.0
Phosphorus to Carbon ratio	57	PCRB	mg PO_4-P/mg C	0.025[1] 0.025-0.05[2]	0.025
Nitrogen to Carbon ratio	58	NCRB	mg N/mg C	0.25[1] 0.05-0.43[2]	0.25
Oxygen to Carbon Ratio	81	OCRB	mg O_2/mg C	2.67[1]	2.67 2.7*

[1] Ambrose et al (1993), [2] Bowie et al (1985), * for Historical data set run

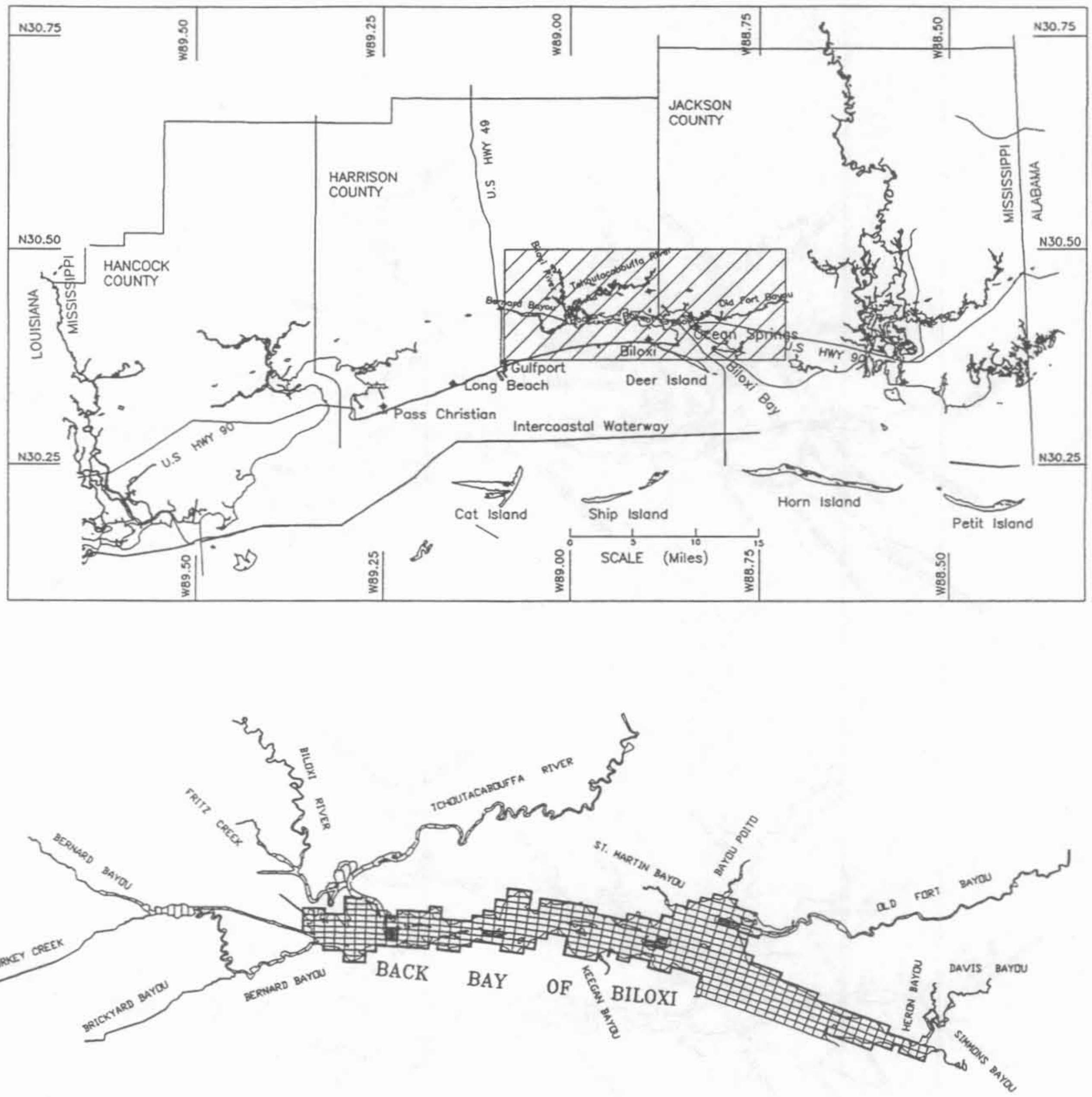
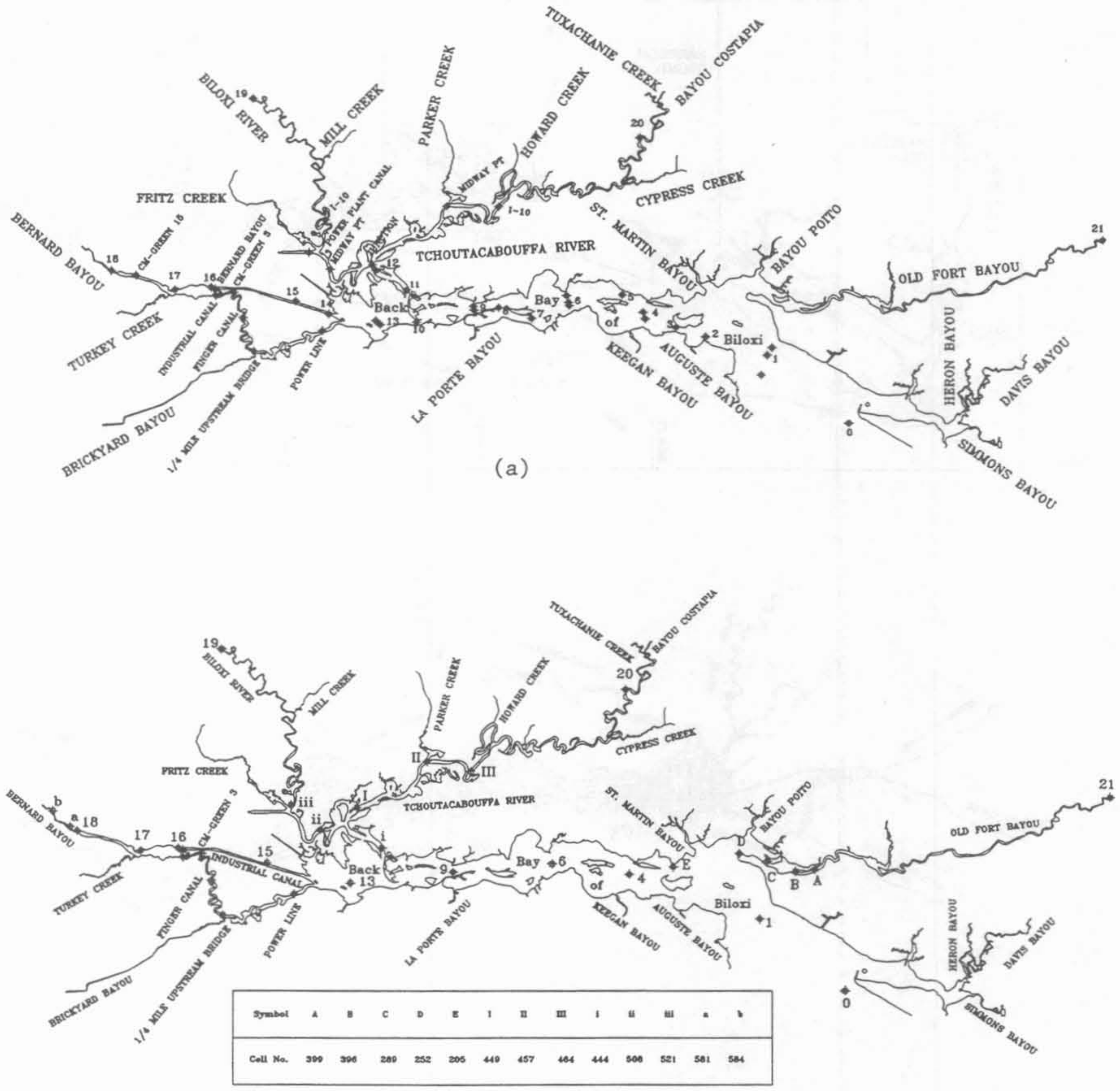


Figure 1: Location and Segmentation Map of Back Bay of Biloxi



Symbol	A	B	C	D	E	I	II	III	i	ii	iii	a	b
Cell No.	399	396	289	252	205	449	457	464	444	506	521	581	584

Figure 2:Location of Water Quality Sampling Stations
(a) September 13-20, 1994 Study (b) April 25-May 2, 1995 Study

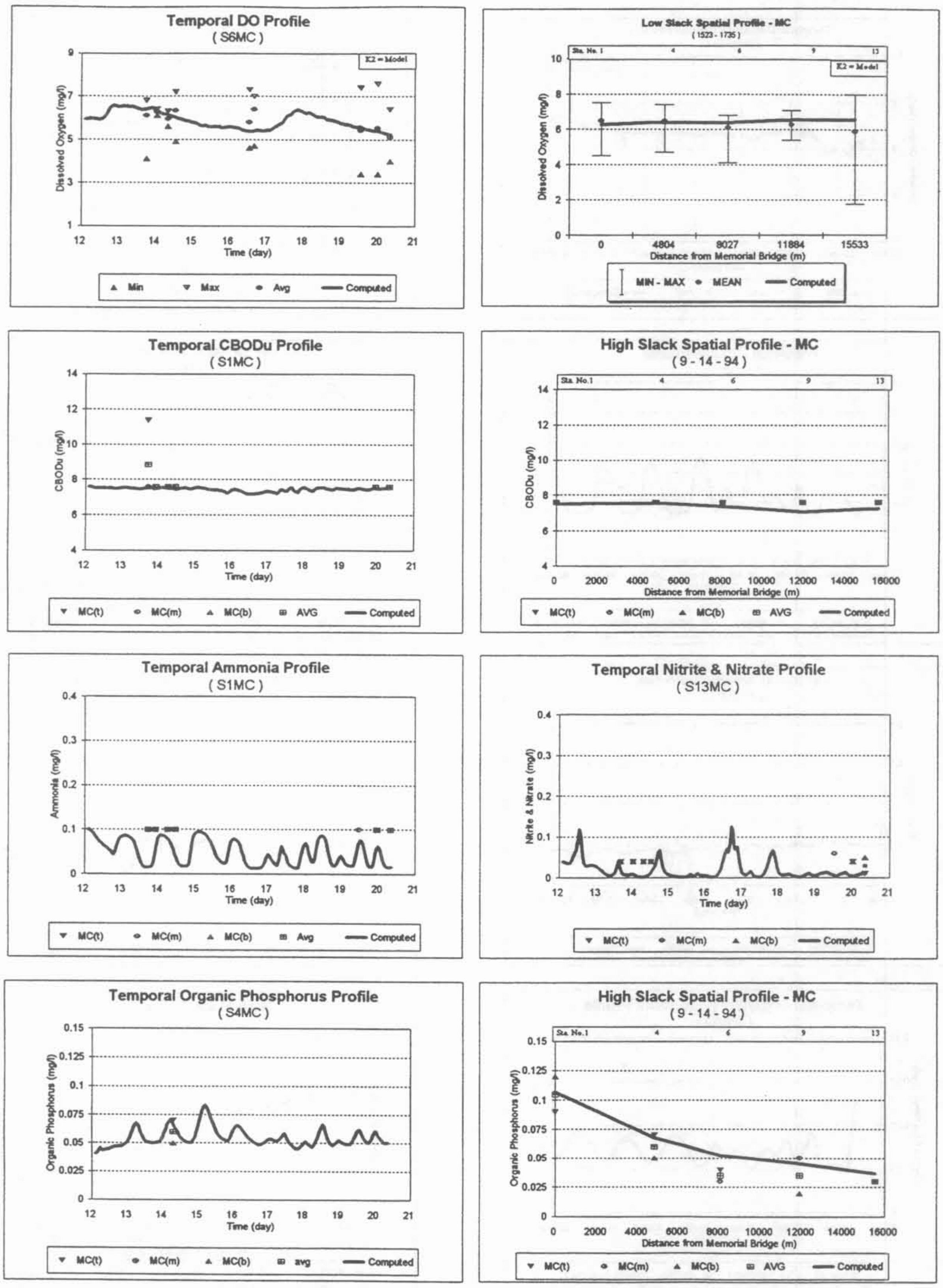


Figure 3: Spatial and Temporal Profiles of Water Quality Constituents at Back Bay of Biloxi
(September 12-21, 1994, USEPA/MSDEQ)

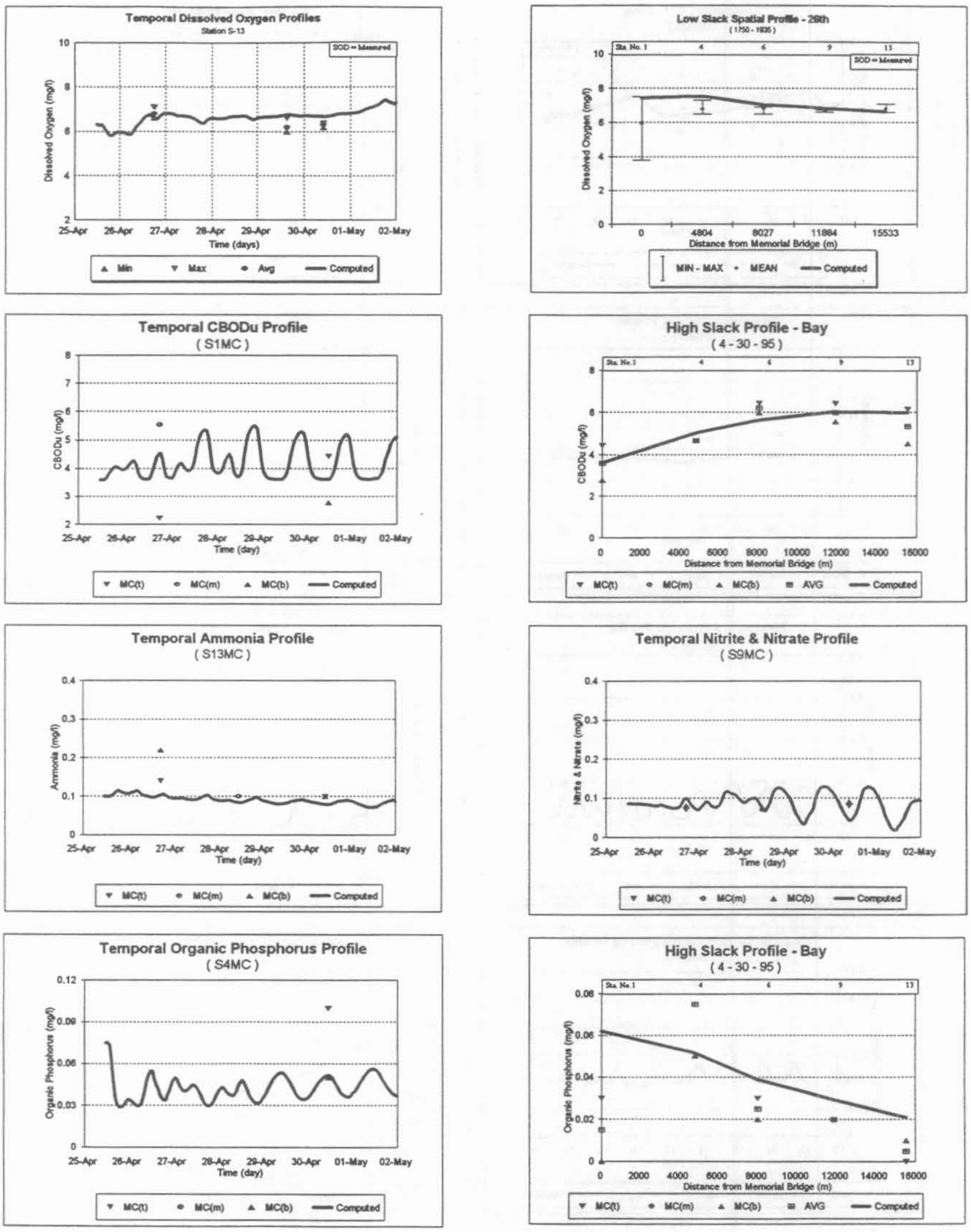


Figure 4: Spatial and Temporal Profiles of Water Quality Constituents at Back Bay of Biloxi
(April 25-May 2, 1995, USEPA/MSDEQ)