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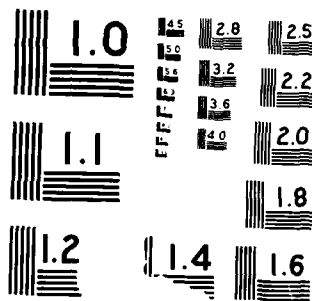
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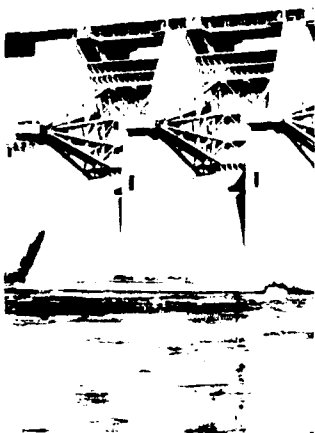
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ENVIRONMENTAL IMPACT
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TECHNICAL REPORT EL-88-7

COUPLING HYDRODYNAMICS TO A
MULTIPLE-BOX WATER QUALITY MODEL

by

Sandra L. Bird, Ross Hall

Environmental Laboratory

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



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PREFACE

This report was prepared by the Environmental Laboratory (EL) of the US Army Engineer Waterways Experiment Station (WES), as part of the Environmental Impact Research Program (EIRP), Work Unit No. 31730, "Environmental Impacts of Modifying Estuarine Circulation and Transport Processes." The EIRP is sponsored by the Office, Chief of Engineers (OCE), US Army, Washington, DC. The OCE Technical Monitors for EIRP are Dr. John Bushman and Dr. David Buelow. Mr. Dave Mathis is the Water Resources Support Center Technical Monitor.

This report describes the use of a box-type model for transport/water quality calculations and the linkage of this model to multidimensional hydrodynamic models. Performance of the coarser grid/time-step box model is compared with directly linked transport codes.

The study was conducted and the report was prepared by Ms. Sandra L. Bird and Mr. Ross Hall of the Water Quality Modeling Group (WQMG), Ecosystem Research and Simulation Division (ERSD), EL, under the direct supervision of Mr. Mark Dortch, Chief, WQMG. General supervision was provided by Mr. Donald L. Robey, Chief, ERSD, and Dr. John Harrison, Chief, EL. Dr. Roger T. Saucier was Program Manager of EIRP. The report was edited by Ms. Lee T. Byrne of the Information Products Division, Information Technology Laboratory.

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CONVERSION FACTORS, NON-SI TO SI (METRIC)
UNITS OF MEASUREMENT

Non-SI units of measurement used in this report can be converted to SI
(metric) units as follows:

<u>Multiply</u>	<u>By</u>	<u>To Obtain</u>
cubic feet	0.02831685	cubic metres
degrees (angle)	0.01745329	radians
feet	0.3048	metres
inches	2.54	centimetres
pounds (mass)	0.4535924	kilograms
square feet	0.09290304	square metres

COUPLING HYDRODYNAMICS TO A MULTIPLE-BOX WATER QUALITY MODEL

PART I: INTRODUCTION

1. Assessment and management of water quality are aided by the use of numerical models. Water body hydrodynamics interact with biological, chemical, and other physical processes to affect water quality variables. Many simplifying assumptions are typically made in the equations governing these processes in order to develop economical numerical models. These assumptions are made in relationship to a particular situation (i.e., an assumption that might be acceptable for analyzing a problem in one water body might provide fallacious results in another).

2. One of the most routinely used assumptions suppresses variation of the variables within a cross section, and the model equations are written in a one-dimensional, longitudinal form. Typically, the cross-sectionally averaged approach is used for riverine applications. For a few well-mixed homogeneous estuaries, this approach may also be appropriate. Reservoir models sometimes assume no variation in the horizontal dimension and solve the one-dimensional, vertical form of the equation. One-dimensional models such as CE-QUAL-R1, a vertical reservoir model (Environmental Lab (EL) 1986) and CE-QUAL-RIV1, a longitudinal riverine model (EL, in preparation) solve the transport/water quality equations quickly and efficiently. The one-dimensional assumption, however, limits the problems that can be adequately addressed with these types of models. Only some reservoir problems and a very limited number of problems in estuaries and coastal embayments can be adequately addressed using this one-dimensional approach.

3. In recent years, many two-dimensional and, even more recently, three-dimensional hydrodynamic models have been developed and applied to reservoirs, estuaries, and coastal embayments. No single model can appropriately describe currents and mixing in all of these water bodies. Highly stratified estuaries require consideration of vertical variation of velocity and water quality constituents; wide estuaries require consideration of lateral variations; and large estuaries (which may be both wide and stratified) can require resolution in all three spatial dimensions. Reservoirs may be deep and stratified or broad and shallow. Because of this variety in water bodies, several different two- and three-dimensional hydrodynamic models have been developed

and used in estuarine and reservoir applications at the US Army Engineer Waterways Experiment Station (WES) by the Hydraulics Laboratory (HL) and the Coastal Engineering Research Center (CERC).

4. The necessity of evaluating environmental impacts of US Army Corps of Engineer (USACE) activities on a variety of water bodies was the impetus for the development of multidimensional water quality modeling capabilities by the EL. Three considerations guided the selection and development of a multidimensional water quality modeling approach:

- a. Long-term multidimensional water quality modeling can become cumbersome and computationally very time consuming when water quality algorithms are directly linked to hydrodynamic models.
- b. The EL should be able to perform water quality modeling studies in conjunction with hydrodynamic studies performed by both the HL and CERC.
- c. Water quality kinetics rarely require the spatial and temporal resolution required for accurate hydrodynamic calculations. To meet these requirements, a multiple-box (also known as a mixed segment, cells in series, or integrated compartment) model was chosen as the transport framework for a versatile, computationally efficient, water quality model. This type of model can be overlaid on the same grid as, or a coarser grid than, the hydrodynamic model, and it can use a larger time-step. Hydrodynamic model output can be averaged over time and space to drive the water quality model.

5. This report first describes the formulation and limitations of a multiple-box model. The Water Quality Analysis Simulation Program (WASP), developed under the auspices of the US Environmental Protection Agency (USEPA), was adapted for the purposes of this study; and the linkage of WASP to two different hydrodynamic models is described. Transport applications of the multiple-box model were made to three different water bodies with different physical characteristics: the Savannah River Estuary, DeGray Reservoir, and the Mississippi Sound. Results are analyzed and discussed.

PART II: MULTIPLE-BOX MODEL FORMULATION

General Formulation

6. WASP, the USEPA multiple-box model, was adapted for use in this study. Concentrations in this model are determined by simple mass balance around a series of completely mixed reactors, from the following equation (Ditoro, Fitzpatrick, and Thomann, 1983):

$$V_i \frac{dc_i}{dt} = \sum_j Q_{j,i} C_j + \sum_j \frac{E_{i,j} A_{i,j}}{L_{i,j}} (C_j - C_i) \pm W_i \pm K_i V_i \quad (1)$$

(1) (2) (3) (4) (5)

where

- V_i = segment volume, L^3
- i = segment index
- j = index of adjoining segment
- $Q_{j,i}$ = net advective flow from segment j to segment i , L^3/T
- C_j = concentration in segment j , M/L^3
- $E_{i,j}$ = dispersion coefficient for the i,j interface, L^2/T
- $A_{i,j}$ = cross-sectional area of the i,j interface, L^2
- $L_{i,j}$ = mixing length between segment i and j
- C_i = segment concentration, M/L^3
- W_i = point or distributed sources and sinks of the constituent, M/T
- K_i = kinetic degradation or transformation rate, M/L^3T

This ordinary differential equation is solved in the WASP model using Euler's Method.

7. Figure 1 is a schematic illustrating the processes described by Equation 1. " A_{in} " and " A_{out} " (term 2 in Equation 1) represent the flux of material into and out of the cell by the net advection of the velocity field. "D" (term 3 in Equation 1) represents the concentration flux from some equal exchange flow between the two cells accounting for dispersive transport resulting from velocity and concentration fluctuations across the dimensions averaged. "B" (term 4 in Equation 1) is the flux of material to/from the segment boundary. "K" (term 5 in Equation 1) represents the change in

concentration arising from reactions occurring within the segment including both degradation and transformation reactions.

8. The multiple-box model is the result of a volume average for each segment of the three-dimensional advective diffusion equation; i.e., it becomes a zeroth-dimensional type equation. Individual box segments can then be arranged in any arbitrary manner forming a one-, two-, or three-dimensional network. Although Figure 1 is an example of a one-dimensional alignment of segments, the processes shown can occur between two- and three-dimensional segment arrangements as well. This geometric flexibility allows the segments to intermesh with any hydrodynamic model grid as long as box volumes and flows between the boxes can be calculated.

Dispersive Properties

9. Dispersion presents the most difficulty in the application of the multiple-box model. Two major problems arise regarding dispersion in the application of the multiple-box model. First, calculation of an appropriate dispersion coefficient for use in the multiple-box model is difficult. Second, the multiple-box model may be numerically overdiffusive. The numerical diffusion introduced by the solution technique may be greater than the physical dispersion of the system unless relatively small segments are used.

10. Calculating dispersion for any transport model is difficult. In a dimensionally averaged model, the primary contribution to dispersion arises from nonuniformity of concentration and velocity in the dimension of averaging. Although the choice of dispersion coefficients is very difficult for one- and two-dimensional estuarine transport, some systematic guidelines are available in the literature (Fischer 1976 and Fischer et al. 1979). For the multiple-box model, no systematic guidelines are available in the literature for estimating these parameters.

11. However, one potential procedure for adjustment of the dispersion coefficient is based on duplicating dye transport simulated with the hydrodynamic model. Typically, if the multiple-box model is used in conjunction with a multidimensional hydrodynamic model, the hydrodynamic model will include a transport algorithm for calculating salinity in an estuary or temperature in a reservoir. Hydrodynamic/transport models are generally calibrated against field measurements of salinity and/or temperature distribution or a dye study

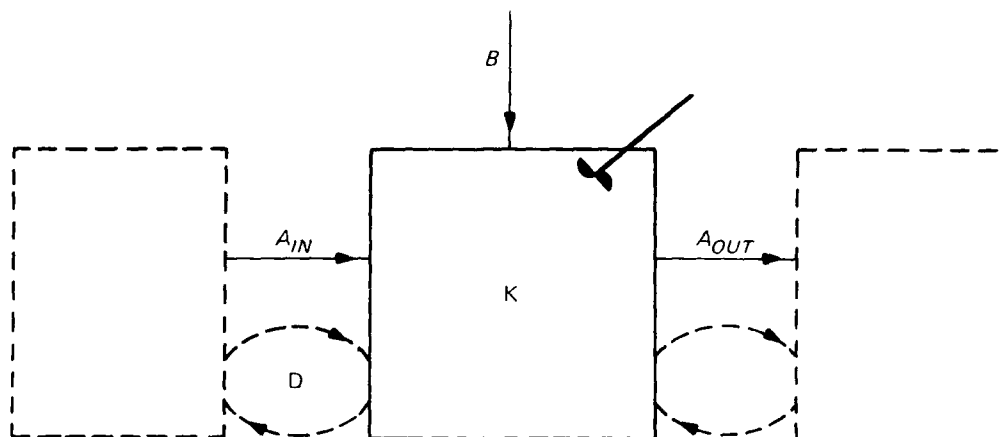


Figure 1. Schematic representation of box model processes

in the water body. Injection and transport of a conservative tracer in the hydrodynamic model, compared with the transport of an identical injection in the multiple-box model over a short period of time (i.e., a period of time typical for the hydrodynamic model runs), can be used as a guide for the adjustment of the dispersion coefficient in the multiple-box model. Additionally, this procedure would be effective in assessing the errors introduced in the use of tidally averaged values for advective transport.

12. Excessive numerical diffusion is often a critical limitation in the multiple-box concept. Shanahan and Harleman (1984) evaluated the diffusive properties of a multiple-box model using a one-dimensional arrangement of boxes, compared with a one-dimensional advective dispersion model for steady uniform flow

$$A \frac{\partial C}{\partial t} + Q \frac{\partial C}{\partial x} = A \frac{\partial}{\partial x} D \frac{\partial C}{\partial x} \quad (2)$$

where

A = cross-sectional flow area, M^2

Q = system through flow, M^3/T

x = the coordinate in the direction of flow, L

D = one-dimensional dispersion coefficient, M^2/T

Their analysis is based on conceptual reactor models used in sewage treatment plant design. A pecllet number (Pe) is defined as

$$Pe = \frac{QX}{AD} \quad (3)$$

where X is the total length of the system in the direction of flow. Their analysis indicates that, to keep the box model from being inherently over-diffusive, there must be at least n segments where n is defined as (for n being a large number)

$$n = \frac{Pe}{2} \quad (4)$$

They point out that for a given spatial step size, $\Delta x = X/n$, Equation 4 is equivalent to numerical diffusion in an upwind spatial finite difference approximation of Equation 2, i.e., $D_n = U \Delta x / 2$, where D_n is the numerical diffusion coefficient introduced by the solution scheme and U is the cross-sectionally averaged velocity (L/T).

13. However, according to Roache (1982), numerical diffusion for upwind differencing in a one-dimensional system is of the form

$$D_n = \frac{U \Delta x}{2} (1 - \alpha) \quad (5)$$

where

$$\alpha = \frac{U \Delta t}{\Delta x}$$

Δt = time

α is referred to as the Courant number. As the Courant number approaches one, numerical diffusion approaches zero. The condition where $\alpha = 1$ is the stability limit for the upwind differencing scheme. In a one-dimensional system when $\alpha = 1$, then the value of Δt represents the time that it takes for a particle to travel the length of a cell (Δx). This stability criterion applied to the box model takes the form $Q_{t,j} \Delta t / V_i = 1$ and can be interpreted

as the total flow into or out of a segment during a time-step must not exceed the volume of the segment. This interpretation lends itself to extrapolation to multidimensional problems. Restating Equation 5 in terms of multiple-box model parameters, numerical diffusion D_n at each segment interface in the multiple-box model can be described for equal length segments by

$$D_n = \frac{Q_{i,j} L_{i,j}}{2A_{i,j}} \left(1 - \frac{Q_{i,j} \Delta t}{V_i} \right) \quad (6)$$

One-Dimensional Example

14. The transport properties of the multiple-box model are illustrated by considering steady uniform flow in a rectangular channel with the following characteristics:

$H = 1.0 \text{ ft}^*$
 $W = 20.0 \text{ ft}$
 $L = 2,000 \text{ ft}$
 $U = 0.2 \text{ fps}$
 $Mn = 0.017$
 $D = 14.7 \text{ ft}^2/\text{sec}$
 $A = 20.0 \text{ ft}^2$
 $Q = 4.0 \text{ cfs}$
 $Pe = 27.2$, pecllet number

where H is the channel depth, W is the channel width, L is the total channel length, U is the average longitudinal velocity, and Mn is Manning's roughness coefficient. The dispersion coefficient, D , was calculated using the method of Fischer et al. (1979). For a very small time-step $\alpha \ll 1$, the channel must be divided into at least 14 segments ($n > Pe/2$) to avoid excessive numerical diffusion in the model.

* A table of factors for converting non-SI units of measurement to SI (metric) units is presented on page 3.

15. The effect of increasing the time-step on numerical diffusion in the box model is illustrated in Figure 2. For an initial concentration of 10 mg/l in the most upstream box, concentration versus time profiles in box 13 calculated with four time-steps ranging from 0.001 to 0.0082 days are shown in this figure. No physical dispersion was input for these test cases. Numerical diffusion decreases as the time-step increases, dropping dramatically as the time-step limit ($\Delta t = 0.008275$ days) is approached. This behavior is consistent with Equation 6.

16. The box model results were compared with the analytical solution of the one-dimensional advective diffusion equation for an instantaneous point source of material injected into steady flow in a uniform channel. The solution is given by Crank (1984):

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}} \exp \frac{-x^2}{4Dt} \quad (7)$$

where x is the downstream distance from the point of injection, t is the time since the injection, M is the mass injected, and D is the one-dimensional dispersion coefficient. Figure 3 shows the results for an injection of $M = 809$ g (the amount of mass equal to 10 mg/l injected into segment 1 of the 14-segment box model discretization) injected at $x = 0$, $t = 0$, and a value of $14.7 \text{ ft}^2/\text{sec}$ for the dispersion coefficient D compared with a 14-segment box model simulation using a 0.001-day time-step. The numerical diffusion for the box model simulation was calculated as $12.6 \text{ ft}^2/\text{sec}$. A value of $2.1 \text{ ft}^2/\text{sec}$ was input for the dispersion coefficient in the model to give a total model dispersion of $14.7 \text{ ft}^2/\text{sec}$. Peak concentrations are slightly lower in the upstream segments of the multiple-box model since the initial mass injection must be spread over the entire box, rather than being a true point source injection. This difference is reduced at the end of the channel, and box model transport approaches the analytical solution.

Model Modifications

17. WASP was developed for lake applications using constant volume boxes and steady flows. The constant volume and steady flow assumptions are not acceptable for intratidal estuarine applications; i.e., the time-step is

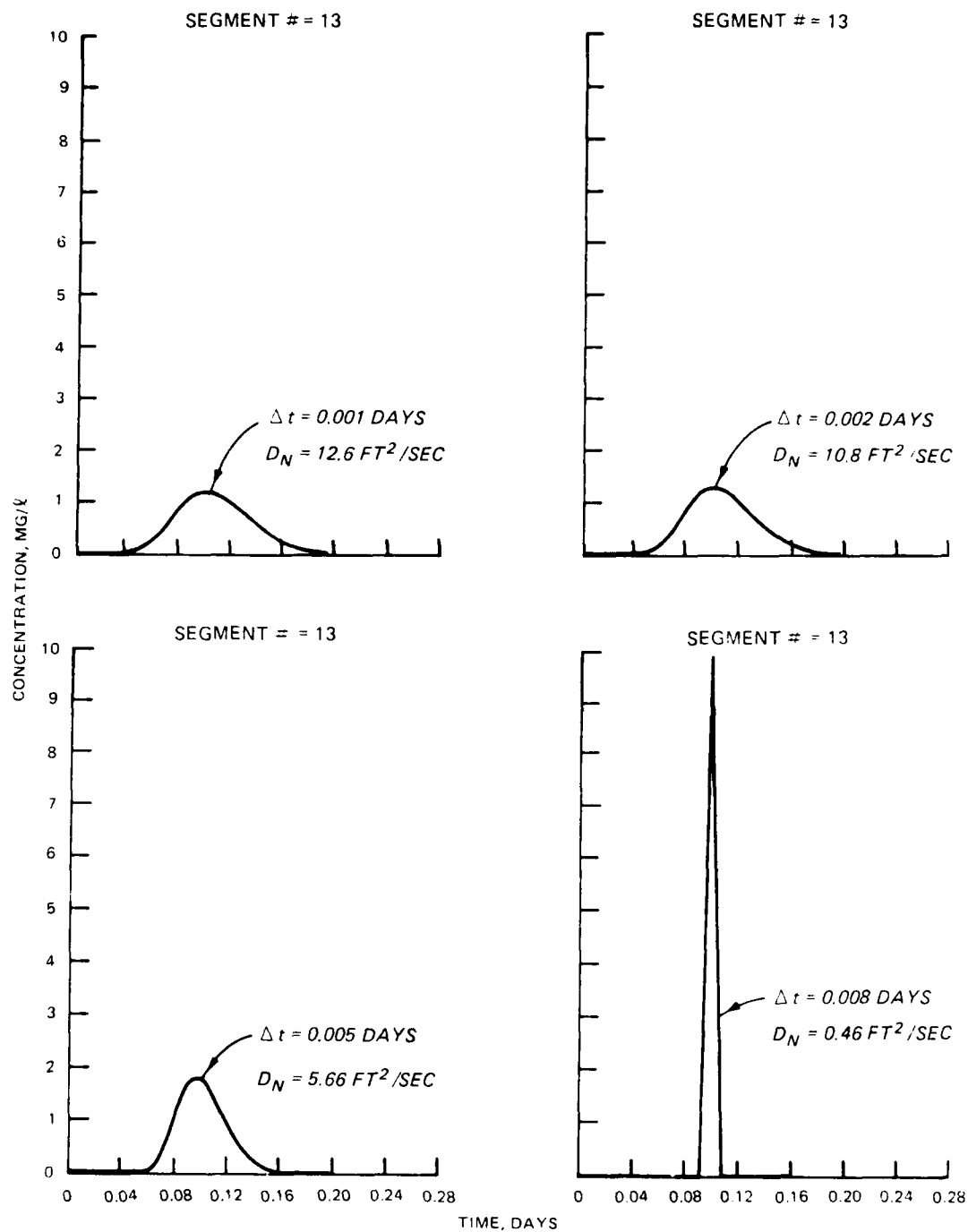


Figure 2. Effect of time-step on dispersion in the box model for a one-dimensional channel

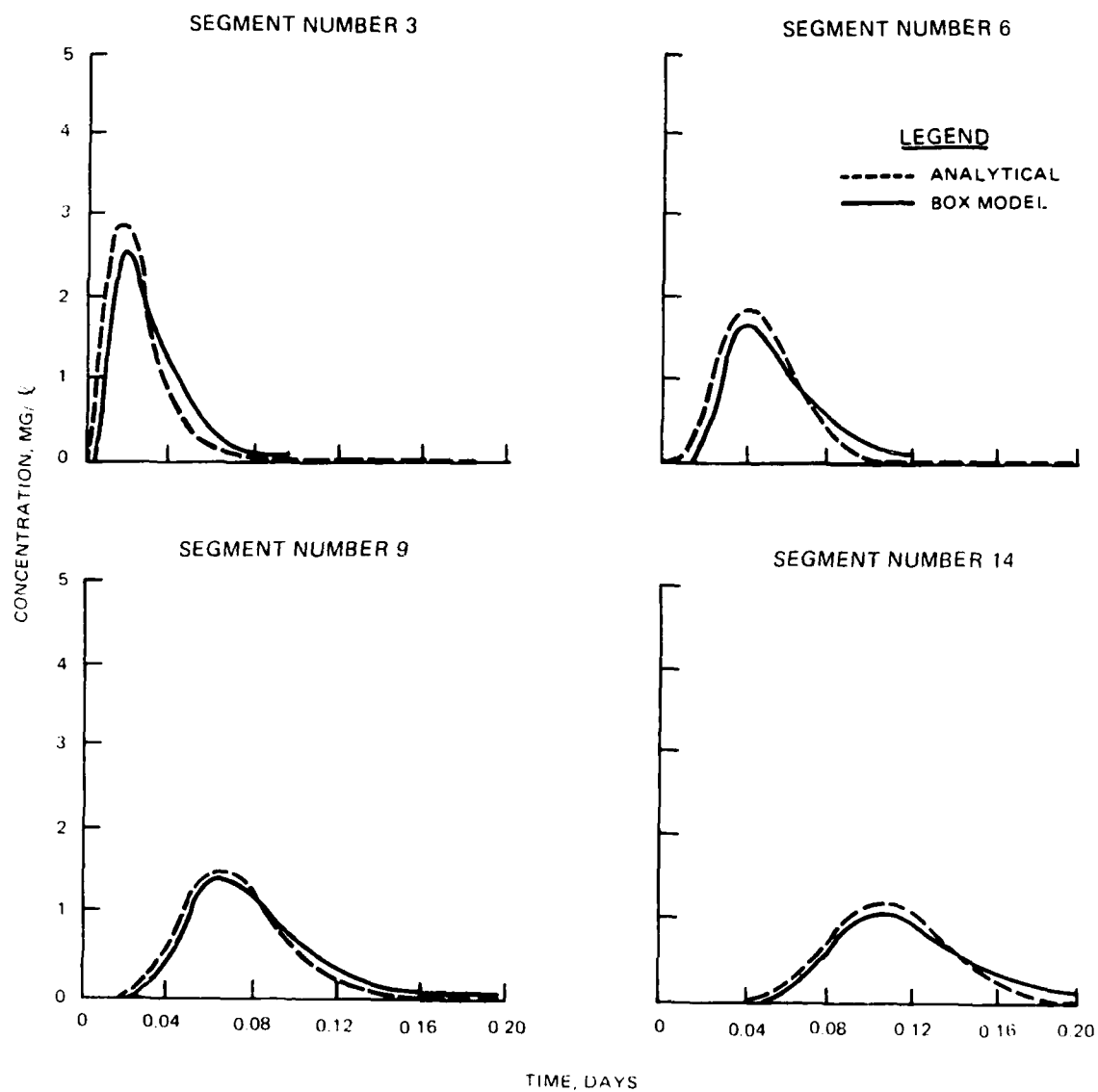


Figure 3. Comparison of box model solution to analytical solution for flow in a one-dimensional channel

less than a tidal cycle. For variable volume applications, the volume on the left hand side of Equation 1 must be written within the time differential, i.e., $D(V_1 C_1)/dt$. The value for the quantity $V_1 C_1$ was found using a Euler solution scheme and solving for the concentration at the new step. The modified formulation conserves mass for both constant and variable volume applications. For variable volume/unsteady flow applications, the model must be altered to read values for volumes and flows at every computational time rather than to read them once during the initial data input.

PART III: HYDRODYNAMIC INTERFACING

General

18. In this study, the multiple-box model is interfaced with hydrodynamic output generated by two different models. The first is CE-QUAL-W2, a two-dimensional, laterally averaged hydrodynamic model developed for the USACE (EL and HL 1986). This model was originally developed for two-dimensional reservoir modeling and extended for use in deep, narrow, stratified estuaries with the addition of estuarine boundary conditions (Edinger and Buchak 1981). Applications of the Savannah River Estuary (Hall 1987) and DeGray Lake (Martin 1987) are used herein as case studies for utilization of CE-QUAL-W2 output as the hydrodynamic driver of a multiple-box model.

19. The second model used to generate hydrodynamic output for the multiple-box model in this study is WIFM-SAL (WES Implicit Flooding Model with constituent transport) (Schmalz 1985b), a vertically averaged model employing an exponentially stretched grid. WIFM-SAL was developed for the analysis of shallow estuaries and embayments that could be assumed to be vertically well mixed. An application of WIFM-SAL to the Mississippi Sound and adjacent areas (Schmalz 1985a) was used as the test case for the interface with the multiple-box model.

Interface with CE-QUAL-W2

Savannah River application

20. Figure 4 shows the computational grid for the main channel and tide gate branches for the application of CE-QUAL-W2 to the Savannah River Estuary with the multiple-box model segments overlaid on it. A relatively coarse grid overlay of 18 box model segments was made on a total of 377 active computational cells in CE-QUAL-W2. In the upper end of the estuary where the reach is predominantly riverine and unstratified, a single vertical layer of boxes was overlaid on the CE-QUAL-W2 grid and expanded to a double layer in the partially stratified downstream sections. Thus, fine-scale vertical resolution was not maintained in this box model overlay.

21. Variables in CE-QUAL-W2 are defined as shown in Figure 5. Water surface elevation (Z), cell width (B), and constituent concentrations are

GEOMETRIC SCHEMATIZATION SAVANNAH RIVER ESTUARY APPLICATION

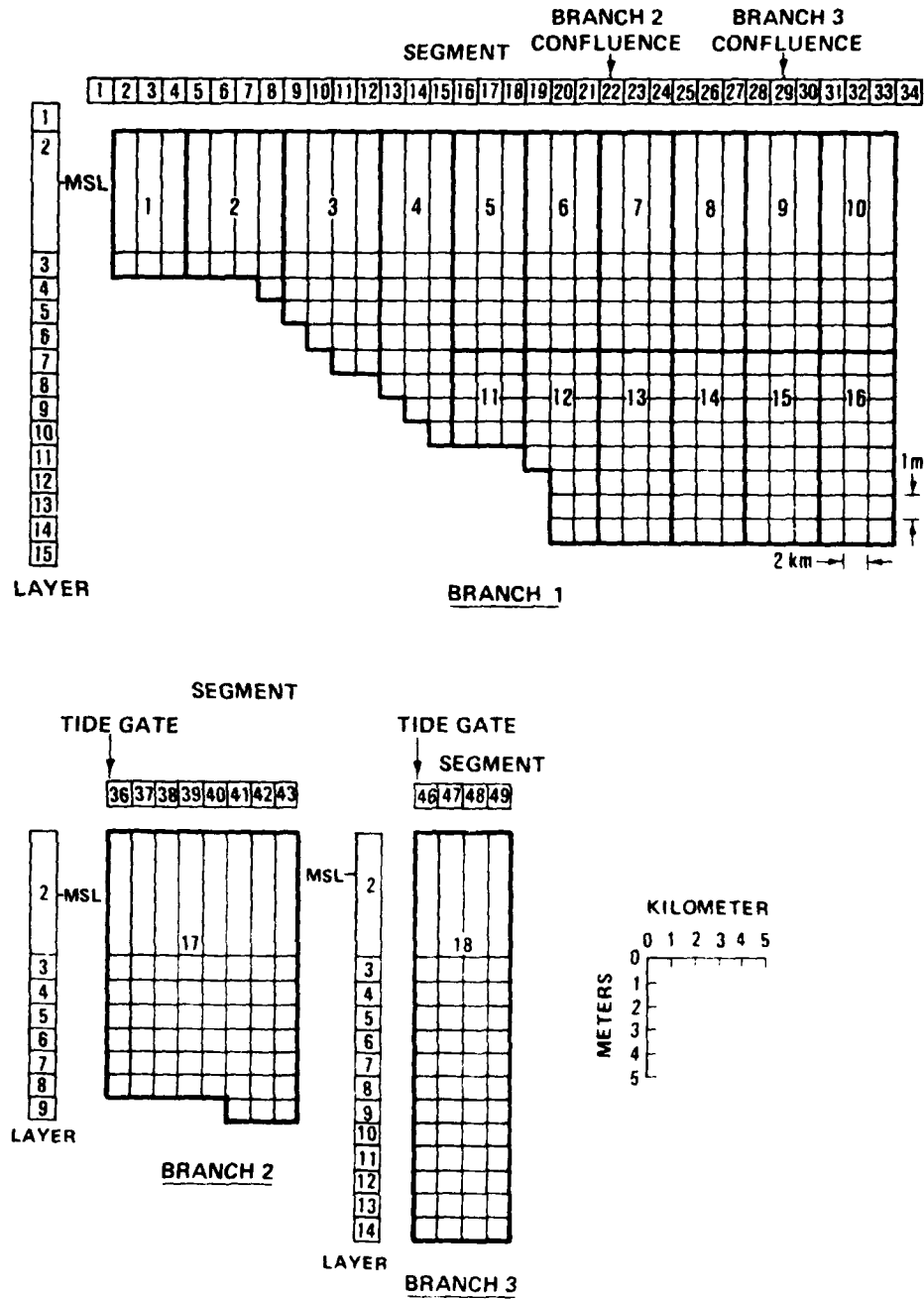


Figure 4. Savannah River Estuary grid for CE-QUAL-W2 with box model overlay shown by heavier lines

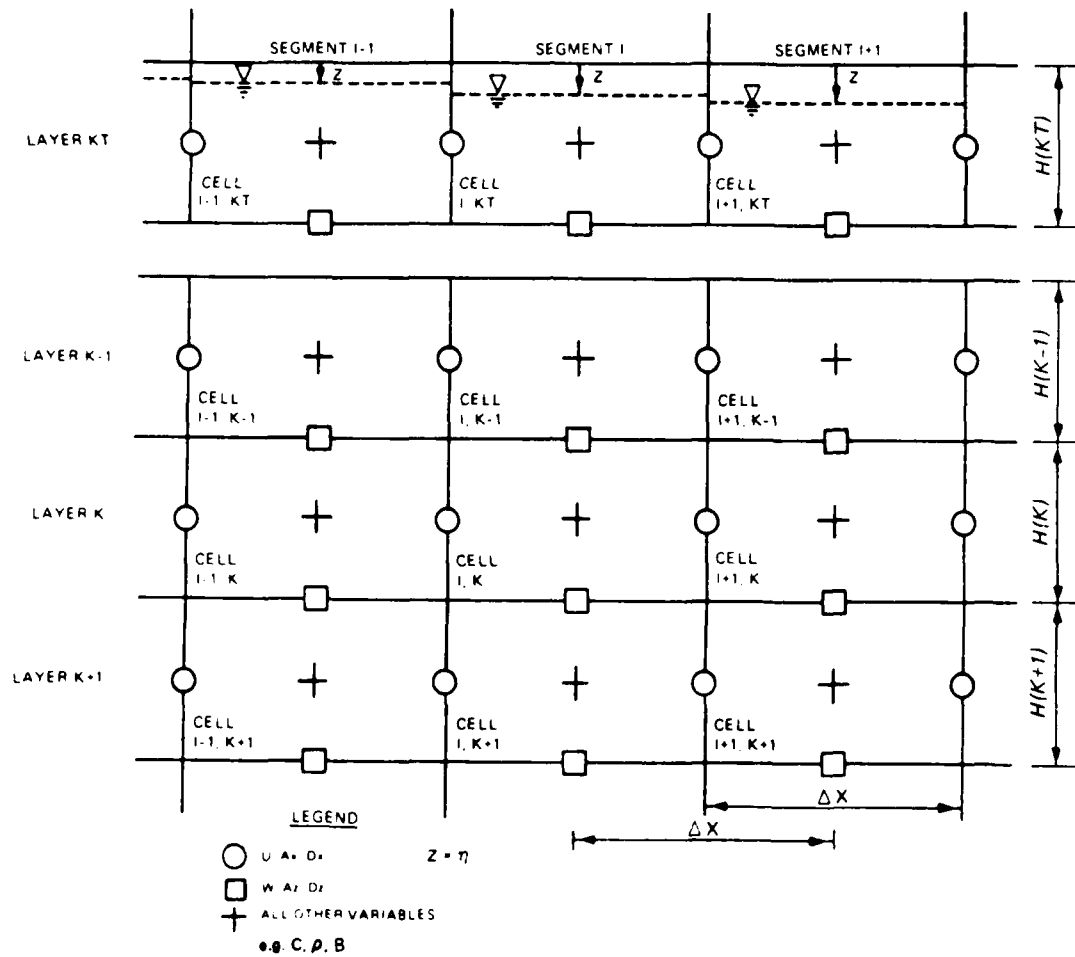


Figure 5. Variable definition sketch for CE-QUAL-W2

defined at the center of each cell. Layer thickness is a constant (H) for all except the top layer, which is variable ($H-Z$). Velocities (u, w) and diffusion coefficients (D_x, D_z) are defined at the cell faces.

22. Box model segment volumes were calculated at each CE-QUAL-W2 time-step by summing the CE-QUAL-W2 cell volumes within each box segment. The CE-QUAL-W2 cell volume $[V(I, K)]$ was calculated by

$$V(I, K) = B(I, K) \times H(K) \times \Delta x \quad K > K_T$$

$$V(I, K) = B(I, K) \times [H(K) - Z(I)] \times \Delta x \quad K = K_T \quad (8)$$

The flow across each box segment face was calculated by summing corresponding CE-QUAL-W2 cell flows at each box face. K is the layer number, and KT is the surface layer. CE-QUAL-W2 flows are given by

$$Q_h(I-1, K) = U(I-1, K) \times H(K) \times \frac{[B(I-1, K) + B(I, K)]}{2} \quad K \neq KT, I > 1$$

$$Q_h(I-2, KT) = U(I-1, KT) \times \frac{[H(KT) - Z2(I)] + [H(KT) - Z2(I-1)]}{2} \\ \times \frac{[B(I-1, K) + B(I, K)]}{2} \quad K = KT, I > 1$$

$$Q_v(I, K-1) = W(I, K-1) \times \Delta x \times \frac{[B(I, K-1) + B(I, K)]}{2} \quad K > 1 \quad (9)$$

where Q_h and Q_v represent flows in the horizontal and vertical directions. The flow across the upstream face at $I = 1$ into the first multiple-box segment is simply the upstream boundary flow specified in CE-QUAL-W2. Box model flows are calculated by summing the flows across each of the CE-QUAL-W2 cell faces that align with the box model face.

23. The time-averaged flow (\bar{Q}_t) was calculated as the arithmetic average of the flows, as follows:

$$\bar{Q}_t = \sum_{n=1}^N \frac{Q_n}{N} \quad (10)$$

where N is the number of time-steps averaged. However, in the time-averaged data set, the volume at the beginning of each averaging interval was used since the average net flow into a segment over the averaging interval added to the volume at the beginning of the interval equalled the volume at the beginning of the next interval. In this way, continuity was assured.

DeGray Lake application

24. Whereas the Savannah River is a strongly advective system with a residence time on the order of days, DeGray Lake typically has a residence time of several months and exhibits very strong thermal stratification during the summer. Relatively fine vertical resolution is required for accurate

water quality modeling. The DeGray application of CE-QUAL-W2 used a horizontal segment length of 993.6 m and a layer thickness of 2.0 m. The first box model test used a direct grid overlay resulting in 428 segments and 828 flows. The correspondence between CE-QUAL-W2 cells and box model cells in the first box model test is shown in Table 1.

25. A second box model test consisted of a 2 by 2 overlay on the CE-QUAL-W2 grid, i.e., four CE-QUAL-W2 cells per box model segment except for some of the bottom segments. This box model application consisted of 112 segments and 210 flows. Correspondence between CE-QUAL-W2 cells and box model cells in the second box model test is shown in Table 2. Daily averaged values for flow and volume input for both of these box model overlays were calculated using the same general approach as previously described for the Savannah River application.

26. The CE-QUAL-W2 time-step for the DeGray application was 1,500 sec or 0.02+ days. The box model time-step was 0.1 day. The 1,500-sec time-step size selected for CE-QUAL-W2 reflects an internal gravity wave restriction. A subset of CE-QUAL-W2 hydrodynamic output calculated during the summer months was used for model comparisons, since interest centered primarily on erosion of the thermocline resulting from numerical diffusion in the box model. Experimentation revealed that 0.1-day time-steps were computationally stable for the box model during the time interval documented in this report; however, during autumnal overturn, the time-step size in the box model was limited to 0.02 day because of the Courant number restriction. Daily averaged values for the volumes and flows were used repeatedly for the time-steps in a particular simulation day.

Interface with WIFM-SAL

27. Figure 6 shows the transformed coordinate grid with the locations of specific variables used in WIFM-SAL calculations. The velocities (U,V) are defined at the cell faces while depth (h), water surface elevation (n), and constituent concentration are defined at the cell center. The variables α_1 and α_2 are the spatial coordinates in transformed space. Figure 7 shows the computational grid in real space coordinates for the WIFM application to the Mississippi Sound and surrounding areas. The WIFM grid is 59 by 115, i.e., nearly 7,000 cells. More boxes were needed to provide an adequate overlay on

Table 1

WASP-01 Overlay on CE-QUAL-W2 Grid*

CE-QUAL-W2 Grid	WASP-01 Overlay	Elevation M
1	1	400
2	2	399
3	3	398
4	4	397
5	5	396
6	6	395
7	7	394
8	8	393
9	9	392
10	10	391
11	11	390
12	12	389
13	13	388
14	14	387
15	15	386
16	16	385
17	17	384
18	18	383
19	19	382
20	20	381
21	21	380
22	22	379
23	23	378
24	24	377
25	25	376
26	26	375
27	27	374
28	28	373
29	29	372
30	30	371
31	31	370
32	32	369
33	33	368
34	34	367
35	35	366
36	36	365
37	37	364
38	38	363
39	39	362
40	40	361
41	41	360
42	42	359
43	43	358
44	44	357
45	45	356
46	46	355
47	47	354
48	48	353
49	49	352
50	50	351
51	51	350
52	52	349
53	53	348
54	54	347
55	55	346
56	56	345
57	57	344
58	58	343
59	59	342
60	60	341
61	61	340
62	62	339
63	63	338
64	64	337
65	65	336
66	66	335
67	67	334
68	68	333
69	69	332
70	70	331
71	71	330
72	72	329
73	73	328
74	74	327
75	75	326
76	76	325
77	77	324
78	78	323
79	79	322
80	80	321
81	81	320
82	82	319
83	83	318
84	84	317
85	85	316
86	86	315
87	87	314
88	88	313
89	89	312
90	90	311
91	91	310
92	92	309
93	93	308
94	94	307
95	95	306
96	96	305
97	97	304
98	98	303
99	99	302
100	100	301
101	101	300
102	102	299
103	103	298
104	104	297
105	105	296
106	106	295
107	107	294
108	108	293
109	109	292
110	110	291
111	111	290
112	112	289
113	113	288
114	114	287
115	115	286
116	116	285
117	117	284
118	118	283
119	119	282
120	120	281
121	121	280
122	122	279
123	123	278
124	124	277
125	125	276
126	126	275
127	127	274
128	128	273
129	129	272
130	130	271
131	131	270
132	132	269
133	133	268
134	134	267
135	135	266
136	136	265
137	137	264
138	138	263
139	139	262
140	140	261
141	141	260
142	142	259
143	143	258
144	144	257
145	145	256
146	146	255
147	147	254
148	148	253
149	149	252
150	150	251
151	151	250
152	152	249
153	153	248
154	154	247
155	155	246
156	156	245
157	157	244
158	158	243
159	159	242
160	160	241
161	161	240
162	162	239
163	163	238
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165	165	236
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168	168	233
169	169	232
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171	171	230
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173	173	228
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175	175	226
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221	221	180
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229	229	172
230	230	171
231	231	170
232	232	169
233	233	168
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235	235	166
236	236	165
237	237	164
238	238	163
239	239	162
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242	242	159
243	243	158
244	244	157
245	245	156
246	246	155
247	247	154
248	248	153
249	249	152
250	250	151
251	251	150
252	252	149
253	253	148
254	254	147
255	255	146
256	256	145
257	257	144
258	258	143
259	259	142
260	260	141
261	261	140
262	262	139
263	263	138
264	264	137
265	265	136
266	266	135
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268	268	133
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384	384	17
385	385	16
386	386	15
387	387	14
388	388	13
389	389	12
390	390	11
391	391	10
392	392	9
393	393	8
394	394	7
395	395	6
396	396	5
397	397	4
398	398	3
399	399	2
400	400	1

* Numbers in the table indicate box model cell numbers at CE-QUAL-W2 grid locations.

Table 2

WASP-01 Overlay on CE-QUAL-W2 Grid*

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	12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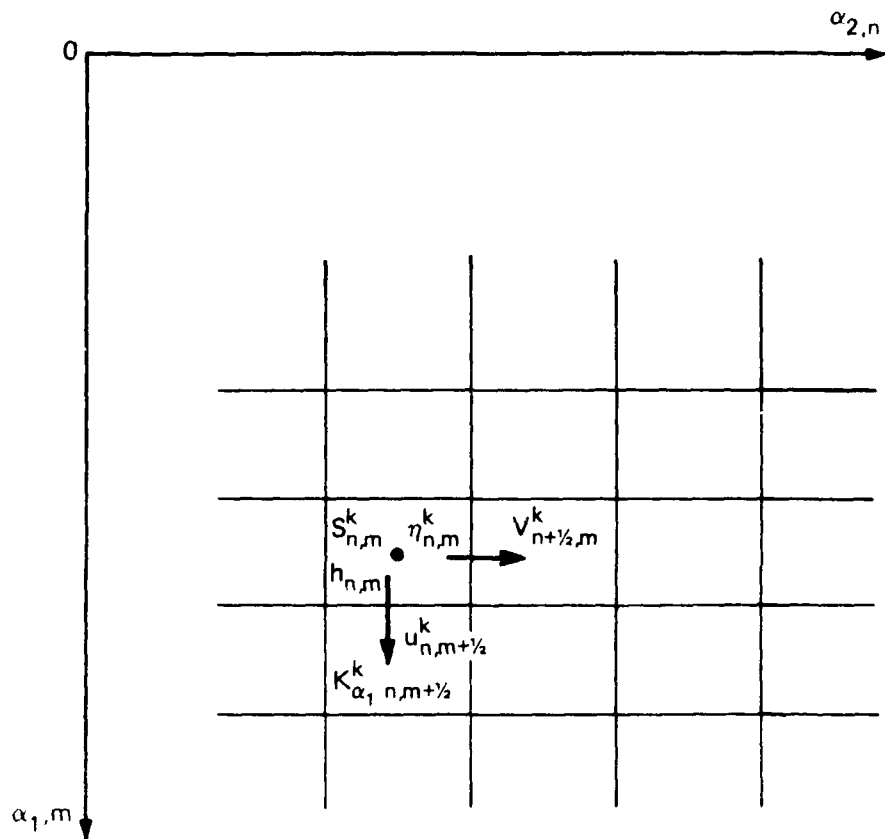


Figure 6. Variable definition sketch for WIFM

this system than were required in the Savannah River application. The overlay, selected to provide adequate resolution within the constraints of reasonable storage requirement and computation time, was a regular 2- by 3-overlay on the WIFM grid (bold outlines on Figure 7), i.e., 6:1 WIFM cells per box model segment resulting in nearly 1,000 box model segments. The use of a regular overlay made it possible to automate generation of the interface file that defined box model segments and flow faces in terms of the WIFM cells. This information is required for the generation of the box model input from hydrodynamic input. For a large number of box model cells, manual generation of this interface is tedious and time consuming.

28. An approach slightly different from that described for CE-QUAL-W2 was used in calculating volumes and flows for box model input from WIFM hydrodynamics. The solution scheme for the continuity equation employed in WIFM was used as a basis for calculation of multiple-box volumes and flows. An approach analogous to that of Schmalz (1985b) in the development of a

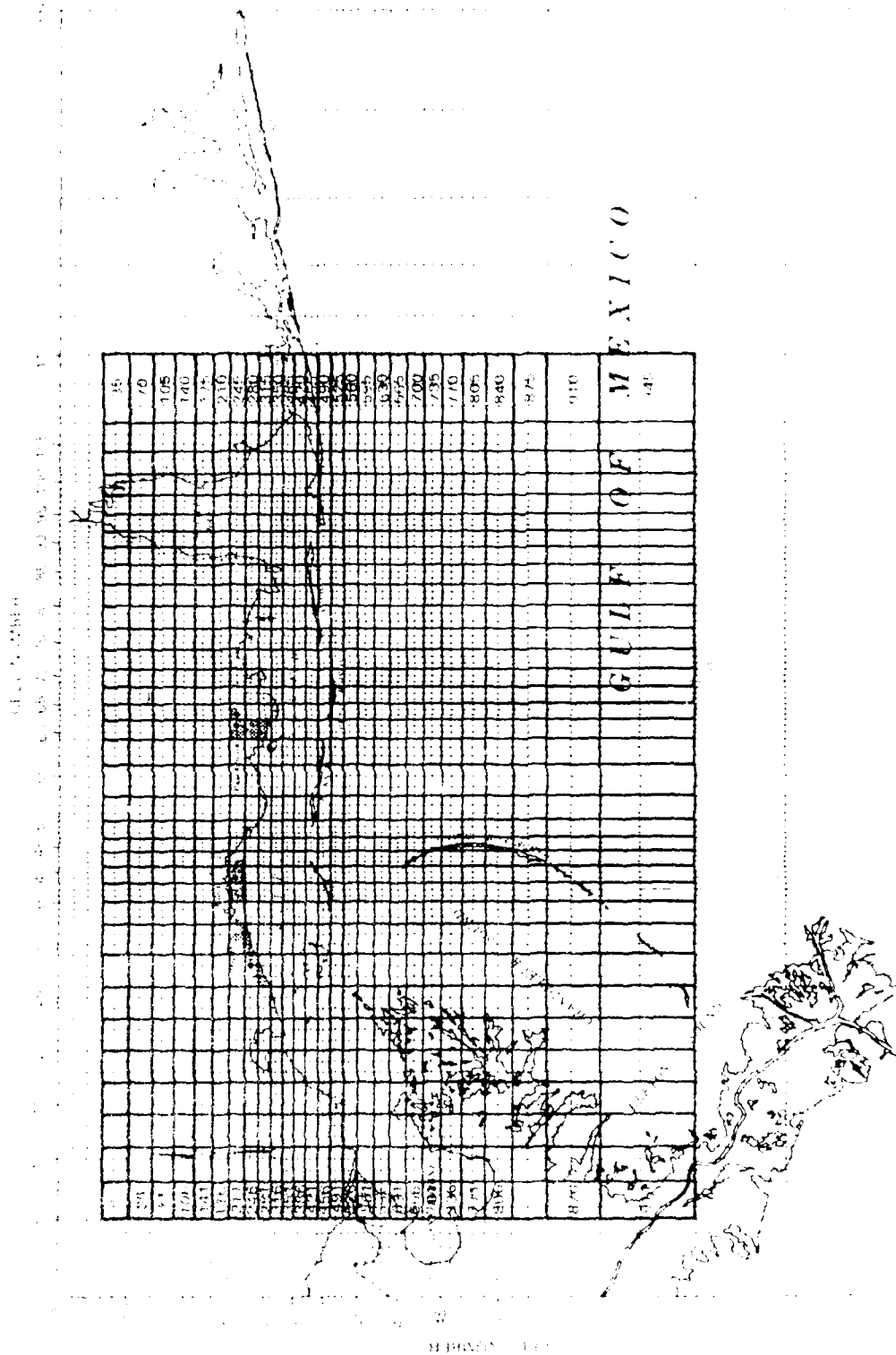


Figure 7. Mississippi Sound computational grid for WFN-SAL with 1:6 box model overlay shown with heavy lines

three-time-level explicit transport scheme for use in WIFM-SAL was employed. The finite difference forms of the continuity equation used in the alternating difference type solution of the two-dimensional hydrodynamics were combined to yield one three-time-level finite difference expression.

$$\begin{aligned} & \frac{\eta_{n,m}^{k+1} - \eta_{n,m}^{k-1}}{2\Delta t} + \frac{1}{2(\mu_1)_m \Delta \alpha_1} \left[\left(u_{n,m+\frac{1}{2}}^{k+1} + u_{n,m+\frac{1}{2}}^{k-1} \right) D_{n,m+\frac{1}{2}}^k - \left(u_{n,m-\frac{1}{2}}^{k+1} + u_{n,m-\frac{1}{2}}^{k-1} \right) D_{n,m-\frac{1}{2}}^k \right] \\ & + \frac{1}{2(\mu_2)_n \Delta \alpha_2} \left[\left(v_{n+\frac{1}{2},m}^{k+1} + v_{n+\frac{1}{2},m}^{k-1} \right) D_{n+\frac{1}{2},m}^k - \left(v_{n-\frac{1}{2},m}^{k+1} + v_{n-\frac{1}{2},m}^{k-1} \right) D_{n-\frac{1}{2},m}^k \right] = 0 \quad (11) \end{aligned}$$

with

$$\begin{aligned} D_{n,m+\frac{1}{2}}^k &= \frac{d_{n,m+\frac{1}{2}}^k + d_{n,m}^k}{2} \\ D_{n+\frac{1}{2},m}^k &= \frac{d_{n+\frac{1}{2},m}^k + d_{n,m}^k}{2} \end{aligned}$$

where

- $\eta_{n,m}^{k\pm 1}$ = water surface elevation at time level $k\pm 1$ in cell (n,m)
- Δt = time-step length
- $(\mu_1)_m$ = stretching coefficient in α_1 direction at cell index n
- $\Delta \alpha_1$ = α_1 direction space increment
- $u_{n,m+\frac{1}{2}}^{k\pm 1}$ = velocity component in α_1 direction for cell (n,m) at time level $k\pm 1$
- $(\mu_2)_n$ = stretching coefficient in α_2 direction at cell index m
- $\Delta \alpha_2$ = α_2 direction space increment
- $v_{n+\frac{1}{2},m}^{k\pm 1}$ = velocity component in α_2 direction for cell (n,m) at time level $k\pm 1$
- $d_{n,m}^k$ = water depth in cell (n,m) at time level k

29. Rearranging Equation 11 and adding the time invariant depth $-h_{n,m}$ to the water surface elevation yields

$$\begin{aligned}
& \left(\eta_{n,m}^{k+1} - h_{n,m} \right) (\mu_1)_m \Delta \alpha_1 (\mu_2)_n \Delta \alpha_2 \quad (1) \\
& = \left(\eta_{n,m}^{k-1} - h_{n,m} \right) (\mu_1)_m \Delta \alpha_1 (\mu_2)_n \Delta \alpha_2 + (\mu_2)_n \Delta \alpha_2 2\Delta t \left[\frac{u_{n,m-\frac{1}{2}}^{k+1} + u_{n,m-\frac{1}{2}}^{k-1}}{2} \right] D_{n,m-\frac{1}{2}}^k \quad (3) \\
& \quad - (\mu_2)_n \Delta \alpha_2 2\Delta t \frac{(u_{n,m+\frac{1}{2}}^{k+1} + u_{n,m+\frac{1}{2}}^{k-1})}{2} D_{n,m+\frac{1}{2}}^k \quad (4) \\
& \quad + (\mu_1)_m \Delta \alpha_1 2\Delta t \frac{(v_{n-\frac{1}{2},m}^{k+1} + v_{n-\frac{1}{2},m}^{k-1})}{2} D_{n-\frac{1}{2},m}^k \quad (5) \\
& \quad - (\mu_1)_m \Delta \alpha_1 2\Delta t \frac{(v_{n+\frac{1}{2},m}^{k+1} + v_{n+\frac{1}{2},m}^{k-1})}{2} D_{n+\frac{1}{2},m}^k \quad (6) \quad (12)
\end{aligned}$$

where term 1 is a finite difference expression for volume of cell (n,m) at the k+1 time level, which is set equal to the volume of the cell at the k-1 time-step (term 2), plus the net volume change resulting from the approximations for flow over two time intervals across the four faces of the cell (terms 3, 4, 5, and 6). Continuity can be guaranteed in the generation of box model parameters if calculation of volume and flow are based on Equation 12.

30. Box segment volume is calculated as the sum of the volume of the cells overlaid where individual WIFM cell volume, $Vol_{n,m}^{k-1}$, is calculated (as suggested by Equation 12) by

$$Vol_{n,m}^{k-1} = \left(\eta_{n,m}^{k-1} - h_{n,m} \right) (\mu_1)_m \Delta \alpha_1 (\mu_2)_n \Delta \alpha_2 \quad (13)$$

Likewise, box model flows are calculated by summing the flows across each of the WIFM cell faces aligned with the box model face. The flow into each WIFM cell is found for α_1 and α_2 directions by dividing terms 3 and 5 respectively by $2\Delta t$ (terms 4 and 6 represent flow out of the WIFM cell). Since Equation 12 is a three-time-level finite difference expression, flows and volumes are calculated at alternate WIFM time-steps since terms 3 and 5 give

the flow from the $k-1$ to $k+1$ time levels and the time interval used for multiple-box input is $2\Delta t$ where Δt is the WIFM-SAL time-step. Additional time-averaging can then be performed as described for the interface with CE-QUAL-W2.

PART IV: TRANSPORT APPLICATIONS

General

31. To identify the potential and limitations for simulating multi-dimensional transport using the relatively coarse grid, long time-step, multiple-box model, movement of a conservative constituent in the box model was compared with movement of the same constituent in the finer scale, directly linked, transport models. Results for the box model and CE-QUAL-W2 simulations were compared using both Savannah River Estuary and DeGray Lake applications; comparison with WIFM-SAL used the Mississippi Sound application.

Comparison with CE-QUAL-W2

Savannah River application

32. A 25-mg/l instantaneous dye injection was made in segment 3 of the box model and in the equivalent area of the CE-QUAL-W2 grid for the Savannah River Estuary, as shown in Figure 4. CE-QUAL-W2 hydrodynamics were averaged as described in Part III and used to drive the box model. Simulations were performed for 3.5 days. CE-QUAL-W2 simulations required a 2-min time-step, whereas the box model was run at a series of time-steps up to 3.5 hr. In order to evaluate the ability of the box model overlay to replicate CE-QUAL-W2 transport, a set of three graphical displays was made for several of the box model segments. The first graph was a time-history of the volume weighted average of the concentrations in the CE-QUAL-W2 cells contained within a given box model segment (represented in the graph by a solid line) and the range of the concentrations (shown with the vertical bar (|)) found in these cells (Figures 8a-14a). The second graph in the set was a time-history of concentrations for the 3.5-hr box model simulations (o____o) compared with the volume weighted CE-QUAL-W2 results (Δ ____ Δ) (Figures 8b-14b). The third graph in the set was concentration time-histories in the segment for the box model simulation using different time-step sizes (Figures 8c-14c), representing 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step results, respectively.

33. The CE-QUAL-W2 cells that overlay segment 4 immediately downstream of the injection location show the greatest variation in concentration for any

of the segments (Figure 8a). The coarse box model overlay did not provide the resolution of the finer CE-QUAL-W2 grid. Excessive information was lost where the variation of concentration within the segment was large compared with the average concentration in the segment. However, the average concentration in the CE-QUAL-W2 cells and the box model simulation agree (Figure 8b) except for the concentration peak value in this segment. The peak concentration in the box model simulation was sensitive to the time-step choice (Figure 8c). For example, the 0.5-hr time-step for the box model simulation substantially decreased the peak concentration compared with the 2.0- and 3.5-hr time-steps. At segment 5, a large variation in the concentrations in the overlaid CE-QUAL-W2 cells diminished substantially downstream (Figures 9a-12a) at segments 6, 7, and 9. The box model replicated the oscillation in concentrations caused by the flow reversals. The phase as well as the magnitude of the oscillations was generally matched.

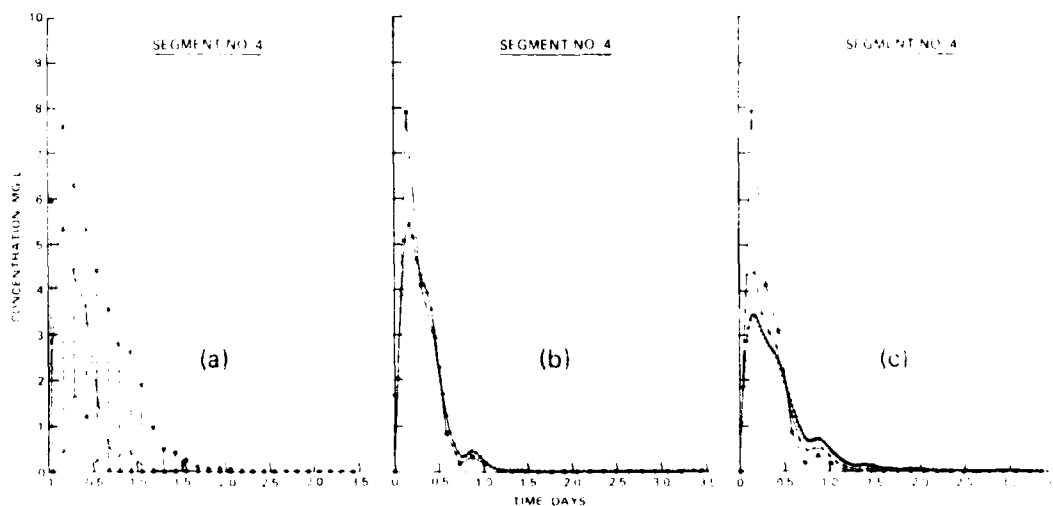


Figure 8. Savannah River application: concentration time-history for box model segment 4 and overlaid CE-QUAL-W2 cells. (a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (|), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

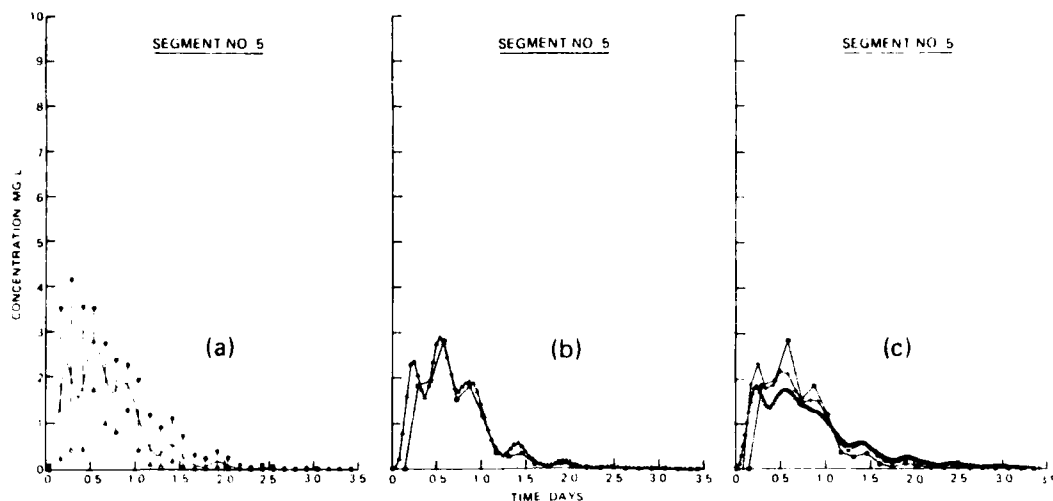


Figure 9. Savannah River application: concentration time-history for box model segment 5 and overlaid CE-QUAL-W2 cells.

(a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (|), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

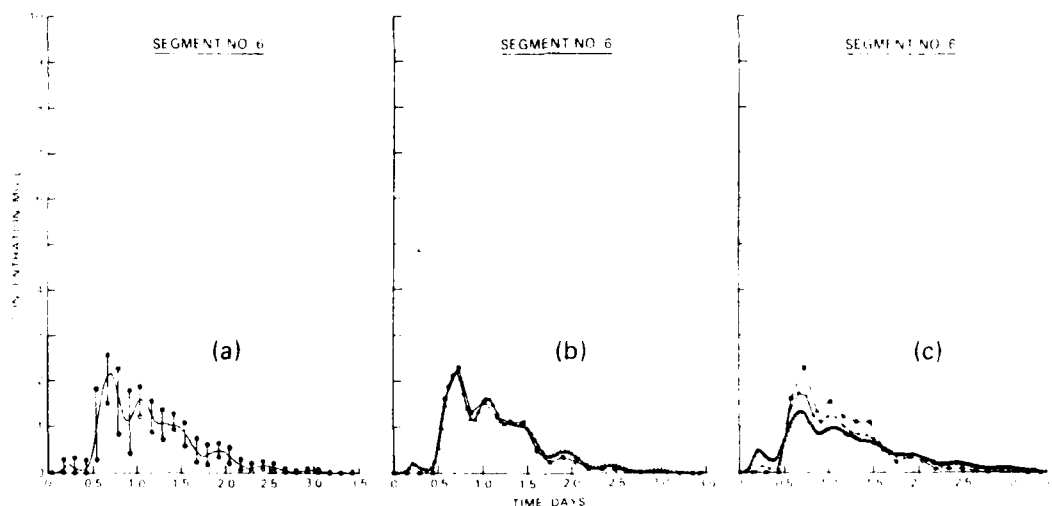


Figure 10. Savannah River application: concentration time-history for box model segment 6 and overlaid CE-QUAL-W2 cells.

(a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (|), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

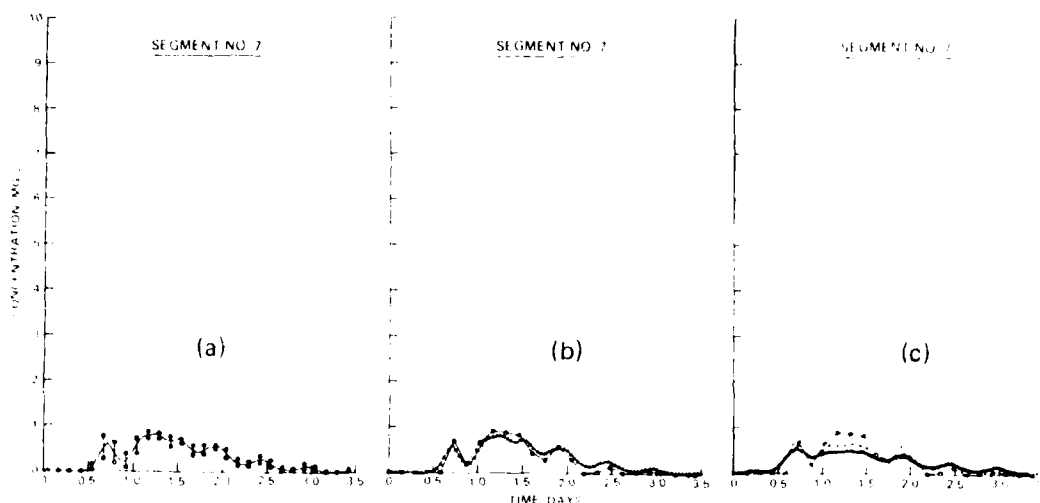


Figure 11. Savannah River application: concentration time-history for box model segment 7 and overlaid CE-QUAL-W2 cells. (a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (---), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

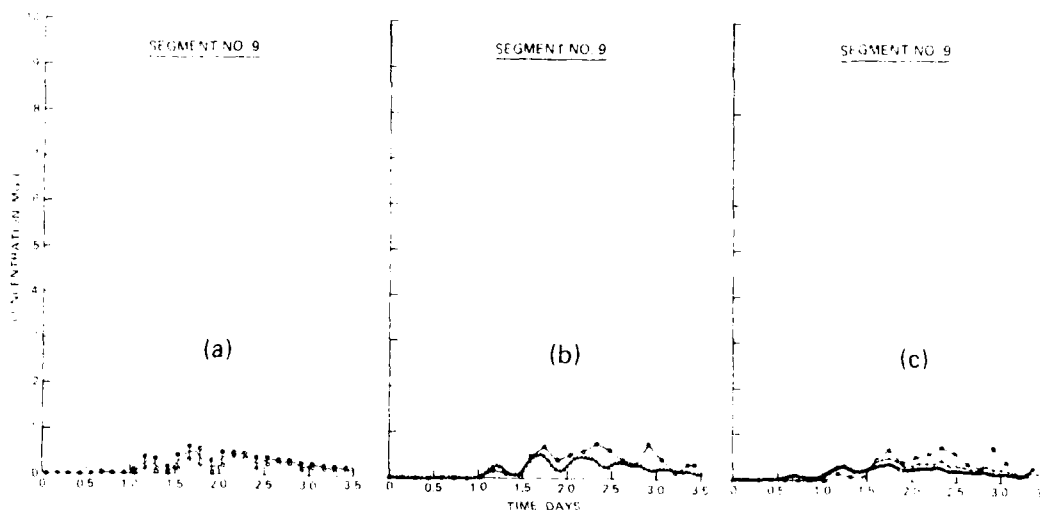


Figure 12. Savannah River application: concentration time-history for box model segment 9 and overlaid CE-QUAL-W2 cells. (a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (---), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

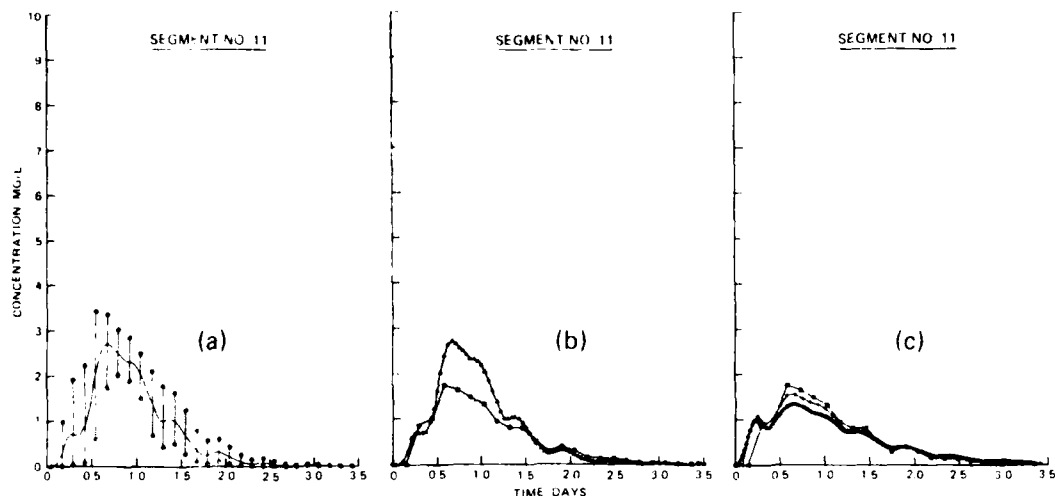


Figure 13. Savannah River application: concentration time-history for box model segment 11 and overlaid CE-QUAL-W2 cells.

(a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (|), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

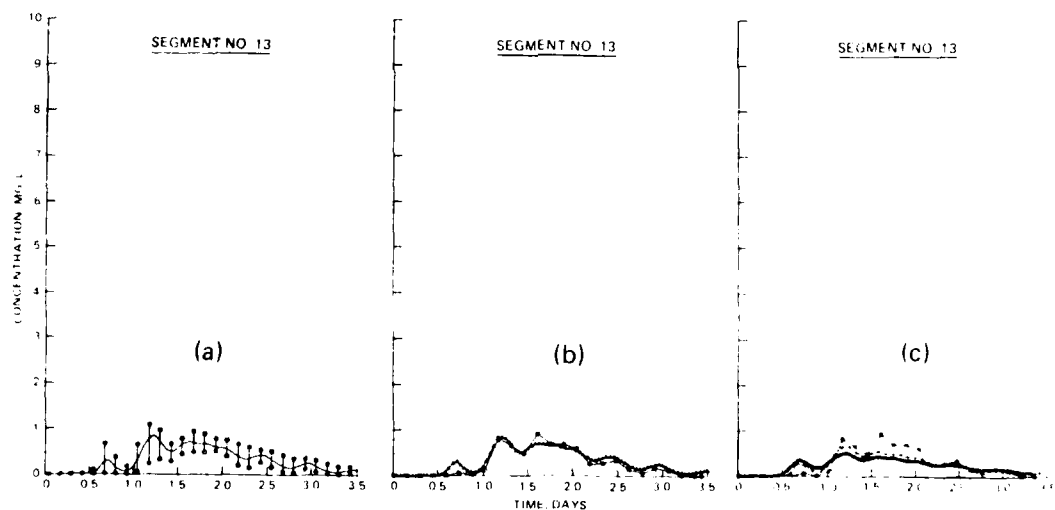


Figure 14. Savannah River application: concentration time-history for box model segment 13 and overlaid CE-QUAL-W2 cells.

(a) Volume weighted average of CE-QUAL-W2 cells overlaid by the box model segment (_____) and the range of concentration in these cells (|), (b) comparison of box model (o____o) and CE-QUAL-W2 (Δ ____ Δ) results, (c) comparison of box model results using a 0.5-hr (Δ ____ Δ), 2-hr (+____+), and 3.5-hr (o____o) time-step

34. However, in segment 11 (Figure 13b) the box model does not adequately simulate the average concentration in the CE-QUAL-W2 cells that it overlays. The box model underestimates the peak concentration in this segment even using the 3.5-hr time-step. The source of this error becomes clear when the large range of concentrations in the CE-QUAL-W2 cells overlaid by segment 4 (Figure 8a), the segment upstream from segment 11, is considered. Circulation in the estuary moved the highest concentration material into the bottom cells of this segment, but the box model transported the average value from segment 4 into segment 11. Given the particular box model overlay and injection condition, this anomaly was the result of lowered spatial resolution of the box model overlay. At segment 13 (Figure 14) farther downstream in the bottom layer of boxes, the box model simulation mimicked the average CE-QUAL-W2 results. The box overlay can impact accuracy of results and should be carefully considered in terms of the problems addressed. If a sharp front is not simulated, results will not be so severe.

DeGray Lake application

35. The primary objective of the DeGray Lake application was to compare the vertical spreading of material in the WASP grids with the CE-QUAL-W2 simulation. A uniform injection of dye was made in the top layers of both the box model and CE-QUAL-W2 grid. For the 1:1 WASP (referred to as WASP01) overlay, a 100-mg/l injection was made into the surface layer of cells in both models. For the 2:1 WASP overlay (referred to as WASP02), the mass injected into the surface layer of the CE-QUAL-W2 cells was distributed through the respective WASP surface layer segments. The initial WASP02 segment tracer concentrations are listed in Table 3.

36. Daily averaged values of flows were calculated from the CE-QUAL-W2 output for WASP input; a time-step of 0.1 day was used in the WASP simulation (i.e., each set of averaged hydrodynamics was used for 10 time-steps). For the WASP01 simulation, 0.1 day approached the time-step limit; for the WASP02 simulation, a 0.5-day time-step could be used without instabilities. However, all results presented here used a 0.1-day time-step in the simulation. If simulations were carried through fall overturn, shorter time-steps had to be used, as mentioned in Part III.

37. Concentration versus elevation plots at six longitudinal segments after 30, 60, and 90 days of simulation are shown respectively in Figures 15-17. In these figures, TEST01 refers to the concentration in the

Table 3
Initial WASP02 Segment Tracer Concentrations (mg/l)

Layer No.	WASP02 Segments														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	78.91	78.70	68.94	67.01	67.55	66.65	67.90	69.98	67.59	67.49	65.60	66.97	68.47	65.55	64.43
2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5					0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6						0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7							0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8								0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9									0.00	0.00	0.00	0.00	0.00	0.00	0.00
10										0.00	0.00	0.00	0.00	0.00	0.00
11											0.00	0.00	0.00	0.00	0.00
12												0.00	0.00	0.00	0.00
13													0.00	0.00	0.00
14														0.00	0.00

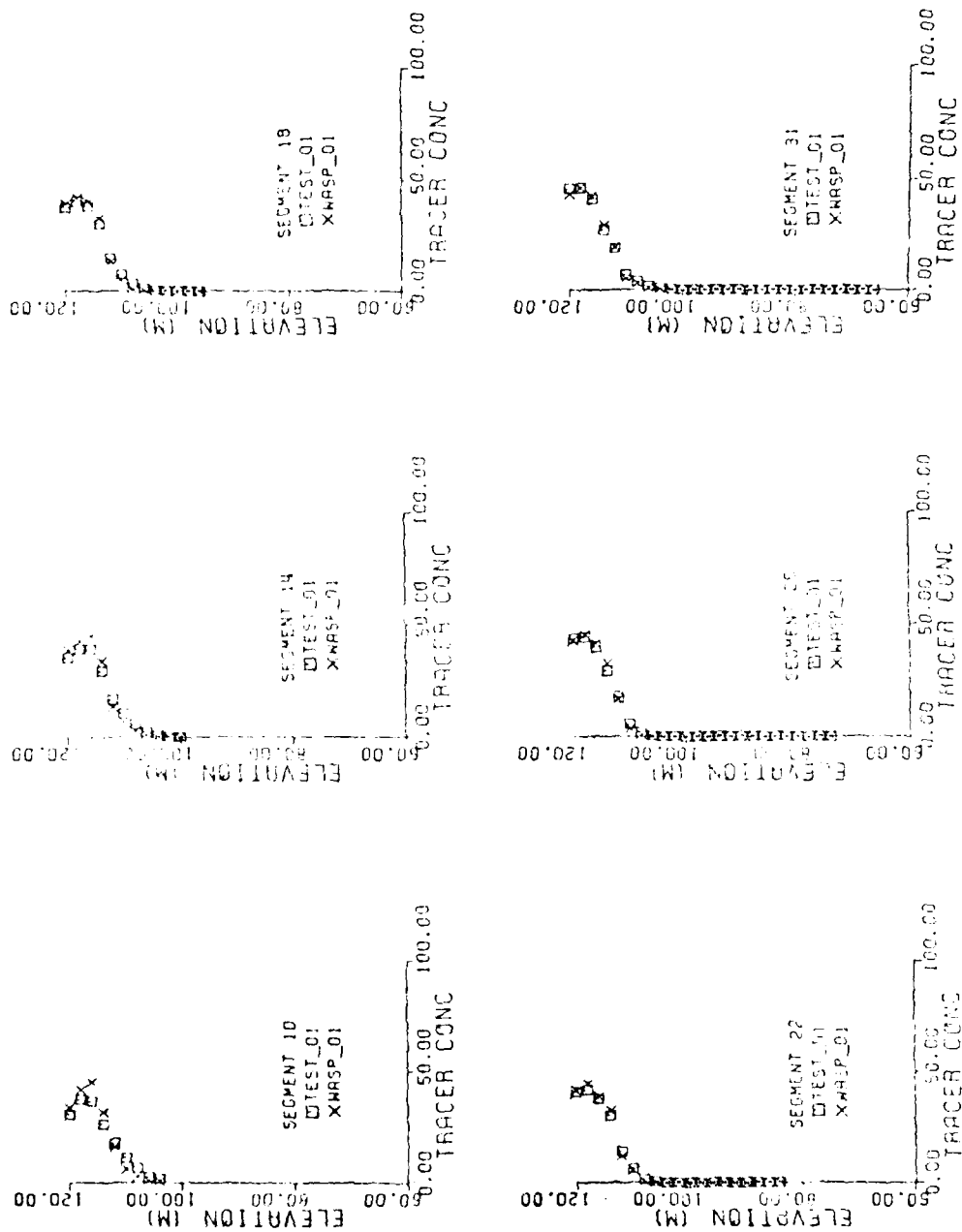


Figure 15. DeGray Lake WASI01 test results compared with CE-QUAL-W2 results after 30-day simulation

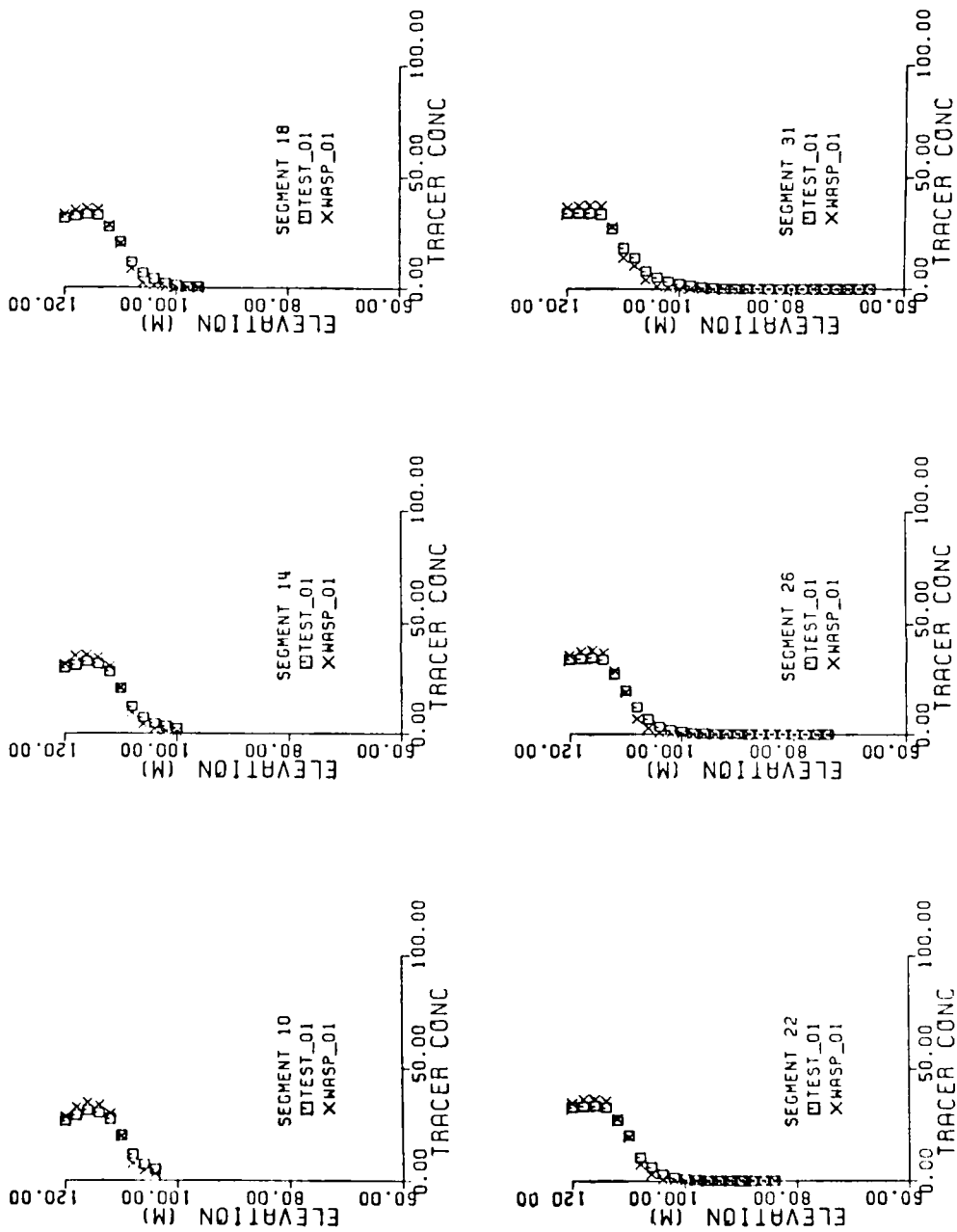


Figure 16. DeGray Lake WASP01 test results compared with CE-QUAL-W2 results after 60-day simulation

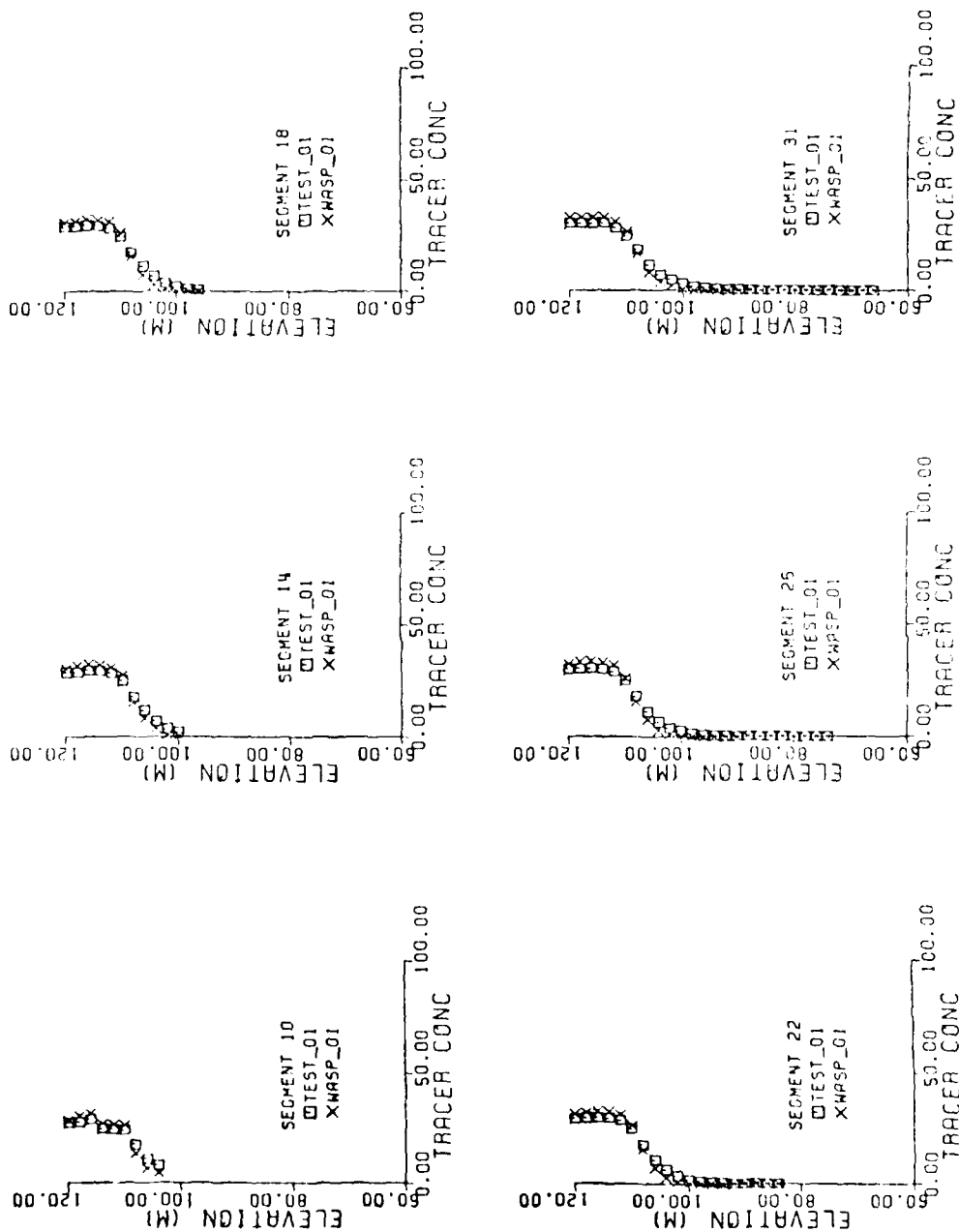


Figure 17. DeGray Lake WASP01 test results compared with CE-QUAL-W2 results after 90-day simulation

overlaid CE-QUAL-W2 cells. Results were very similar for the WASP01 and TEST01 simulations. WASP01 was slightly less vertically diffusive than TEST01. Numerical diffusion may be slightly lower for WASP01 because of the larger time-step. While the CE-QUAL-W2 simulation required over 2 hr of simulation time, the WASP01 required less than 4 min.

38. Similar plots were prepared for the WASP02 simulation (Figures 18-20). In these plots, the TEST02 values refer to the volume weighted average of the concentrations in the CE-QUAL-W2 cells overlaid by the WASP segments. After 30 days of simulation (Figure 18), concentration differences in the upper layers were significant. The greatest deviation between the two simulations occurred in the upper layers. A large portion of this deviation was probably due to the fact that the initial box concentrations represented a distribution of surface CE-QUAL-W2 cell tracer mass over two layers. By 60 days (Figure 19), the tracer was generally mixed through the epilimnion in both cases, and the only remaining significant deviation was in the metalimnion at the segment near the dam. This trend continued, and at 90 days, the deviation, even in the downstream segment, was further reduced. The increased concentration observed for WASP02 in segment 5 between 30 and 60 days was due to reversed surface currents. The VAX 11/750 CPU time requirement for the WASP02 simulation was approximately 1 min.

Comparison with WIFM-SAL

39. Two different injections were made into the 6:1 box model grid overlay and in the analogous areas of the WIFM-SAL grid. First, a 25-mg/l spike was made in segment 683 of the WASP model (see Figure 7) and the six corresponding cells for the WIFM-SAL simulation. Second, a gradient-type initial condition was input in both WASP and WIFM-SAL. Initial concentrations for this injection are tabulated by box number in Table 4 and shown as a contour plot in Figure 21. For a direct (1:1) box model grid overlay of the Mobile Bay area, a 25-mg/l dye injection was made at WIFM-SAL grid location $N = 95$, $M = 8$ (see Figure 7).

40. Results for these test cases are presented as contour plots after 4.5 days of simulation. The large number of grid points and box segments made plotting individual segment concentration histories unwieldy. Concentration contours of WIFM-SAL results after 4.5 days of simulation for the 25-mg/l

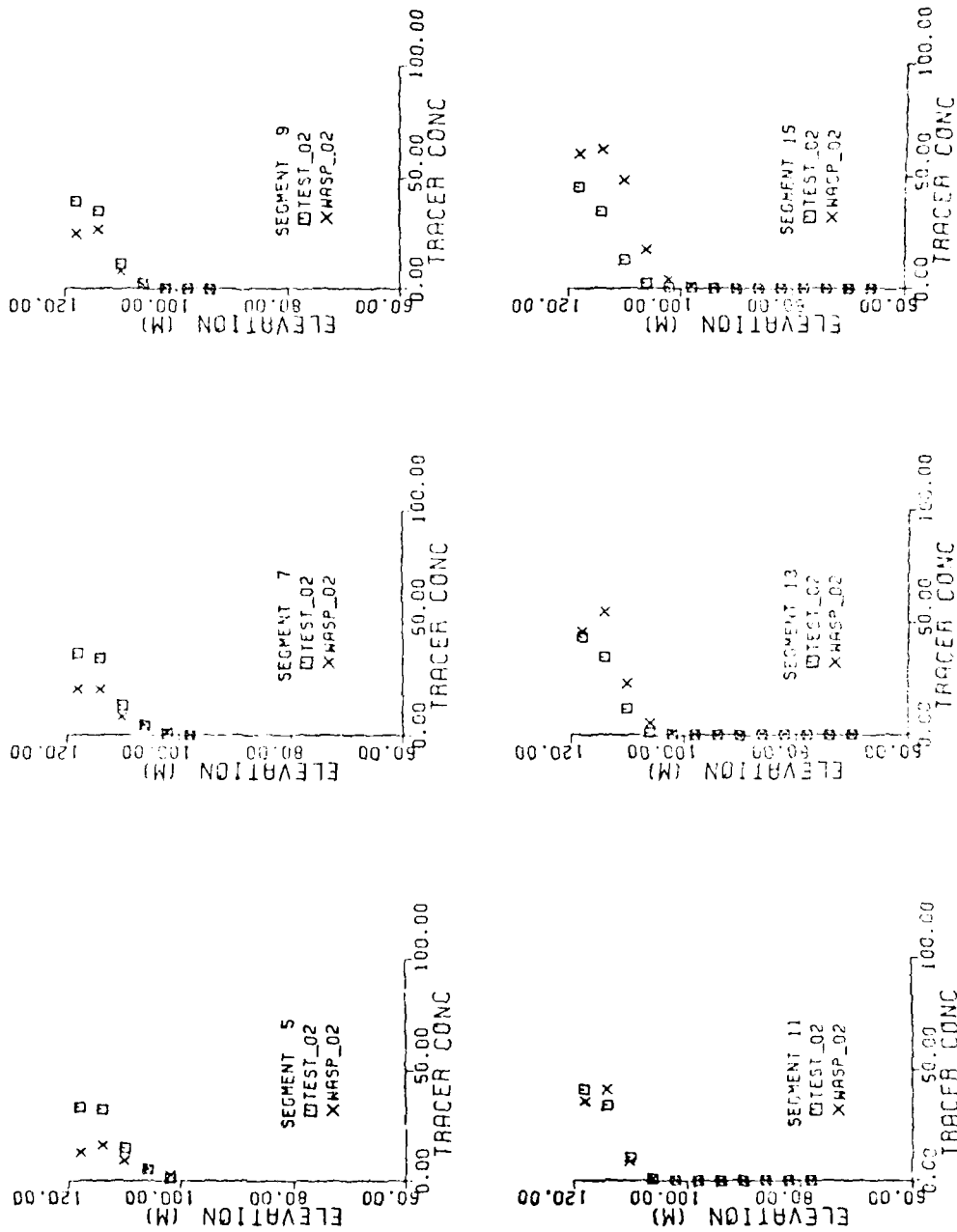


Figure 18. DeGray Lake WASP02 test results compared with
 CH-QUAL-W2 results after 30-day simulation

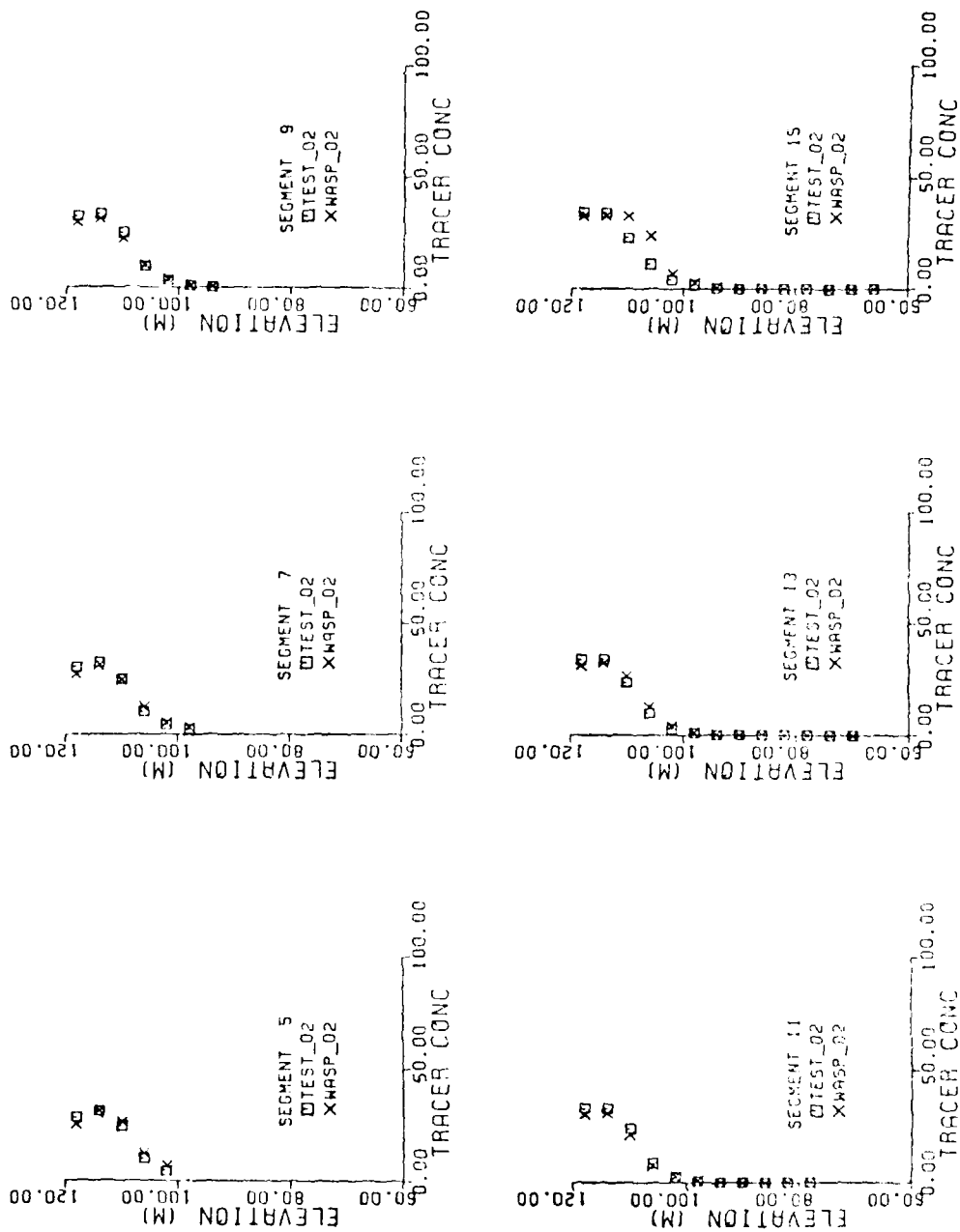


Figure 19. DeGray Lake WASP02 test results compared with
GE-QUAL-W2 results after 60-day simulation

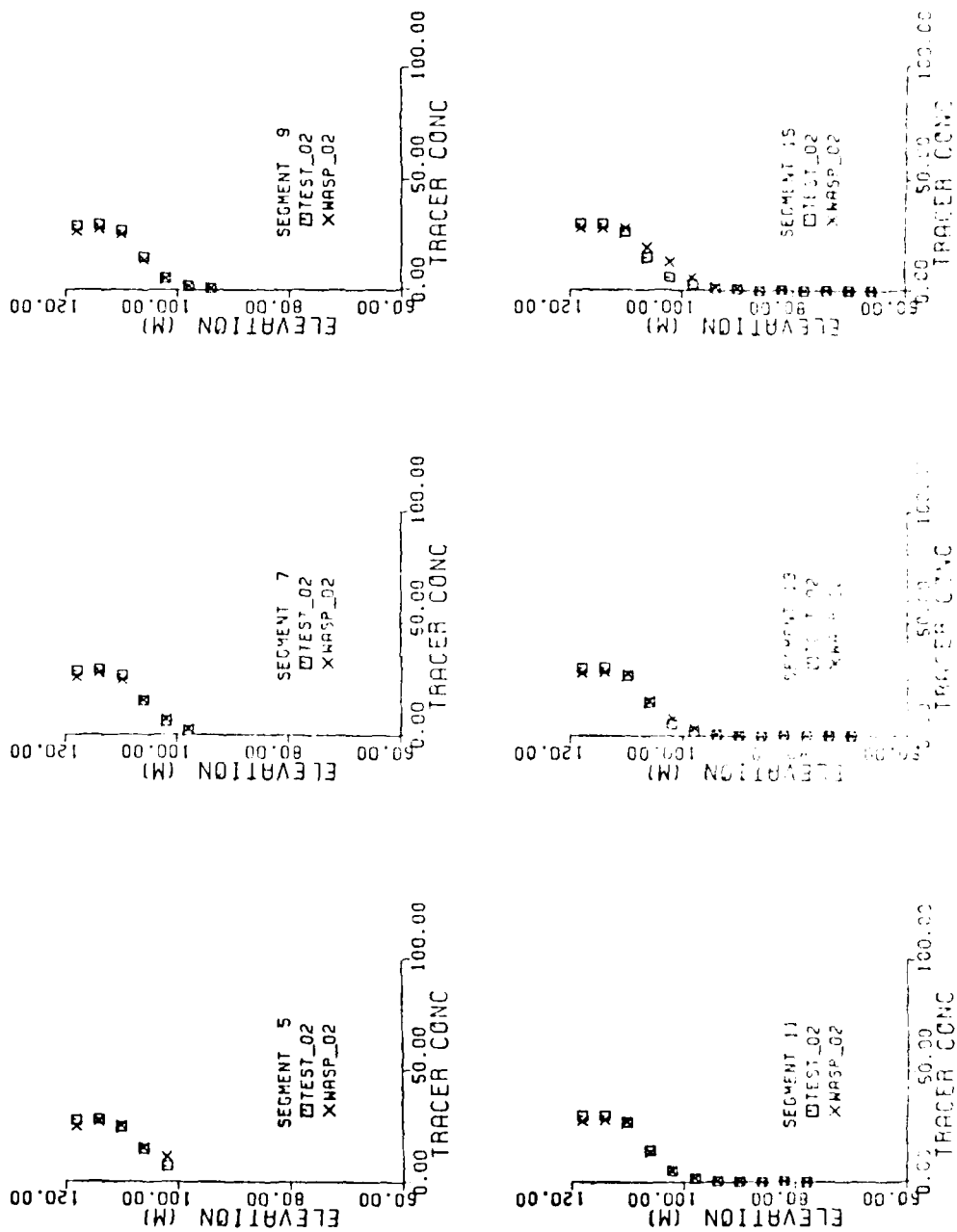


Figure 20. Delay (hr) (0.00) test results compared with
CF-QWASP results after 90-day simulation

Table 4

WASP Gradient Injection, Initial Concentrations, Mississippi Sound

<u>Box No.</u>	<u>Conc</u> <u>mg/l</u>	<u>Box No.</u>	<u>Conc</u> <u>mg/l</u>	<u>Box No.</u>	<u>Conc</u> <u>mg/l</u>
432	0.1	557	5.0	721	5.0
433	0.1	558	5.0	722	1.0
434	0.1	559	5.0	723	0.5
435	0.1	580	5.0	724	0.1
436	0.1	581	3.0	747	0.1
437	0.1	582	1.0	748	0.5
438	0.1	583	0.5	749	1.0
439	0.1	584	0.1	750	3.0
440	0.1	607	0.1	751	3.0
441	0.1	608	0.5	752	3.0
442	0.1	609	1.0	753	3.0
443	0.1	610	3.0	754	3.0
444	0.1	611	5.0	755	3.0
467	0.1	612	7.0	756	3.0
468	0.5	613	7.0	757	1.0
469	0.5	614	7.0	758	0.5
470	0.5	615	5.0	759	0.1
471	0.5	616	3.0	782	0.1
472	0.5	617	1.0	783	0.5
473	0.5	618	0.5	784	1.0
474	0.5	619	0.1	785	1.0
475	0.5	642	0.1	786	1.0
476	0.5	643	0.5	787	1.0
477	0.5	644	1.0	788	1.0
478	0.5	645	3.0	789	1.0
479	0.1	646	5.0	790	1.0
502	0.1	647	7.0	791	1.0
503	0.5	648	9.0	792	1.0
504	1.0	649	7.0	793	0.5
505	1.0	650	5.0	794	1.0
506	1.0	651	5.0	817	0.1
507	1.0	652	1.0	818	0.5
508	1.0	653	0.5	819	0.5
509	1.0	654	0.1	820	0.5
510	1.0	677	0.1	821	0.5
511	1.0	678	0.5	822	0.5
512	1.0	679	1.0	823	0.5
513	0.5	680	3.0	824	0.5
514	0.1	681	5.0	825	0.5
537	0.1	682	7.0	826	0.5
538	0.5	683	7.0	827	0.5
539	1.0	684	7.0	828	0.5
540	3.0	685	5.0	829	0.1
541	3.0	686	3.0	852	0.1
542	3.0	687	1.0	853	0.1
543	3.0	688	0.5	854	0.1
544	3.0	689	0.1	855	0.1
545	3.0	712	0.1	856	0.1

DYE TRANSPORT — GRADIENT INJECTION INITIAL CONDITONS

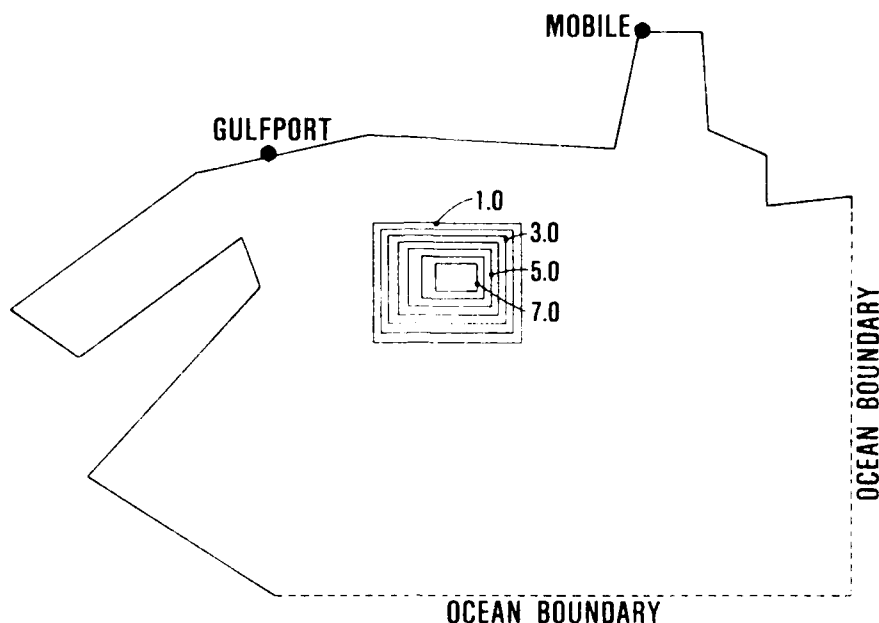
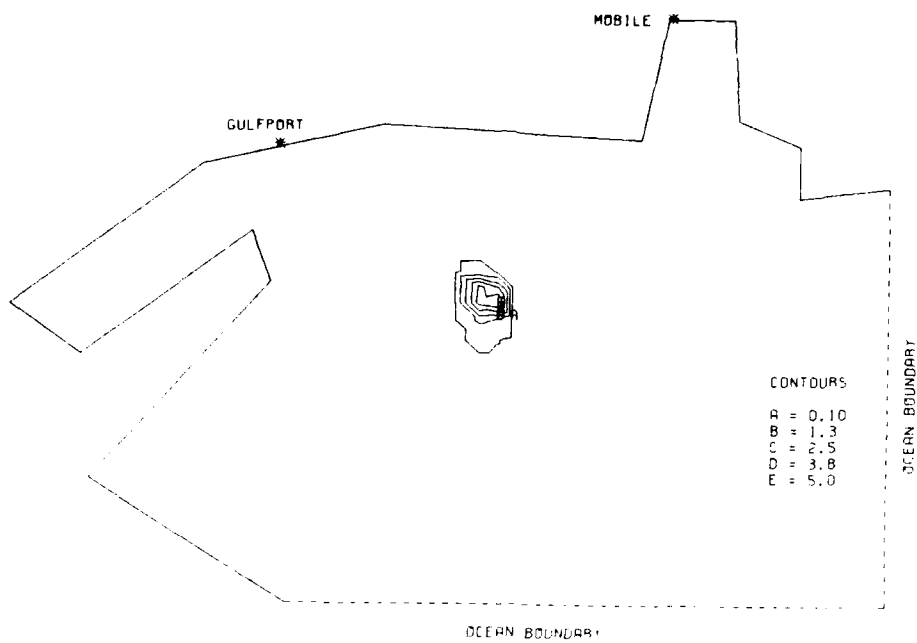
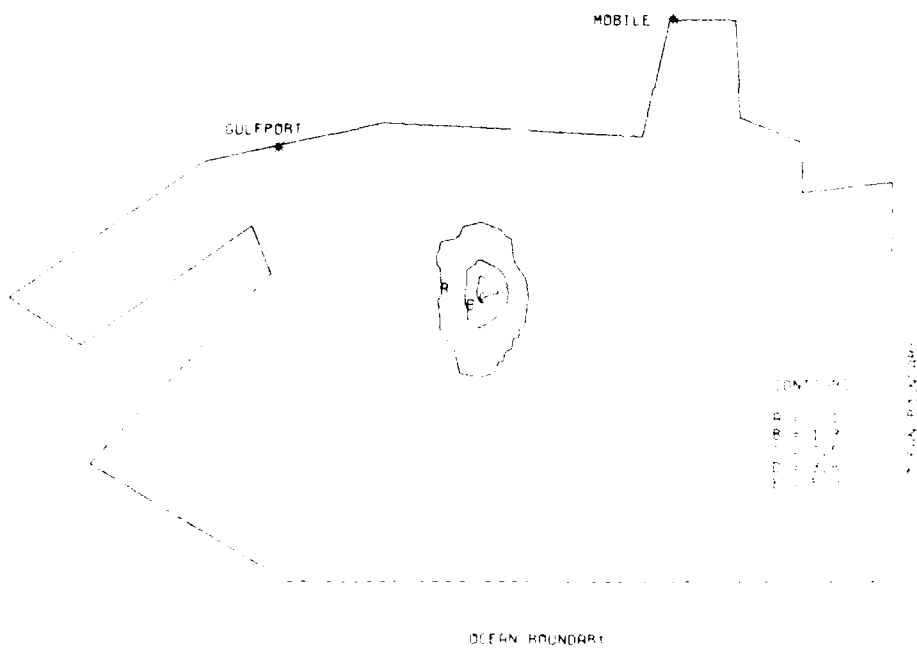


Figure 21. Mississippi Sound, WASP gradient injection initial condition

spike injection are shown in Figure 22a. WASP results for this injection using a 6-hr time-step are shown in Figure 22b. Clearly, the WASP simulation is overdispersive in comparison with the WIFM-SAL results. Unlike the CE-QUAL-W2 solution scheme (i.e., unlike CE-QUAL-W2, WIFM-SAL is not inherently overdispersive), the flux-corrected transport scheme in WIFM-SAL controls numerical dispersion. The spike injection into the Mobile Bay area, using a direct box model overlay on the WIFM-SAL grid, illustrates that for a one-to-one grid overlay, the box model is overdiffusive in comparison with WIFM-SAL transport. Figure 23 demonstrates this using time-steps as long as 6 and 12 hr for the box model simulation. Peak concentrations for the box model simulation are twofold to threefold lower than peak values maintained by WIFM-SAL.

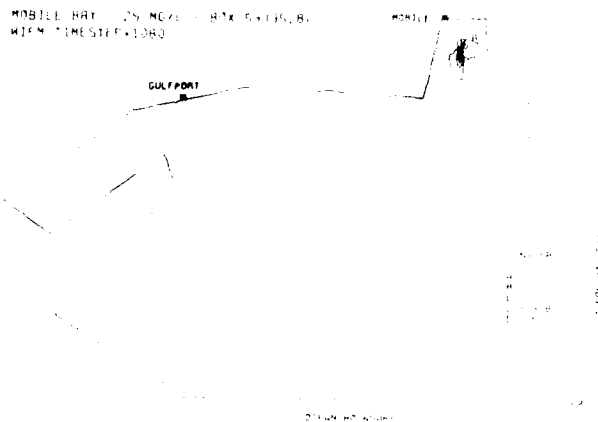


a. WIFM-SAL results

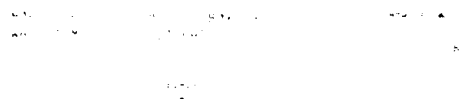


b. Box model results for 1:6 overlay

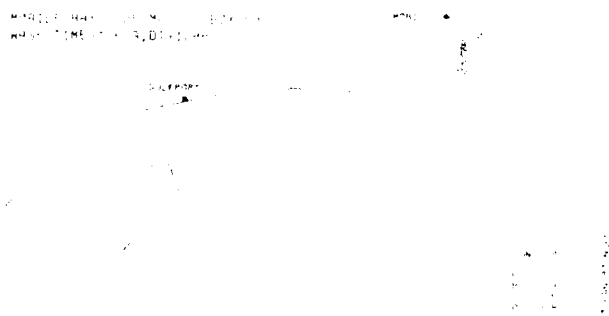
Figure 22. Mississippi Sound, concentration contours after 4.5-day simulation for instantaneous injection in WASP segment 683



a. WIFM-SAL results

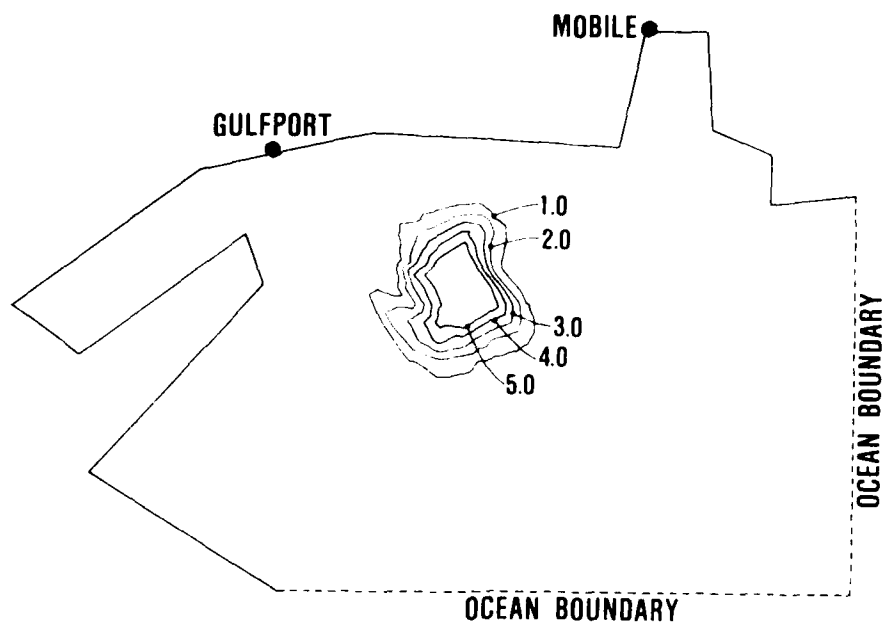


b. Box model results using 1:1 overlay and 6.0-hr time-step

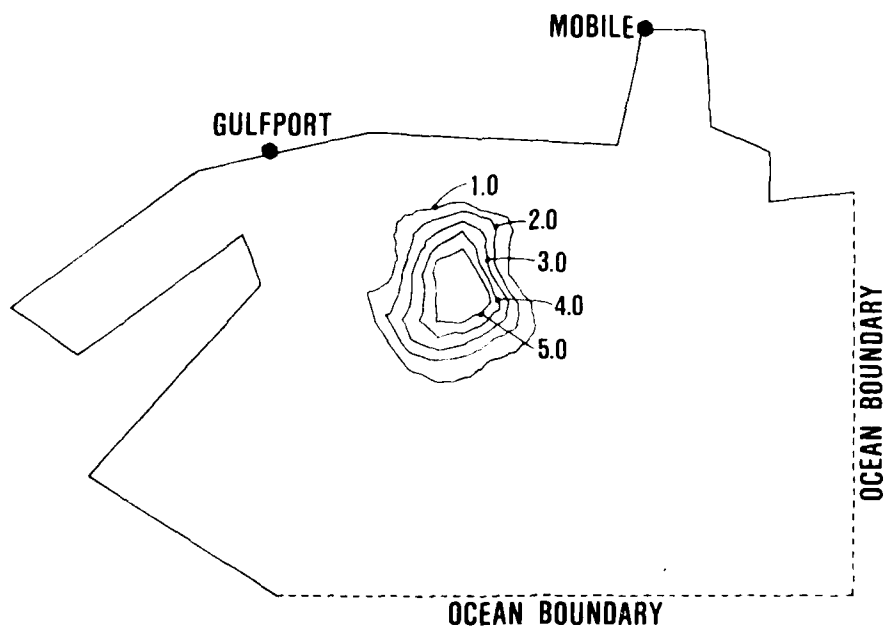


c. Box model results using 1:1 overlay and 12.0-hr time-step

Figure 23. Mobile Bay instantaneous injection after 4.5-day simulation



a. WIFM-SAL



b. 6:1 Model simulation

Figure 24. Mississippi Sound, results of gradient injection after 4.5-day simulation

41. For most water quality considerations, a gradient of the constituents rather than a sharp front exists. For the 6:1 overlay 6-hr time-step and the initial conditions described in Table 4, results are shown in Figure 24. Although the overdispersive character of the box model is still discernible, the box model more closely replicates the transport for the gradient injection condition than for the steep front condition.

PART V: SUMMARY AND RECOMMENDATIONS

42. The box model is a computationally feasible approach for long-term multidimensional water quality modeling. For the applications described in this report, the box model required under 15-min CPU time, whereas the simulations using the directly linked models, CE-QUAL-W2 and WIFM-SAL, required from 3.0- to 20.0-hr VAX 11/750 CPU time. Computational time requirement is an important consideration for a complex water quality application requiring a large number of calibration runs and long-term (seasonal and annual) simulations.

43. The box model is numerically diffusive. An increase in box model segment size increases numerical diffusion. Numerical diffusion decreases as the time-step increases until numerical instabilities occur; i.e., as the Courant number approaches one, numerical diffusion approaches zero.

44. Box model simulation results compare well with results obtained using CE-QUAL-W2. Using a one-to-one grid overlay, box model results are nearly identical to CE-QUAL-W2 results. The upwind difference scheme in CE-QUAL-W2 is also a diffusive scheme and is equivalent to the box model solution. However, even using a one-to-one grid overlay and time-steps up to 12 hr, the box model is overdiffusive in contrast to WIFM-SAL, which has a diffusion-controlled solution.

45. Neither the box model nor CE-QUAL-W2 is appropriate for simulating a situation where movements of sharp fronts of material, such as spills, must be depicted accurately. Both are, at present, numerically overdiffusive; i.e. numerical diffusion at the model in many instances exceeds physical diffusion in the system. However, for situations where concentration gradients are not steep, these models can adequately represent the mass transport in a water body. This limitation is acceptable for many water quality applications. At the time of this publication, both models were being modified to reduce numerical diffusion.

46. Extensive effort to accurately determine the mass dispersion coefficients for a multidimensional modeling study, using either the box model or CE-QUAL-W2 with its current transport algorithm, appears to be unnecessary, since numerical diffusion in these models is typically greater than the physical dispersion for the system. However, where intertidal averaging is

performed, additional dispersion may need to be input, and calculation of this parameter could be crucial.

47. Future activities should focus in the following three areas:

- a. Linkage of the box model with other hydrodynamic models including CELC3D, a three-dimensional stretched grid model; CH2D, the two-dimensional boundary-fitted hydrodynamic model; and CH3D, the three-dimensional boundary-fitted hydrodynamic model.
- b. Integration of a diffusion-controlled solution scheme in the box model and CE-QUAL-W2 (see paragraph 45).
- c. Testing of the use of intertidally averaged hydrodynamics with the box model and development of methods to calculate advective flows and dispersion coefficients for the box model for these intertidal cases from the hydrodynamic model output.

REFERENCES

- Crank, J. 1984. The Mathematics of Diffusion, Clarendon Press, Oxford.
- Ditoro, D. M., Fitzpatrick, J. J., and Thomann, R. V. 1983. "Documentation for Water Quality Analysis Simulation Program (WASP) and Model Verification Program (MVP)," EPA-600/3-81-044, Washington, DC.
- Edinger, J. E., and Buchak, E. M. 1981. "Estuarine Laterally Averaged Numerical Dynamics: The Development and Testing of Estuarine Boundary Conditions in the LARM Code," Miscellaneous Paper EL-81-9, prepared by J. E. Edinger Associates, Inc., for the US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- Environmental Laboratory (EL). 1986. "CE-QUAL-R1: A Numerical One-Dimensional Model of Reservoir Water Quality; User's Manual," Instruction Report E-82-1 (Revised Edition), US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- _____. "A Dynamic One-Dimensional (Longitudinal) Water Quality Model for Streams, CE-QUAL-R1V1: User's Manual," Instruction Report in preparation, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- Environmental and Hydraulics Laboratories. 1986. "CE-QUAL-W2: A Numerical Two-Dimensional, Laterally Averaged Model of Hydrodynamics and Water Quality; User's Manual," Instruction Report E-86-5, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- Fischer, H. B. 1976. "Mixing and Dispersion in Estuaries," Annual Review of Fluid Mechanics 8, pp 107-133.
- Fischer, H. B., et al. 1979. Mixing in Inland and Coastal Waters, Academic Press, Inc., New York.
- Hall, R. W. 1987. "Application of CE-QUAL-W2 to the Savannah River Estuary," Technical Report EL-87- , US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- Kuo, J. T., and Thomann, R. V. 1984. "Phytoplankton Modeling in the Embayments of Lakes," Journal of Environmental Engineering, Vol 109, No 6.
- Martin, L. L. 1987. "Application of a Two-Dimensional Model of Hydrodynamics and Water Quality (CE-QUAL-W2) to DeGray Lake, Arkansas," Technical Report E-87-1, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- Roache, Patrick J. 1982. "Computational Fluid Dynamics," Hermosa Publishers, Albuquerque, N. Mex.
- Schmalz, Richard A., Jr. 1985a. Numerical Model Investigation of Mississippi Sound and Adjacent Areas, Miscellaneous Paper CERC-85-2, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- _____. 1985b. User Guide for WIFM-SAL: A Two-Dimensional Vertically Integrated, Time-Varying Estuarine Transport Model, Instruction Report EL-85-1, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
- Shanahan, P., and Harleman, D. R. F. 1984. "Transport in Lake Water Quality Modeling," Journal of Environmental Engineering, Vol 110, No. 1.

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