Energy and Environment Research; Vol. 2, No. 1; 2012
ISSN 1927-0569 E-ISSN 1927-0577
Published by Canadian Center of Science and Education

WASP_SEDDEER: Incorporation of SEDDEER into WASP

Yi Xiong[1], Vladimir J. Alarcon[2], James L. Martin[1] & William H. McAnally[1]

[1] Department of Civil Engineering, Mississippi State University, Mississippi State, USA

[2] Geosystems Research Institute, 2 Research Blvd, Mississippi State, USA

Correspondence: Yi Xiong, Department of Civil Engineering, Mississippi State University, PO Box 9546, Mississippi State, MS 39762, USA. Tel: 1-662-518-1607. E-mail: xiongyinj@yahoo.com

Received: January 16, 2012 Accepted: January 30, 2012 Online Published: May 22, 2012

doi:10.5539/eer.v2n1p157 URL: http://dx.doi.org/10.5539/eer.v2n1p157

This research was supported by a Grant of the Northern Gulf Institute (NGI)

Abstract

In this study, SEDDEER (Sediment Deposition and Erosion), a stand-alone sediment and contaminant model which simulates one water box and the underlying multiple sediment bed layers, was incorporated into Water Quality Analysis Simulation Program (WASP7.4). WASP7.4 toxic module (TOXI7) was modified to include SEDDEER to develop WASP_SEDDEER model. Tests were designed to ensure that the coupling of the WASP7.4 and SEDDEER bed models is correct. The tests compared WASP_SEDDEER one-box simulations against SEDDEER results to verify fluxes across the sediment-water interface. Also, two-vertical-boxes water-column model tests were performed to compare WASP_SEDDEER output against Environmental Fluid Dynamic Code (EFDC) solutions. The comparisons revealed a good fitting between WASP_SEDDEER and EFDC results (R^2 values above 0.95) verifying a successful incorporation. Exploratory applications of EFDC, WASP7.4, and WASP_SEDDEER to Mobile Bay for simulating sediment and contaminant transport showed the capabilities of WASP_SEDDEER for estimating suspended sediment and contaminant concentrations throughout the computational domain.

Keywords: WASP_SEDDEER, SEDDEER, WASP7.4, EFDC, sediment transport, water quality modeling

1. Introduction

Water quality modeling is an economically feasible mean of predicting water quality and making water resources management decisions. Within all the processes usually modeled by water quality models, the modeling of sediment transport, in particular, could have profound effects on water quality management. Sediments interact with inorganic and organic compounds, and biotic species in the water column and in the sediment bed. Therefore, the proper conceptualization and modeling of sediment transport is fundamental for achieving realistic management scenarios and could influence greatly the design of Total Maximum Daily Loads (TMDLs) or Best Management Practices (BMPs).

Mechanistic water quality models are based on the conservation of mass (Chapra, 1997). Box models capture much of the basic physics of mass conservation and are also of practical value in determining some of the bulk, or overall, properties (Hearn, 2008). A well-established water quality model -the Water Quality Analysis Simulation Program (WASP) (Wool et al., 2002) includes algorithms for implementing multiple sediment layers, sediment settling and resuspension, as well as bed layer alterations and compaction, in a simulation.

WASP is based on the concept of a box model (Ambrose et al., 1993). Therefore, improving the subroutines that take care of contaminant or sediment transport is reasonably easy. Moreover, any improvement made to those subroutines not only could serve WASP but also other models that are based on the stand-alone mass-conservation box-model modeling strategy.

This paper details the incorporation of the Sediment Deposition and Erosion (SEDDEER) model into WASP's toxic module (TOXI7). SEDDEER is a state-of-the-art stand-alone sediment transport model developed by Xiong (2010). This integration seeks to improve the approach currently existing in WASP (version 7.4). The resulting improved WASP model (WASP_SEDDEER) is used for an exploratory study of sediment and contaminant (p,p'-DDT) transport in Mobile Bay, Alabama. Comparisons between EFDC, WASP7.4, and

WASP_SEDDEER sediment and contaminant transport simulation results were performed to demonstrate the capabilities of WASP_SEDDEER.

2. Methods

2.1 Development of WASP_SEDDEER

In this study, SEDDEER (Sediment Deposition and Erosion), a stand-alone mass conservation sediment transport model, was incorporated into WASP to generate the improved WASP_SEDDEER model. SEDDEER is described in detail in Xiong (2010) and Xiong et al. (2010). It simulates one completely mixed water box and the underlying vertically stratified sediment layers, and can be used as a prescreening model before more detailed and complex sediment transport models are applied.

WASP suspended sediment simulation is based on an integrated control-volume equation (Chapra, 1997):

$$\frac{d(VC)}{dt} = \sum Q_{in} C_{in} - \sum Q_{out} C + \sum \frac{E_d A_j}{l_j} \left(C_j - C \right) \pm sources/sinks, \tag{1}$$

where V is the compartment volume; C is the sediment concentration; t is the time; Q_{in} is the volumetric flow rate of inflow; C_{in} in is the average inflow sediment concentration; Q_{out} is the volumetric flow rate of outflow; E_d is the diffusion coefficient; A_j represents the cross-sectional area of the interface; l_j is the turbulent mixing length; and C_j is the sediment concentration in the adjacent compartment.

Since WASP solves the advection and diffusion terms, the remaining computational task to include a new sediment transport algorithm consist of modifying the existing settling velocity model and sink/source terms for sediments. By looping SEEDEER through all sediment surface bed cells, WASP applies SEDDEER to the whole domain (see Figure 1).

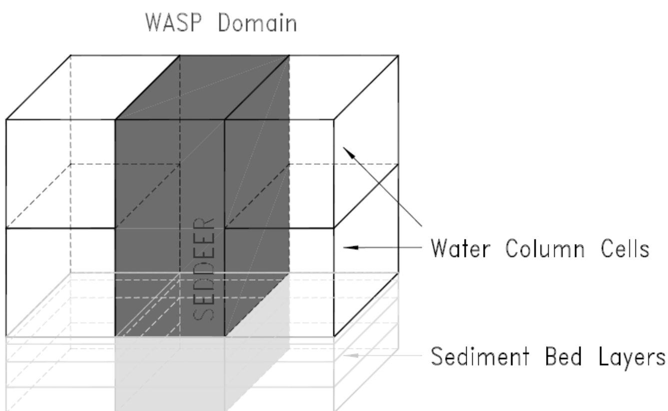


Figure 1. Linkage of SEDDEER and WASP. SEDDEER, an easy-to-use, stand-alone mass conserved box sediment transport is incorporated into WASP. Looping SEEDEER through all sediment surface bed cells, WASP applies SEDDEER to the whole computational domain

SEDDEER adds seven additional solid types (one size silt, one size sand, and five classes of flocs) to the existing WASP TOXI7 module, modifying the formulation of sediment settling velocity, sediment bed scheme, and sediment-water interactions. One simple contaminant was added to WASP by introducing an additional state variable. Thus, in the modified WASP TOXI7, SYSTEM 8 is silt; SYSTEM 9 is sand; SYSTEMs 10 through 14 are flocs; and SYSTEM 15 is the contaminant. Consequently, significant coding modifications were made to the WASP subroutines. Specifically, the new code modifies: the WASPB kinetic subroutine (WASPB.f) (Lung, 2001; Wool et al., 2002), and the SOLIDS subroutine – SOLID.f. Other WASP subroutines modified were: Run_Model.f, WASP1.f, WASP2.f, WASP4.f, and WASP5.f, input/output subroutines, and other common blocks and dependencies (WASP_PARAM.inc, etc). Figure 2 shows the WASP TOXI7 modification as described above.

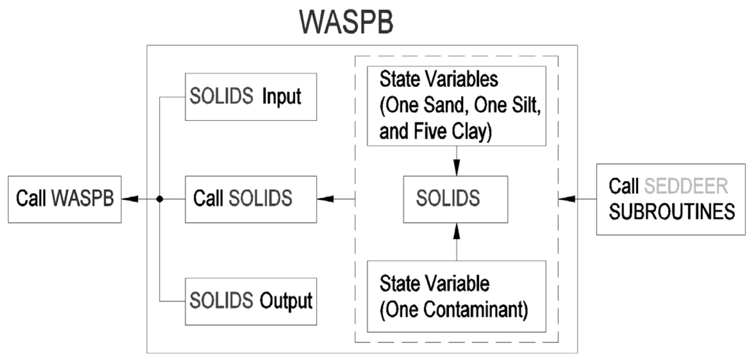


Figure 2. WASP TOXI7 Modification. SEDDEER was incorporated into the WASP TOXI7 module. Seven additional solid types (one size silt, one size sand, and five classes flocs) were implemented. Changes to the main block in the WASP code - WASPB kinetic subroutine (WASPB.f) and solids subroutine – SOLID.f, and WASP subroutines (Run_Model.f, WASP1.f, WASP2.f, WASP4.f, and WASP5.f, etc.), were performed

2.2 WASP_SEDDEER Testing

Model tests were designed to ensure that the coupling of the WASP's water-column and SEDDEER's bed models is correct. Simple tests were conducted comparing WASP_SEDDEER one-box models against SEDDEER one-box models. Results were compared at the water column and at the top sediment layer to verify the fluxes across the sediment-water interface. Then, further simulations were performed to compare a WASP_SEDDEER two-vertical-boxes water column model with a similar two-vertical-boxes EFDC model. Coefficients of determination (R^2) values were calculated to assess the goodness of fit of model simulated results to EFDC-simulated results.

2.2.1 One-box Model Test

WASP_SEDDEER was configured to model an individual completely-mixed water box and underlying vertically stratified sediment layers model, so that the coupling could be verified by comparing WASP_SEDDERR output to SEDDEER output. Five floc classes of clay were specified in both models in order to compare the models under the same conditions. The one-box system was set up assuming constant values for volume of water, depth, salinity, and water temperature (Table 1). Five days were simulated with a time step of 432 seconds. Table 2 shows the boundary and initial conditions for the four state variables.

Table 1. Constants for the one-box model test

Water Volume, V (m^3)	20,000
Water Depth, H_{wat} (m)	2
Salinity, Sa (ppt)	15
Water Temperature, T (°C)	20

Table 2. Parameters and constants for deposition and resuspension test

	State Variables			
	Clay	Silt	Sand	Contaminant
Sediment density (kg/m^3)	2,600	2,600	2,600	---
Initial sediment concentrations in water column (mg/L)	300	100	50	1
Initial sediment concentration in top bed layer (kg/m^3)	325			---
Initial contaminant concentrations in top bed layer (mg/g)	---	---	---	1
Initial sediment bed layer mass fraction	0.30	0.40	0.30	---
Partition coefficient for contaminant (L/kg)	10,000	5,000	1,000	---

2.2.1.1 Deposition and Resuspension

Since the bottom shear stress has significant influence on the modeling of sediment transport, five bottom shear stress scenarios were set up: 0.01 N/m^2, 0.10 N/m^2, 0.50 N/m^2, 0.70 N/m^2, and 1.11 N/m^2.

2.2.1.2 Sediment-Water Diffusion

Contaminant diffusion across the sediment-water interface was tested without considering sediment settling and resuspension. To simplify the test, only the water column and the top sediment layer are considered. It is assumed that no suspended sediment exists in the water column. Diffusions from the water column to the top sediment bed layer and from the top bed layer to the water column were tested. Table 3 shows the parameter values for the sediment-water diffusion test. To explore diffusion from the top bed layer to the water column, the initial contaminant concentration in the water column was specified as zero, while the contaminant concentration in the bed was set to 1 mg/g.

Table 3. Parameter values for the water-column to sediment-bed diffusion test

Paramters and Constants	Values
Initial Contaminant Concentration in Water Column (mg/L)	1
Initial contaminant concentration in bed (mg/g)	0
Sediment-water diffusive transfer coefficient (m/s)	5.0×10^{-7}

In addition, bioturbation diffusion from the sediment bed to the water column was tested by assuming a bioturbation diffusion coefficient equal to 1.0×10^{-9} m^2/s.

2.2.2 Two-Vertical Boxes Test

An additional test of WASP_SEDDEER was performed by comparing its simulation results to EFDC simulated output. A two-vertical-boxes model was set up in both WASP_SEDDEER and EFDC to check the accuracy of vertical transport in the water column. Each segment was set up with a depth of 2 m and a volume of 20,000 m^3. Initial conditions for clay, silt, and sand for each segment were set as shown in Table 2. A constant settling velocity 1.5×10^{-4} m/s was specified.

2.3 Model Applications to Mobile Bay

An exploration of the use of WASP_SEDDEER to model sediment and contaminant transport in Mobile Bay, Alabama, was performed. The contaminant in this test was p,p’- DDT (a DDT isomer). WASP_SEDDEER output was compared against EFDC and WASP7.4 simulated results. Simulations were conducted to test WASP_SEDDEER coupling implementation and to demonstrate the capabilities of WASP_SEDDEER in a hypothetical sediment and contaminant transport case occurring in a real coastal estuary.

A Mobile Bay EFDC hydrodynamic model developed by Wool et al. (2003) was used as a starting point in this exploration. EFDC, WASP7.4, and WASP_SEDDEER were applied to Mobile Bay for a simplified DDT modeling (only p,p’- DDT was considered) based on previous EFDC hydrodynamic models developed by EPA & Tetra Tech, Inc..

2.3.1 Mobile Bay Study Area

Mobile Bay (Figure 3) is a major regional and national resource, providing abundant fisheries, waterborne transportation routes from the Gulf of Mexico to the United States heartland, and vibrant recreational opportunities and serving as home to more than half a million residents. It receives the runoff from the nation’s fourth largest river system, draining most of Alabama and parts of Mississippi, Georgia, and Tennessee. The size and complexity of the drainage system creates the potential for the delivery of large amounts of harmful contaminants, including mercury (Collins, 2007; Martin et al., 2009) leading to water quality impairments.

Sediments that are discharged into Mobile Bay are dominated by silts and clays containing a clay mineral assemblage composed essentially of kaolinite and montmorillonite with some illite presented as a major component (Clay Minerals Society, 1966).

According to Raines (2003), DDT concentrations from monitoring Gulf oyster since 1986, Mobile Bay appears to have some of the most severe DDT contamination recorded in any Gulf Coast estuary.

Figure 3. Mobile Bay Receives runoff from the nation's fourth largest river system, draining most of Alabama and parts of Mississippi, Georgia, and Tennessee

2.3.2 Computational Domain and Simulation Details

The computational grid (developed by Wool et al., 2003) consists of 1,758 cells on the horizontal plane, and each cell is further divided into 1 to 4 vertical layers with an equal depth. Figure 4 represents the grid and locations of observed data.

There are 42 fresh water streams draining into Mobile Bay, being Mobile River discharge most significant. Sediment and daily flow data from Tombigbee River at Coffeeville, AL, and Alabama River at Claiborne, AL, were extracted from USGS databases (USGS, 2010) to estimate the Mobile River discharge and sediment load. A detailed description of this approach can be found in Xiong (2010). The calibrated hydrodynamic model was used to generate a hydrodynamic linkage file (containing the hydrodynamic simulation simulated results) to feed the WASP and WASP_SEDDEER models. The simulation period was two years from 01/01/2003 to 12/31/2004 with a time step of 20 seconds. The simulation corresponding to year 2004 (day 365 through day 725) was employed for results analysis and discussion.

Four cases were simulated: peak tidal elevation; minimum Mobile River discharge; peak freshwater discharge; lowest tidal elevation.

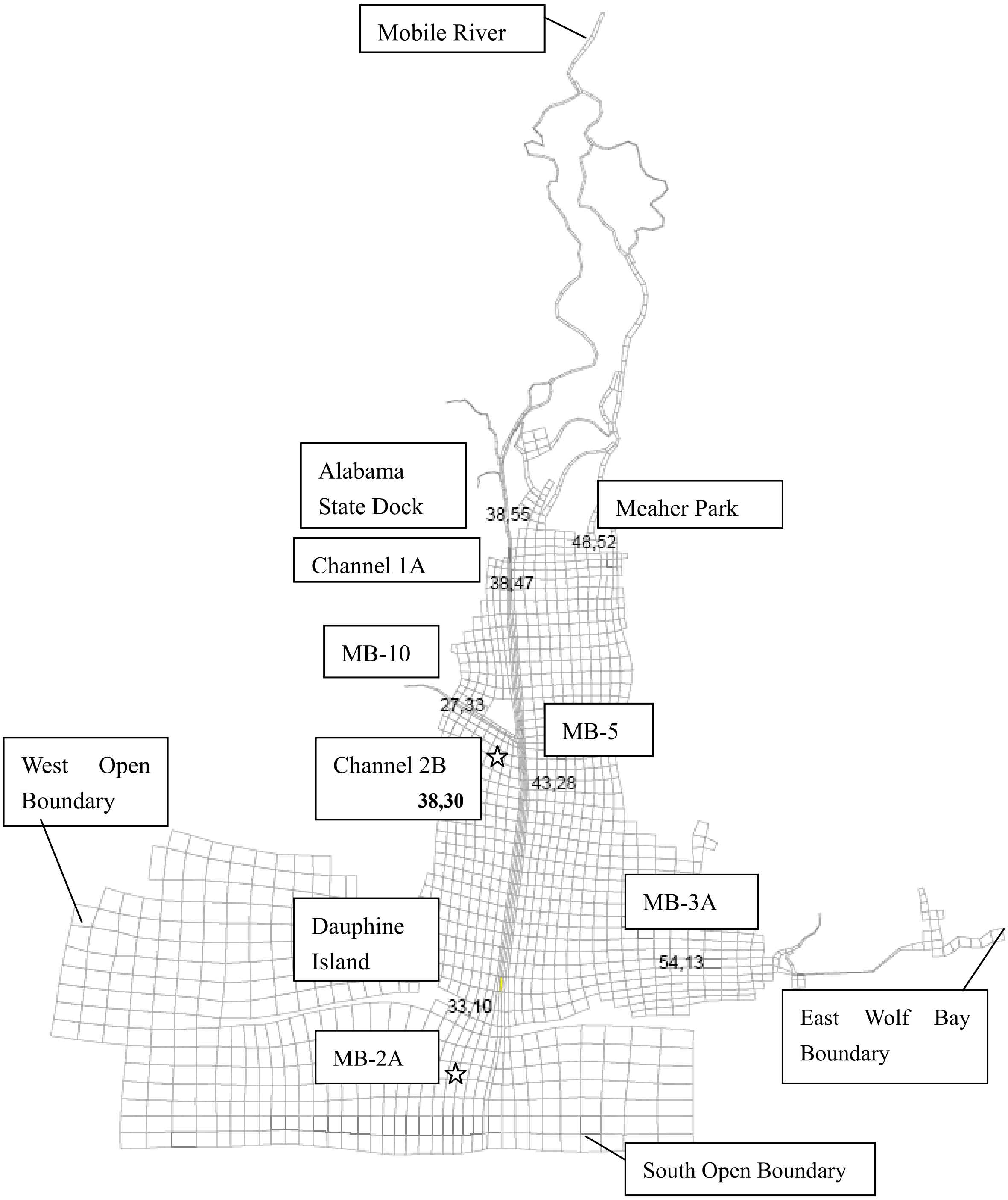


Figure 4. Mobile Bay Computational Domain. The computational grid developed by Wool et al., (2003), conformed by 1,758 cells on the horizontal and 4 vertical layers, was used. The figure includes locations of observed control points

2.3.3 Sediment Transport Modeling

EFDC, WASP7.4, and WASP_SEDDEER were used to simulate Mobile Bay sediment transport. Table 4 lists the modeling parameters and Sections 2.3.3.1 through 2.3.3.3 describe the settings in detail.

Table 4. Parameters and constants for sediment transport modeling

Parameters and Constants	EFDC	WASP7.4	WASP_SEDDEER
Segmentation			
Water column			
Grid type	EFDC grid	WASP grid	WASP grid
Number of horizontal water cells	1,758	1,467	1,467
Water depth and velocity	From EFDC simulation		
Benthic Sediment			
Number of sediment bed layers	1	2	2
Number of horizontal bed cells	1,758	1,467	1,467
Sediment bed depth (m)	1.50	1.50	1.50
Sediment classification			
Number of sediment classes	2	2	7
Sediment classes	Cohesive	Silts & fines	5 classes of clay
	Noncohesive	Sand	1 class silt
			1 class sand
System Parameter			
Water column			
Initial sediment concentration (mg/L)	Corresponding to above sediment classes		
	10	10	7
	0	0	3
			0
Sediment Loading	Monthly time series sediment load		
Benthic Sediment			
Sediment bed porosity	0.65	0.65	0.65
Sediment bed mass fraction	Corresponding to above sediment classes		
	0.80	0.80	0.50
	0.20	0.20	0.30
			0.20
Other Parameter			
Primary sediment density (kg/m^3)	2,600		
Sediment settling velocity (m/s)	Corresponding to above sediment classes		
	3.0×10^{-4}	3.0×10^{-4}	Calculated
	Calculated	3.0×10^{-4}	Calculated
			Calculated
Critical shear stress for deposition (N/m^2)	Corresponding to above sediment classes		
	0.07	--	Calculated
	Calculated	--	Calculated
			Calculated
Critical shear stress for resuspension (N/m^2)	0.50	--	Calculated

2.3.3.1 EFDC

Only two sediment classes (one cohesive and one noncohesive) can be modeled with EFDC (EPA version). Table 5 details cohesive sediment sizes for the test. Parameters in the sediment transport model were specified based on an initial calibration. A simple concentration-dependent cohesive sediment settling velocity method was chosen and the reference settling velocity was set equal to 3.0×10^{-4} m/s. To check the results sensitivity, a reference settling velocity of 2.0×10^{-4} m/s was later assigned. Critical shear stresses for deposition and resuspension were set to 0.07 N/m^2 and 0.50 N/m^2, respectively. A surface resuspension rate of 0.005 $g/m^2\cdot s$ was also specified. Both the settling velocity and critical shear stress for noncohesive sediment were internally computed by EFDC.

Table 5. Sediment classification

	Cohesive Sediment	Noncohesive Sediment
Class No.	1	1
Size Range (m)	0-6.2×10^{-5}	6.2×10^{-5}-1.0010^{-3}
Size (m)	2.1×10^{-5}	4.3710^{-4}

Initial concentrations and boundary conditions for cohesive and noncohesive sediment are required for both water column and sediment bed. Spatially constant initial water column concentrations of 10.0 mg/L and 0 mg/L were specified for cohesive sediment and noncohesive sediments, respectively. These initial concentrations for cohesive and noncohesive sediment were also used for the open boundary average conditions. A representative seasonal monthly sediment load time-series was employed. Only one bed layer was set up in the EFDC application with layer thickness 1.5 m. An initial ratio of 80% to 20% cohesive-sediment to noncohesive-sediment was specified for the sediment bed mass fraction.

2.3.3.2 WASP7.4

For the WASP7.4 application to Mobile Bay, 1467 surface and 1467 subsurface benthic segments were set up in addition to the water column segments associated with the hydrodynamic linkage file generated by EFDC. Silts, fine sediments, and sand transport were simulated by the model. Spatially constant sediment settling and resuspension velocities were set to 3.0×10^{-4} m/s and 1.0×10^{-10} m/s, respectively.

Constant initial concentrations of 10.0 mg/L and 0 mg/L were specified in the water column. Two uniform sediment layers were initially set up in the sediment bed (a thickness of 0.01 m for the top layer, and 1.5 m for subsequent layer) all over the domain. Additionally, initial 80% content of silts and fine sediments, and 20% sand were specified for the sediment bed mass fraction.

2.3.3.3 WASP_SEDDEER

The WASP_SEDDEER simulation included: 5 floc classes of clay, 1 class silt, and 1 class sand. The calculated median sediment settling velocity was set up to 3.0×10^{-4} m/s, approximately.

Constant initial concentrations of 7.0 mg/L, 3.0 mg/L, and 0 mg/L were specified for clay, silt and sand, respectively, in water column. Two sediment layers were initially identified for the sediment bed (a thickness of 0.01 m for the top layer, and 1.5 m for the second layer). Initial contents of 50% clay, 30% silt, and 20% sand were specified for the sediment bed mass fraction in the whole domain.

2.3.4 Isomer p,p'-DDT transport mmodeling

DDT is one of the most widely known synthetic insecticides. The Isomer p,p'- DDT is the major component (77%) of the DDT compound.

The transport of isomer p,p'- DDT was modeled using the same time step and simulation period to that of the hydrodynamic and sediment transport models. In addition to advection and dispersion that are modeled by EFDC or WASP, adsorption to sediment fractions, volatilization, and biotransformation were simulated using SEDDEER (through the linking of SEDDEER and WASP, i.e., WASP_SEDDEER).

WASP_SEDDEER simulations for p,p'- DDT were compared with EFDC and WASP7.4 modeling results for year 2004 to explore the quantitative and qualitative differences between simulation results. Table 6 shows the input parameters and constants for Mobile Bay simplified p,p'- DDT models.

Initial and boundary conditions for p,p'- DDT were specified for both, the water column and the sediment bed. A constant initial concentration was set to 1.0×10^{-5} µg/L in the water column (also used for the open boundary average conditions). A constant p,p'- DDT concentration carried by Mobile River was set up (2.0×10^{-5} µg/L).

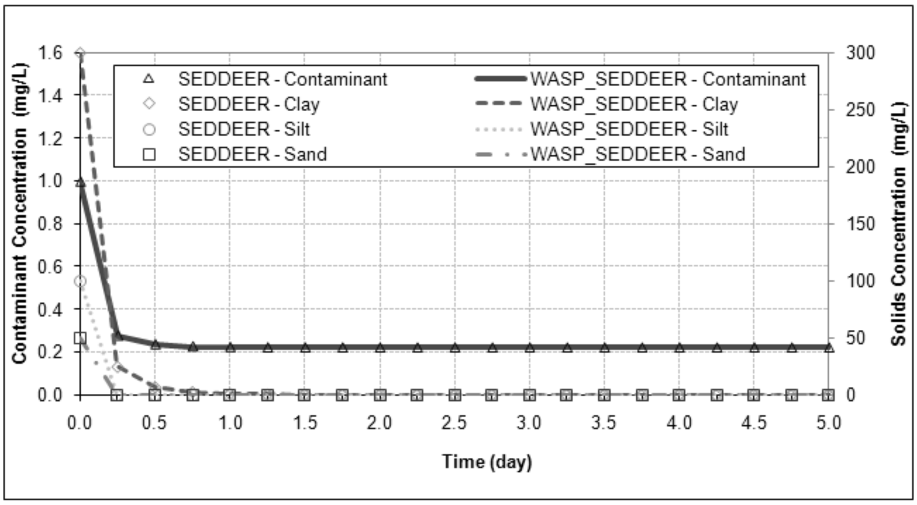
Table 6. Input Parameters and Constants for simulation of p,p'-DDT transport in Mobile Bay.

Input Parameters	Value
System Parameter	
Water Column	
Initial DDT Concentration (μg/L)	p,p'-DDT (1.0×10^{-5})
Benthic Sediment	
Initial DDT Concentration (μg/g)	p,p'-DDT (1.3×10^{-4})
Other Parameter	
Molecular Weight	p,p'-DDT (354)
Partition Coefficient to Silts and Fines (L/kg)	p,p'-DDT (2270)
Partition Coefficient to Sands (L/kg)	p,p'-DDT (454)
Henry's Law Constant, (atm-m^3/mol)	p,p'-DDT (8.3×10^{-6})
Degradation Constants (s^{-1}) for p,p'-DDT	$k_{DDE}=2.50\times10^{-9}$ (in water column)
(Converted to DDD in bed and DDE in water column)	$k_{DDD}=2.44\times10^{-9}$ (in sediment)
Diffusion Coefficient in Sediment Bed Pore Water (m^2/s)	1.0×10^{-9}
Flux Velocity between Water Column and Pore Water (m/s)	1.736×10^{-7}
Exchange (Molecular Diffusion Coefficient, m^2/s)	1.0×10^{-10}

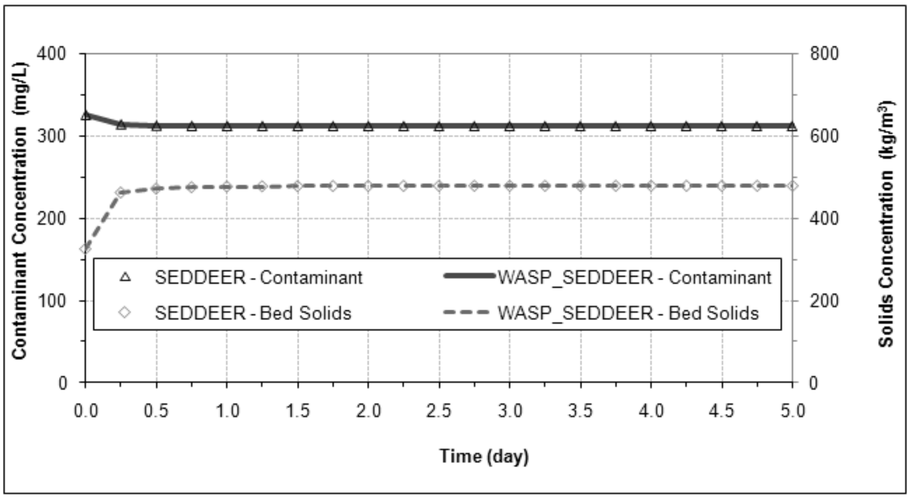
3. Results and Discussion

3.1 One-Box Model Testing

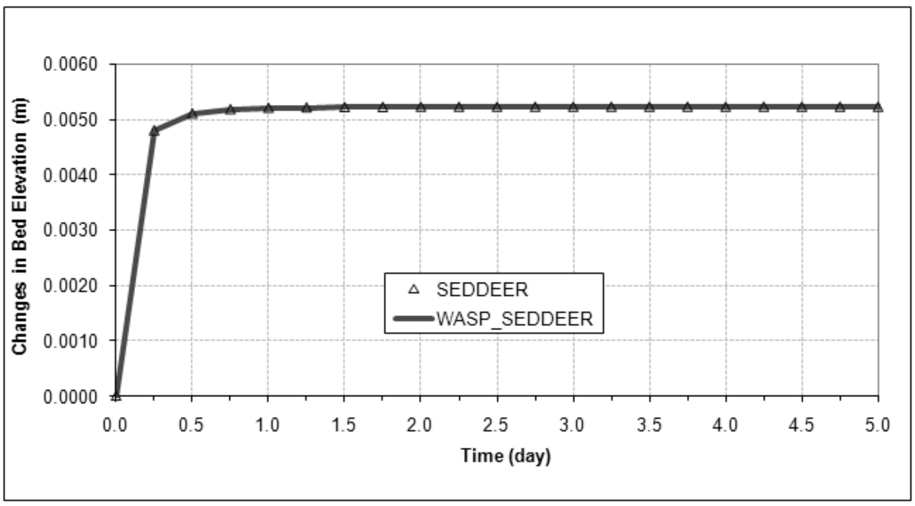
Figures 5 through 9 present comparisons of sediment & contaminant and bed elevation simulations between WASP_SEDDEER and SEDDEER under the five scenarios included in the test. The results demonstrate that WASP_SEDDEER and SEDDEER generate the same output, indicating that the incorporation of sediment into WASP TOXI7 has been performed correctly for sediment deposition and resuspension in a single box. Similar conclusions can be drawn from Figures 10 and 11 that show simulated results for diffusion across the sediment-water interface. As can be seen in the figures, WASP_SEDDEER and SEDDEER results are exactly the same. With regards to bioturbation diffusion across the sediment-water interface WASP_SEDDEER and SEDDEER solutions are also identical (Figure 12).



(a)



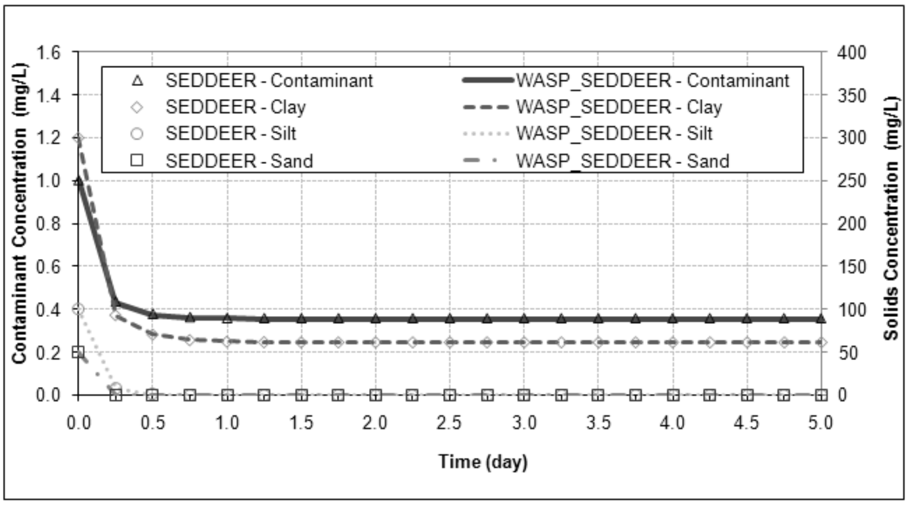
(b)



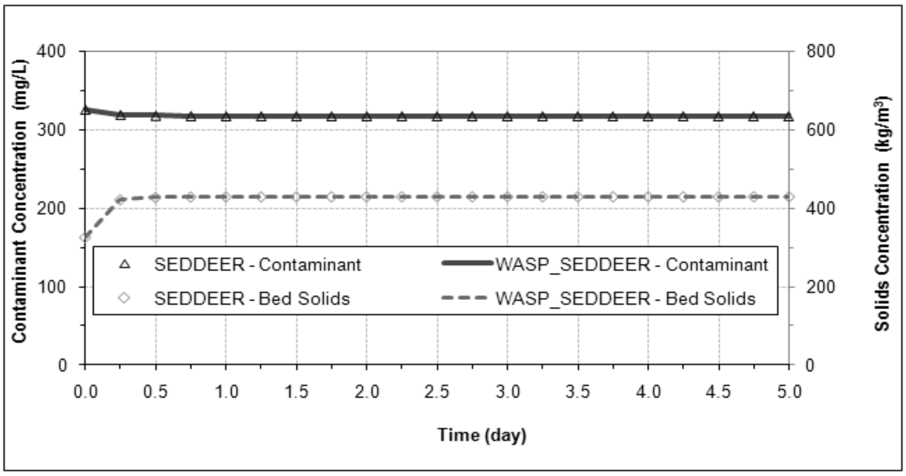
(c)

Figure 5. Comparison between SEDDEER and WASP_SEDDEER solutions (Bottom Shear Stress = 0.01 N/m^2)

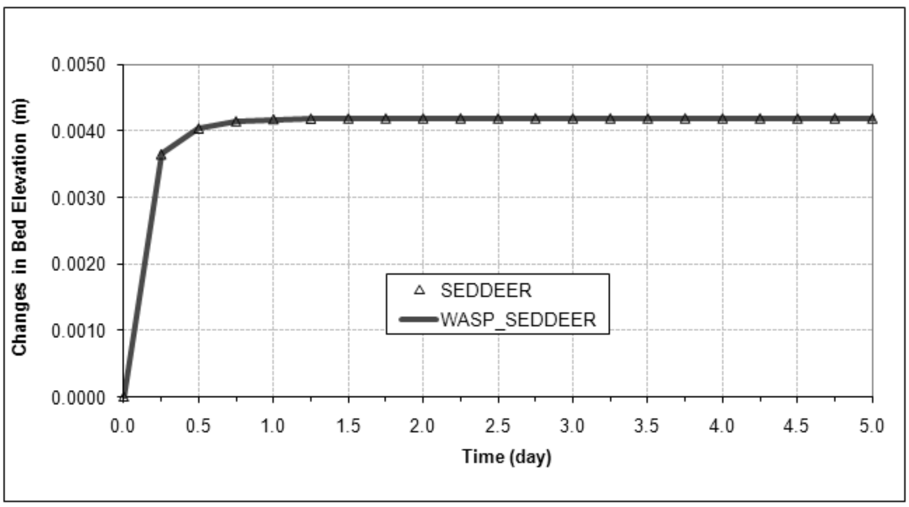
a) Contaminant and sediment concentration at Water Column; b) Changes in Bed Elevation; c) Comparison between SEDDEER and WASP_SEDDEER at Top Bed Layer. WASP_SEDDEER output is identical to SEDDEER solution (R^2 =1)



(a)



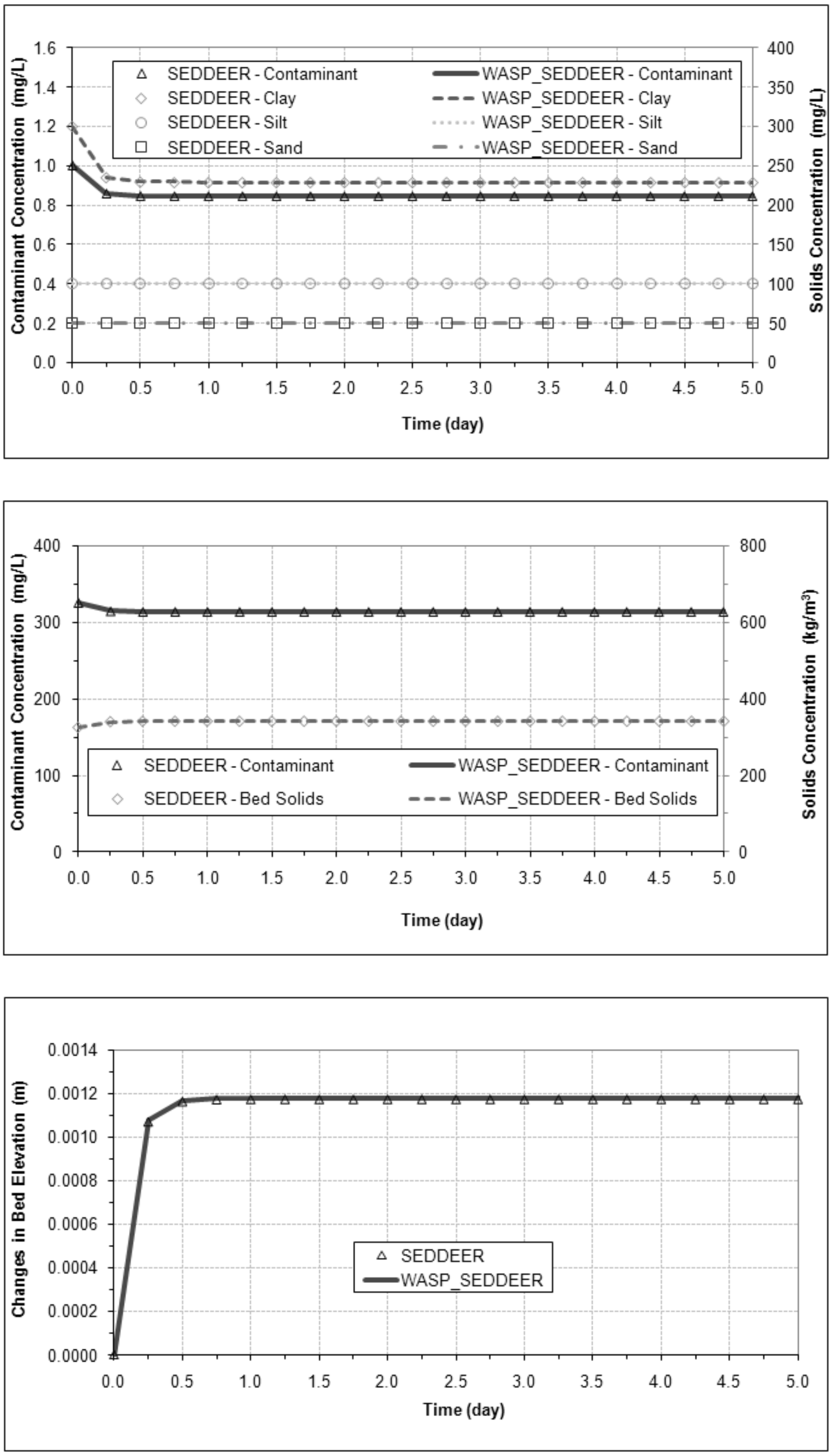
(b)



(c)

Figure 6. Comparison between SEDDEER and WASP_SEDDEER solutions (Bottom Shear Stress = 0.10 N/m^2)

a) Contaminant and sediment concentration at Water Column; b) Changes in Bed Elevation; c) Comparison between SEDDEER and WASP_SEDDEER at Top Bed Layer. WASP_SEDDEER output is identical to SEDDEER solution (R^2 =1)



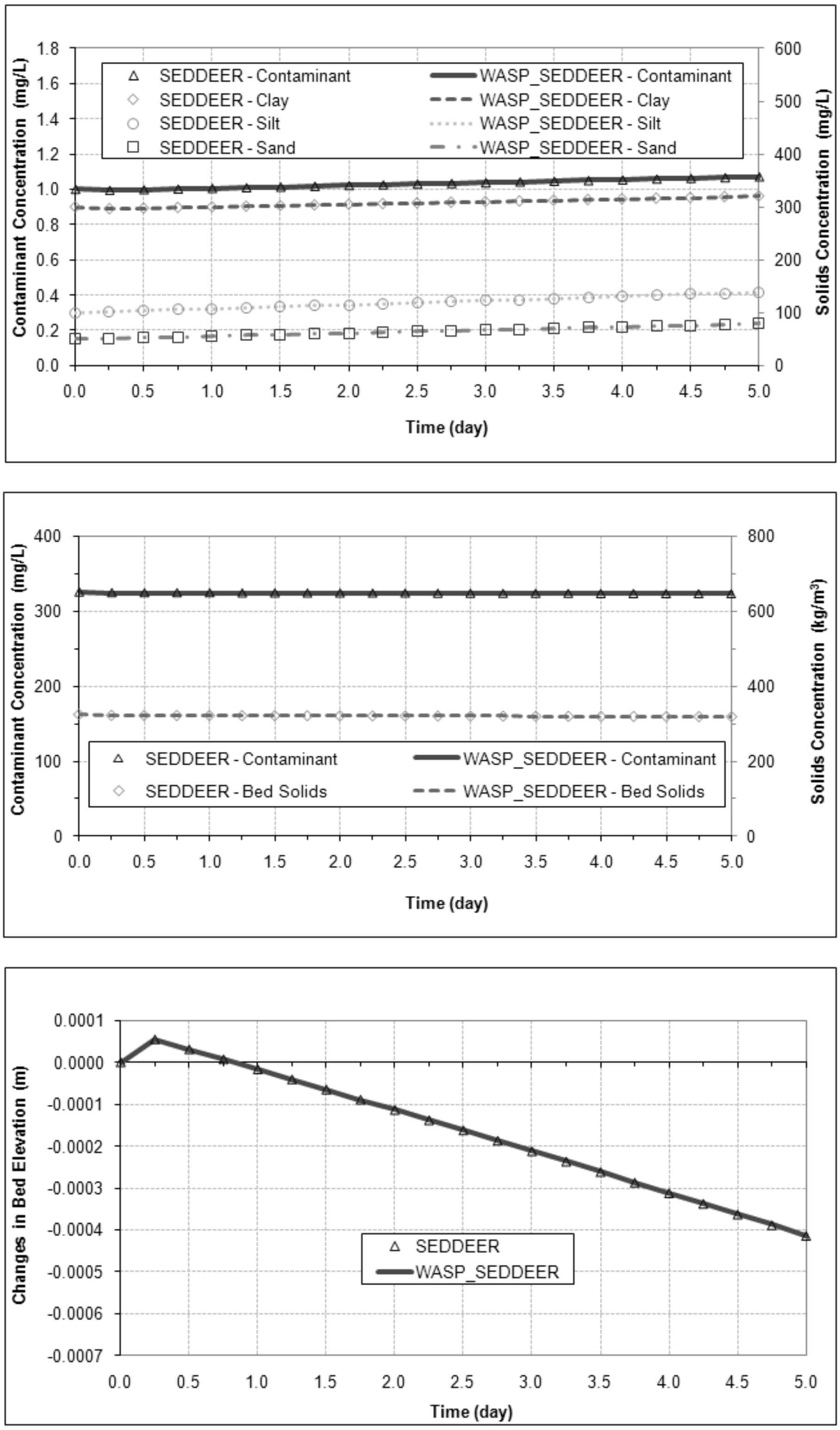
(a)

(b)

(c)

Figure 7. Comparison between SEDDEER and WASP_SEDDEER solutions (Bottom Shear Stress = 0.50 N/m^2)

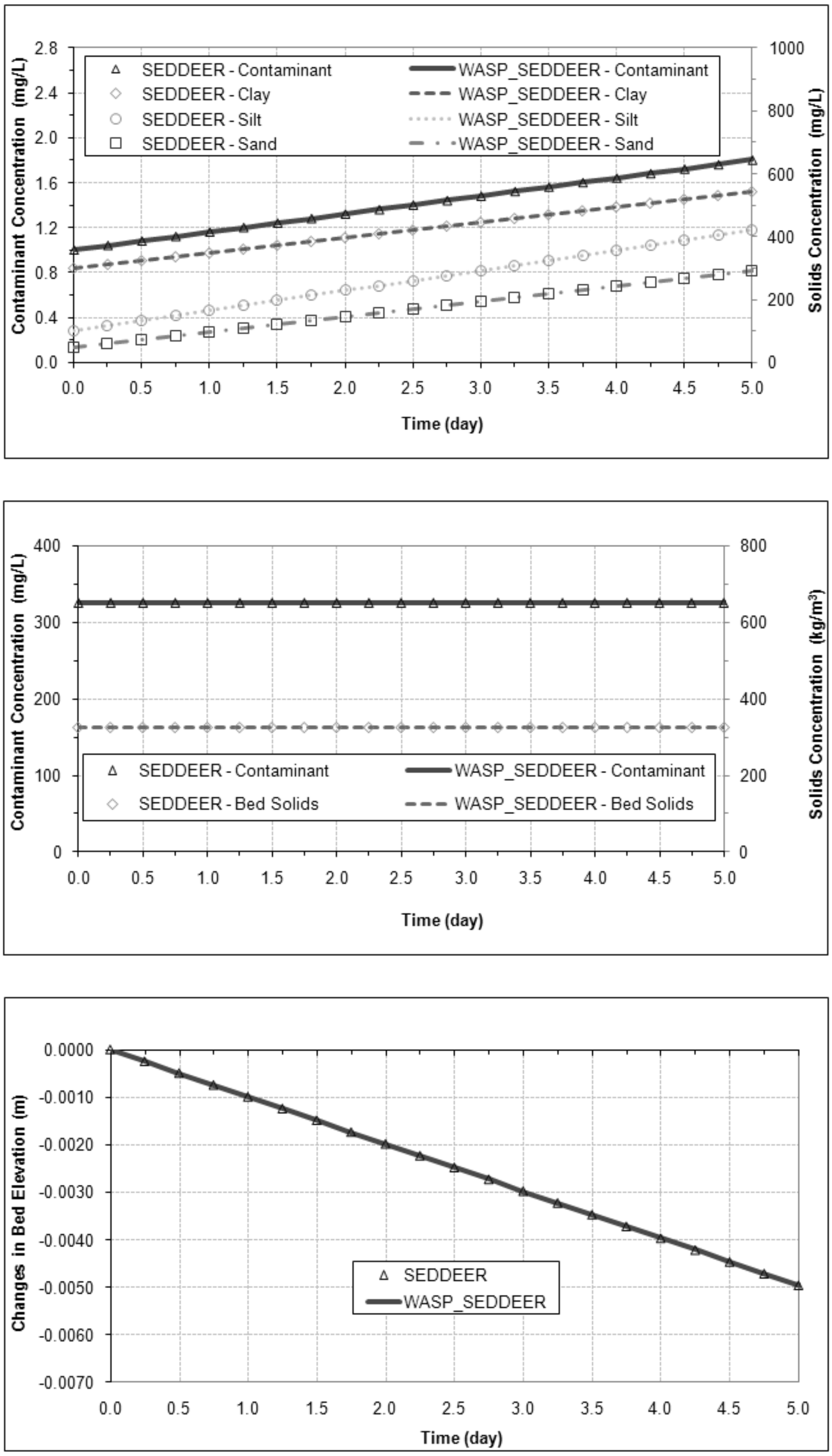
a) Contaminant and sediment concentration at Water Column; b) Changes in Bed Elevation; c) Comparison between SEDDEER and WASP_SEDDEER at Top Bed Layer. WASP_SEDDEER output is identical to SEDDEER solution (R^2 =1)



(a) (b) (c)

Figure 8. Comparison between SEDDEER and WASP_SEDDEER solutions (Bottom Shear Stress = 0.70 N/m^2).

a) Contaminant and sediment concentration at Water Column; b) Changes in Bed Elevation; c) Comparison between SEDDEER and WASP_SEDDEER at Top Bed Layer. WASP_SEDDEER output is identical to SEDDEER solution (R^2 =1)



(a) (b) (c)

Figure 9. Comparison between SEDDEER and WASP_SEDDEER solutions (Bottom Shear Stress = 1.11 N/m^2)

a) Contaminant and sediment concentration at Water Column; b) Changes in Bed Elevation; c) Comparison between SEDDEER and WASP_SEDDEER at Top Bed Layer. WASP_SEDDEER output is identical to SEDDEER solution (R^2 =1)

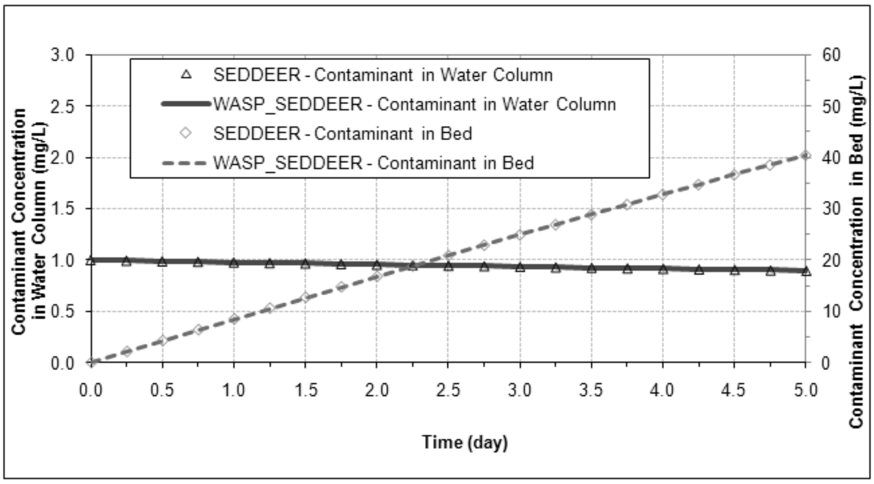


Figure 10. Test of Sediment-Water Diffusion from Water Column to Top Sediment Layer

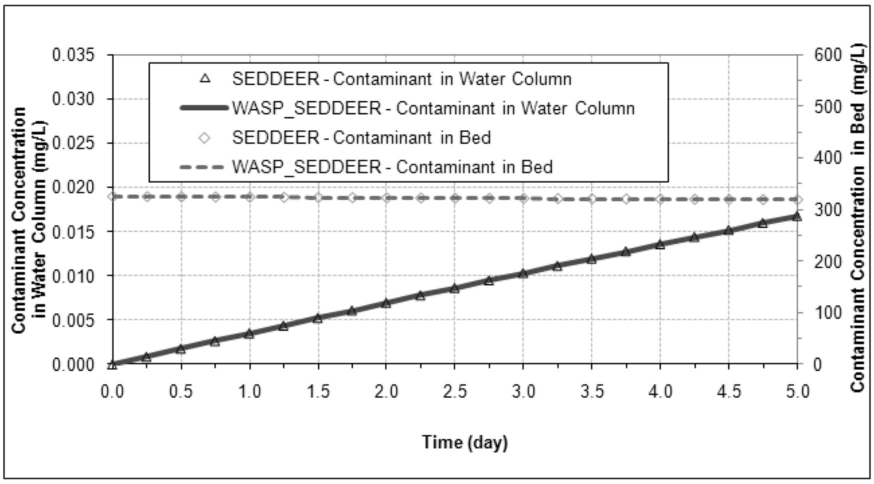


Figure 11. Test of Sediment-Water Diffusion from Top Sediment Layer to Water Column

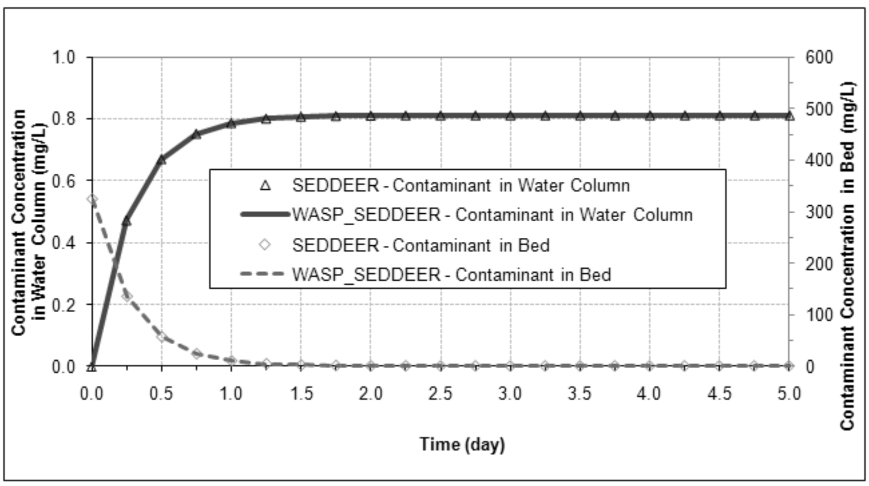


Figure 12. Test of Bioturbation Diffusion from Top Sediment Layer to Water Column

3.2 Two-Vertical Boxes Test

Simulation results for two-vertical boxes test are illustrated in Figures 13 and 14. Despite minor differences (which evidence the fact that WASP_SEDDEER uses multiple sediment classes) the comparison of simulation results between EFDC and WASP_SEDDEER are very similar, evidenced by the high R^2 values.

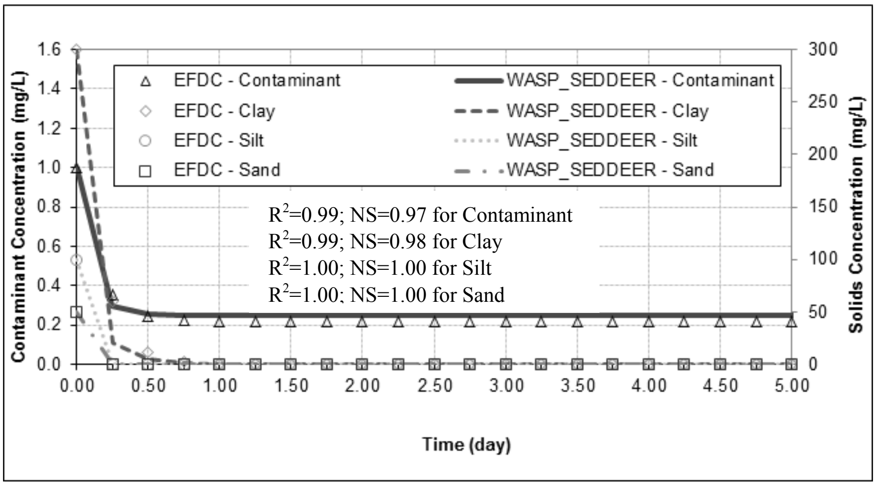


Figure 13. Comparison between EFDC and WASP_SEDDEER for Upper Segment WASP_SEDDEER agrees well with EFDC (R^2 >0.95)

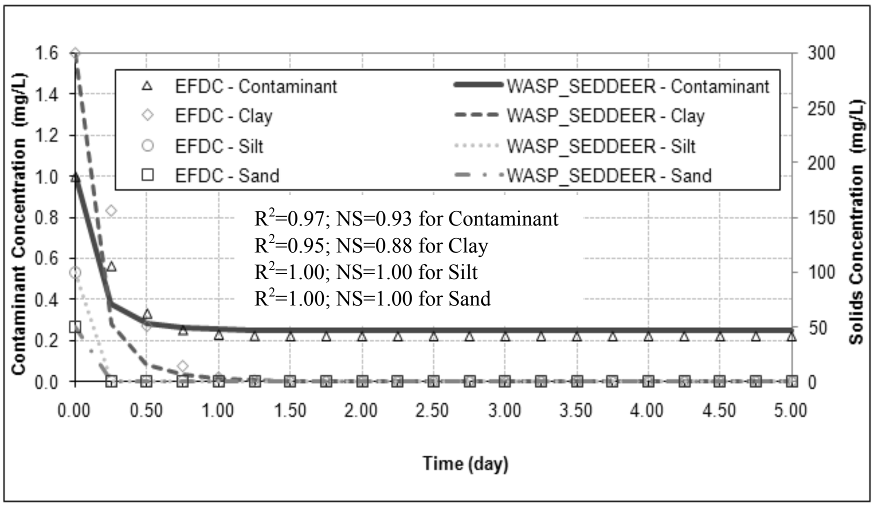


Figure 14. Comparison between EFDC and WASP_SEDDEER for Lower Segment. Comparison between EFDC and WASP_SEDDEER for Upper Segment. WASP_SEDDEER agrees well with EFDC (R^2 >0.95)

3.3 Application to Mobile Bay

3.3.1 Sediment Transport Modeling

Figures 15 through 17 represent the simulated average suspended sediment concentrations at navigation channel cells (38, 30), (38, 47), (38, 55) in 2004 (for days 365 through 725 in a 2-year simulation) using EFDC, WASP7.4, and WASP_SEDDEER, respectively. The WASP_SEDDEER simulated output generally agrees with the trend of EFDC and WASP7.4 simulated output. By involving a flocculation model with 5 classes of flocs, WASP_SEDDEER has the advantage of maintaining a more realistic sediment concentration. Since WASP_SEDDEER includes flocculation in its settling and deposition algorithms, suspended sediment concentrations are generally lower than EFDC and higher than WASP7.4. These results account for the fact that flocculated sediments tend to settle and deposit and not remain suspended as EFDC predicts (EFDC sediment and deposition algorithms only depend on the values of predetermined settling velocity). Similarly, WASP 7.4 does not model sediment resuspension, bioturbation, or flocculation. Therefore, it is expected that WASP_SEDDEER predicted suspended sediment concentrations be higher than WASP.

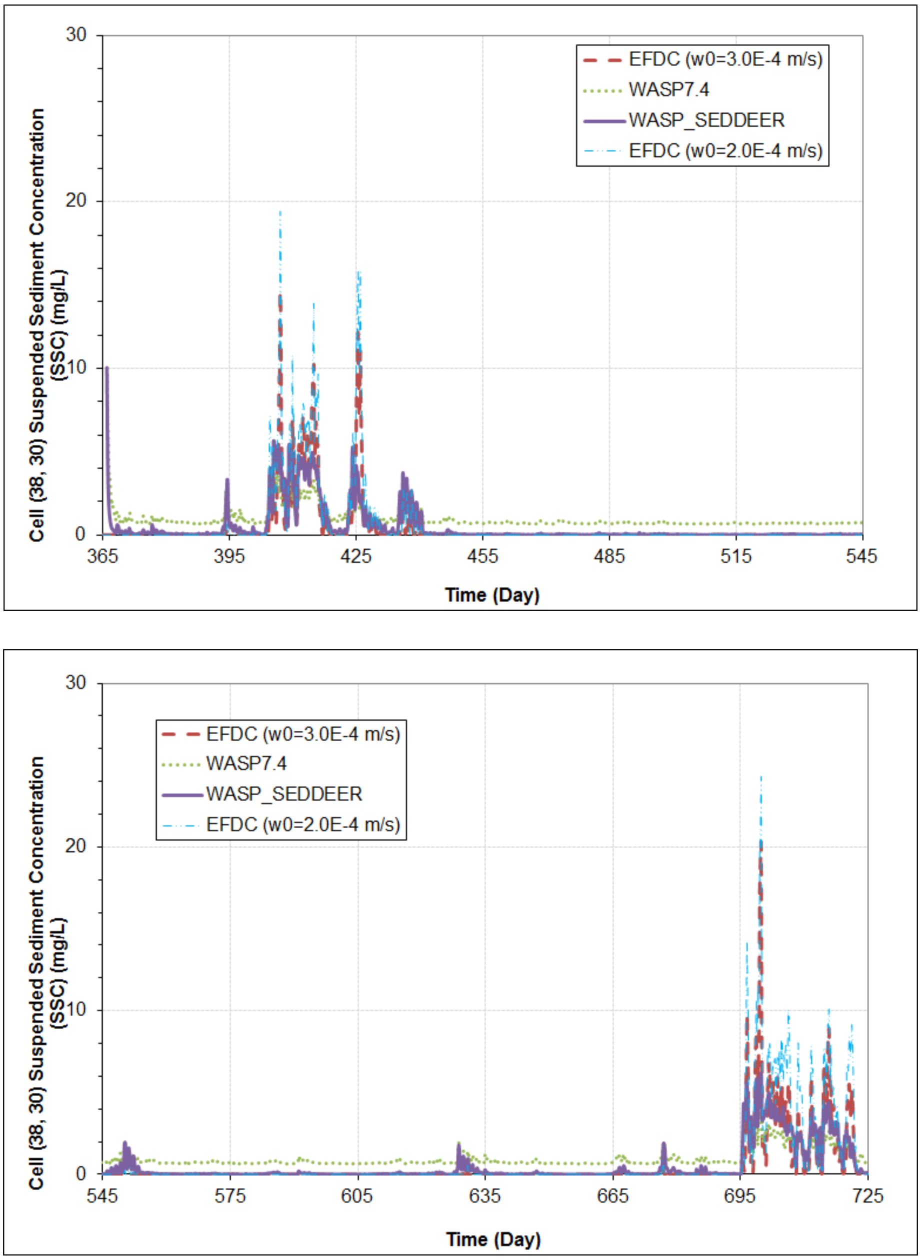


Figure 15. Simulated Average Suspended Sediment Concentration at Navigation Channel Cell (38, 30)

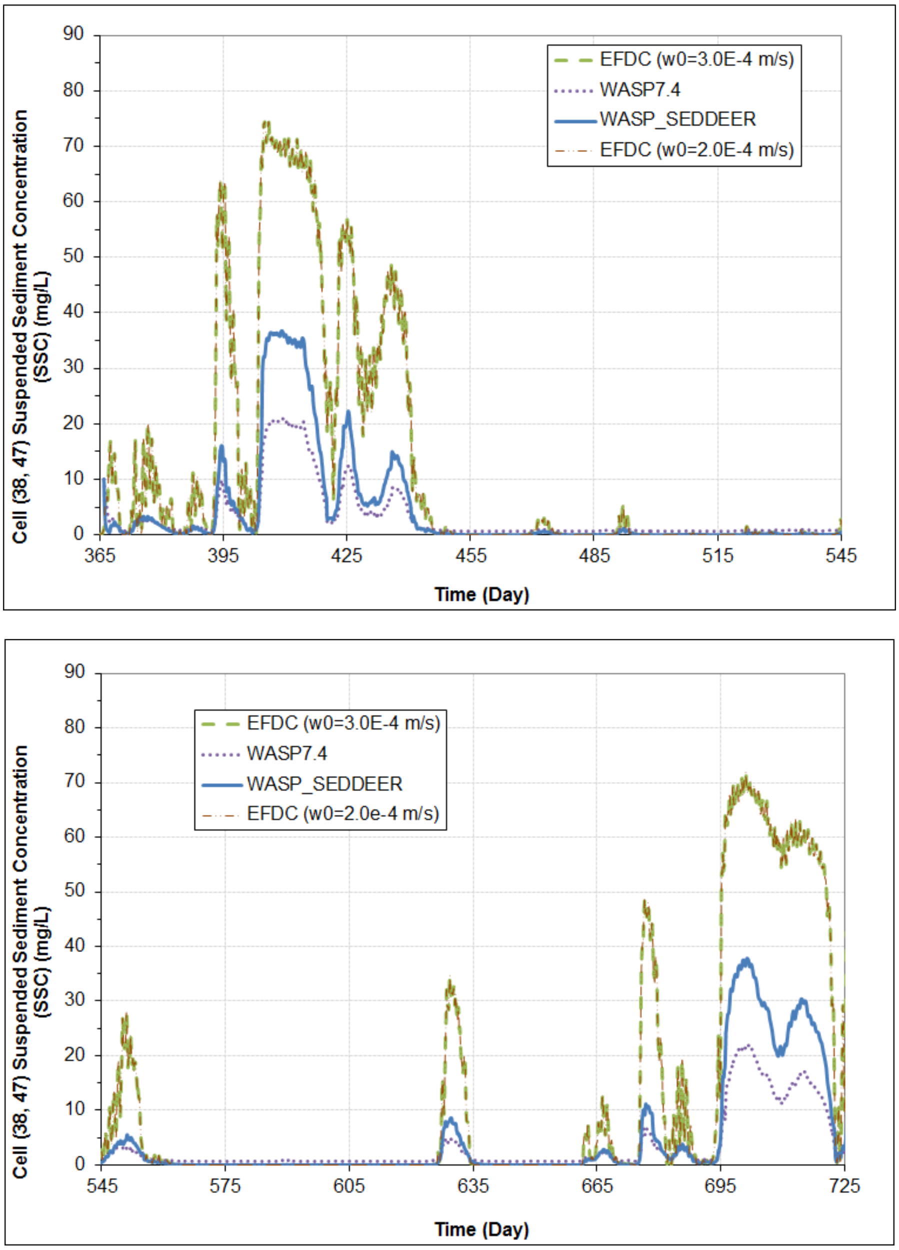


Figure 16. Simulated Average Suspended Sediment Concentration at Navigation Channel Cell (38, 47)

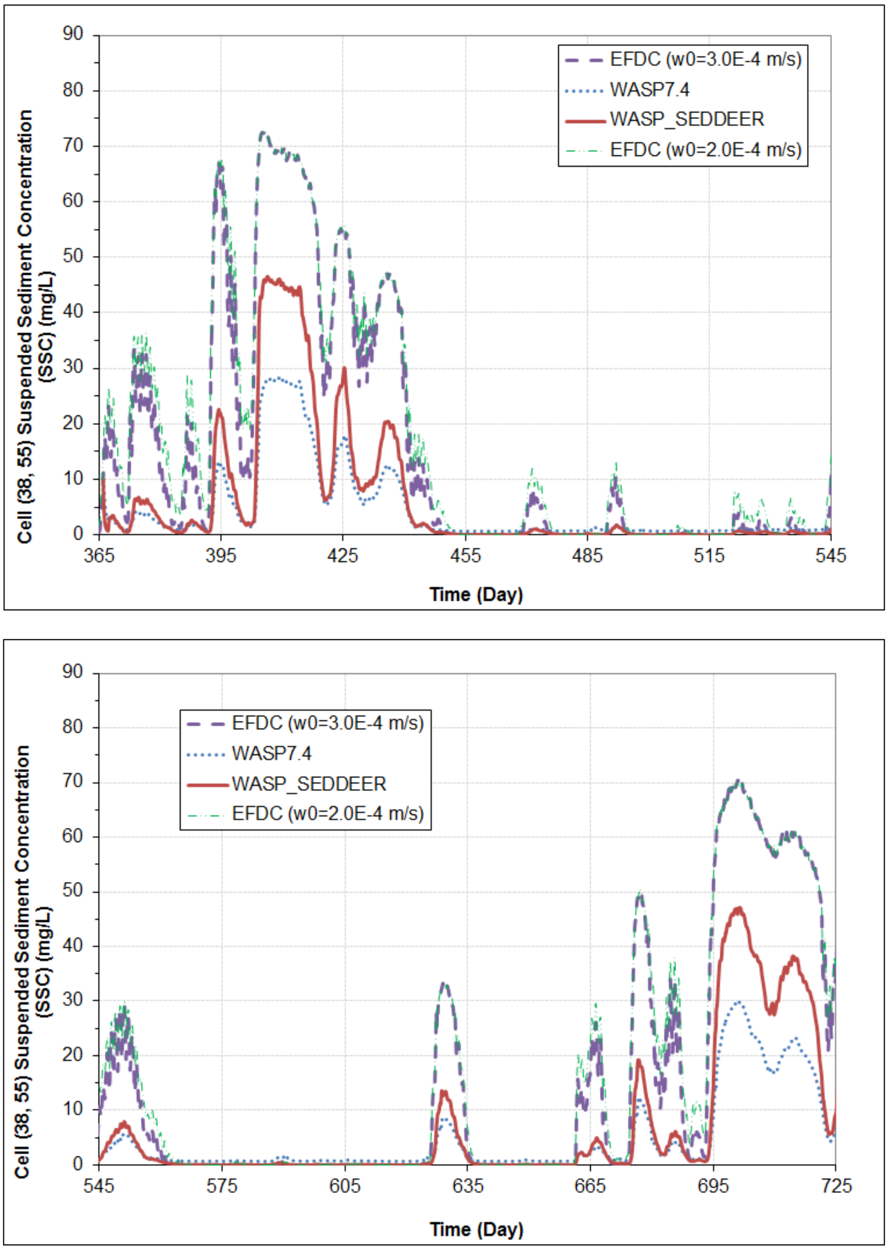


Figure 17. Simulated Average Suspended Sediment Concentration at Navigation Channel Cell (38, 55)

3.3.2 Contaminant Modeling

EFDC, WASP7.4, and WASP_SEDDEER were used to track the p,p'- DDT input concentration from Mobile River throughout the computational domain. Figures 18 through 20 show simulated p,p'- DDT concentrations at the Mobile Bay navigation channel: cells (38, 30), (38, 47), (38, 55). The figures correspond to simulation for year 2004. Isomer p,p'-DDT concentrations follow a similar trend to suspended sediment concentrations reported in previous sections, i.e., isomer concentration values simulated by WASP_SEDDEER are consistently lower than those estimated by EFDC, and greater than those simulated by WASP 7.4. The results seem to be reasonable because it is expected that contaminant concentrations in the water column -when flocculation, resuspension and bioturbation are included in the simulation (as WASP_SEDDEER does)- be lower than algorithms purely dependent from predetermined settling velocities (such as in EFDC), and higher than concentrations calculated by algorithms that do not consider resuspension or flocculation. Figures 21 and 22 show simulated surface layers for p,p'- DDT using WASP_SEDDEER. Figure 21 was captured at the beginning of the simulation, and Figure 22 corresponds to the end of the simulation. The figures illustrate

WASP_SEDDEER capabilities for estimating contaminant and sediment concentrations throughout the computational domain.

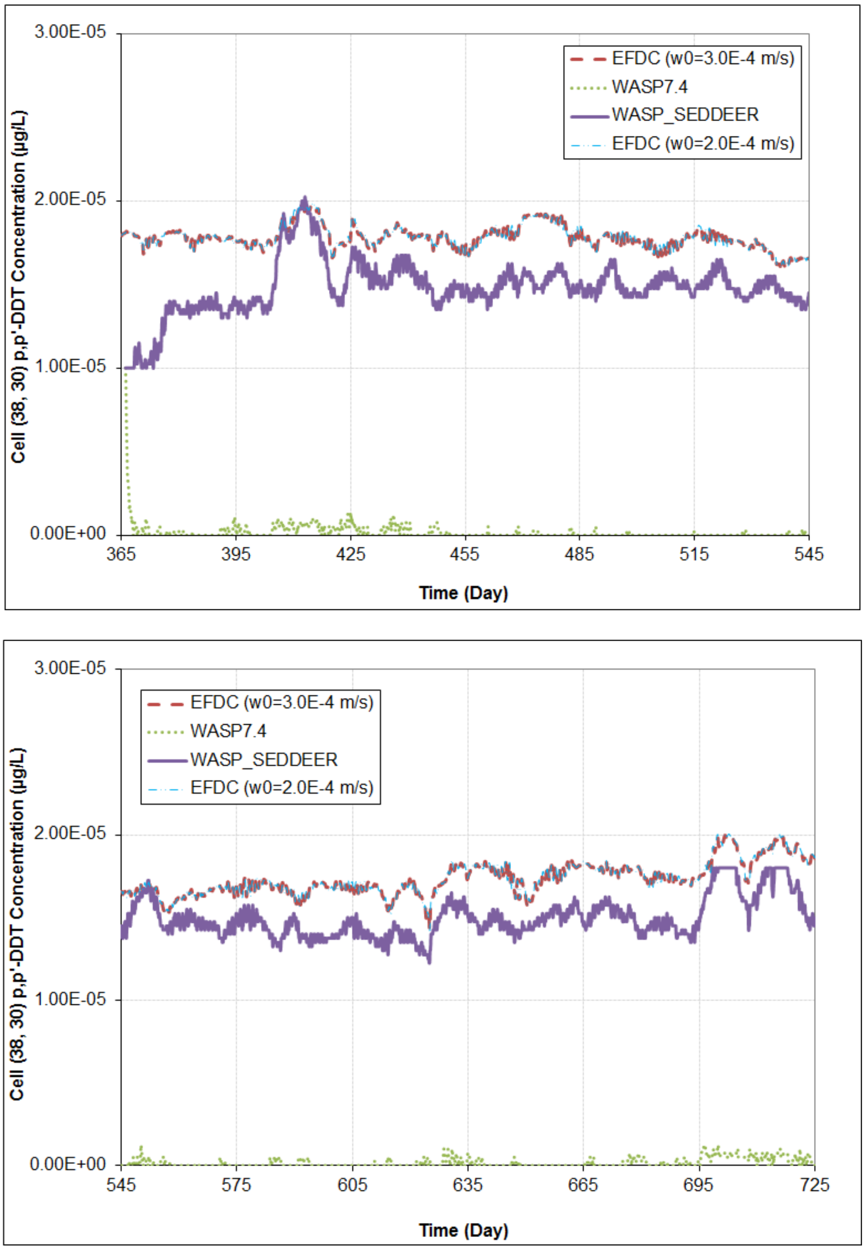


Figure 18. Simulated p,p'-DDT Concentration at Navigation Channel Cell (38, 30)

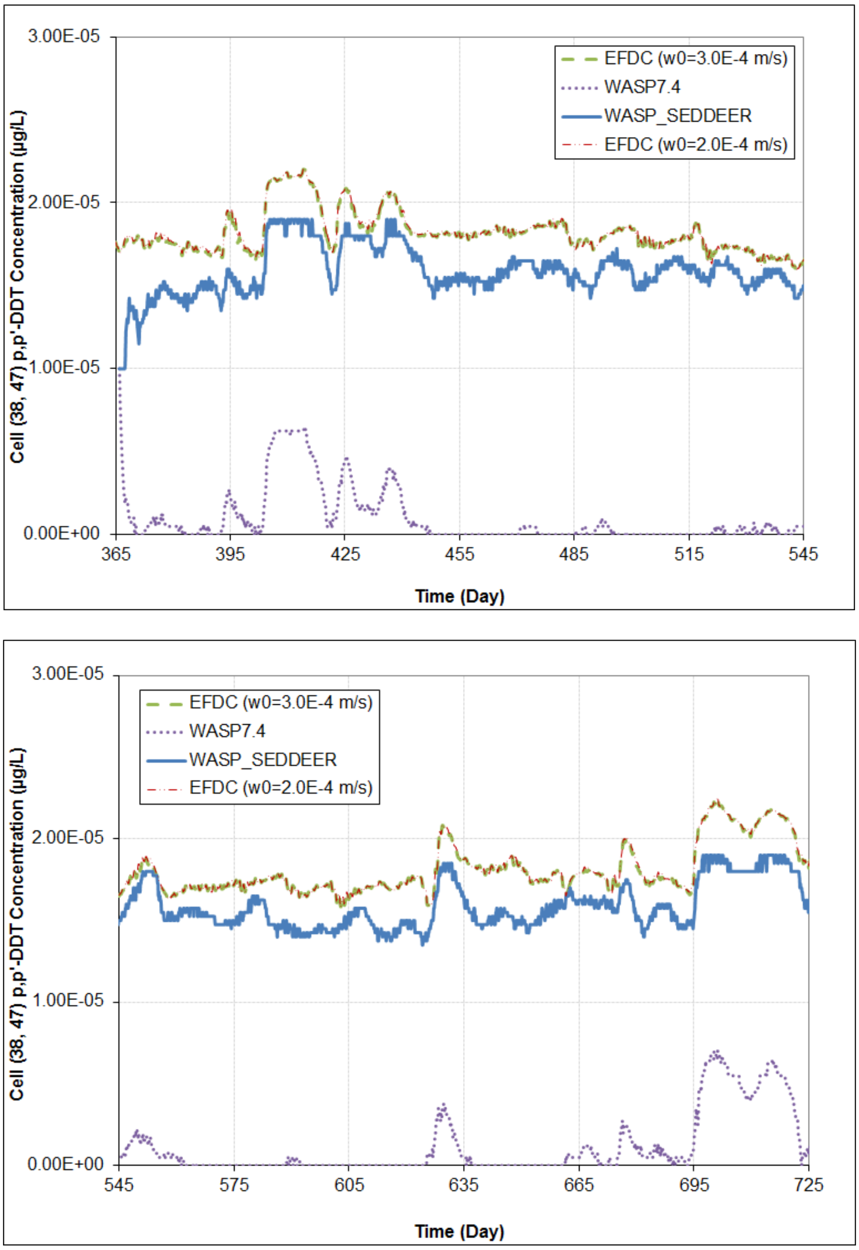


Figure 19. Simulated p,p'-DDT Concentration at Navigation Channel Cell (38, 47)

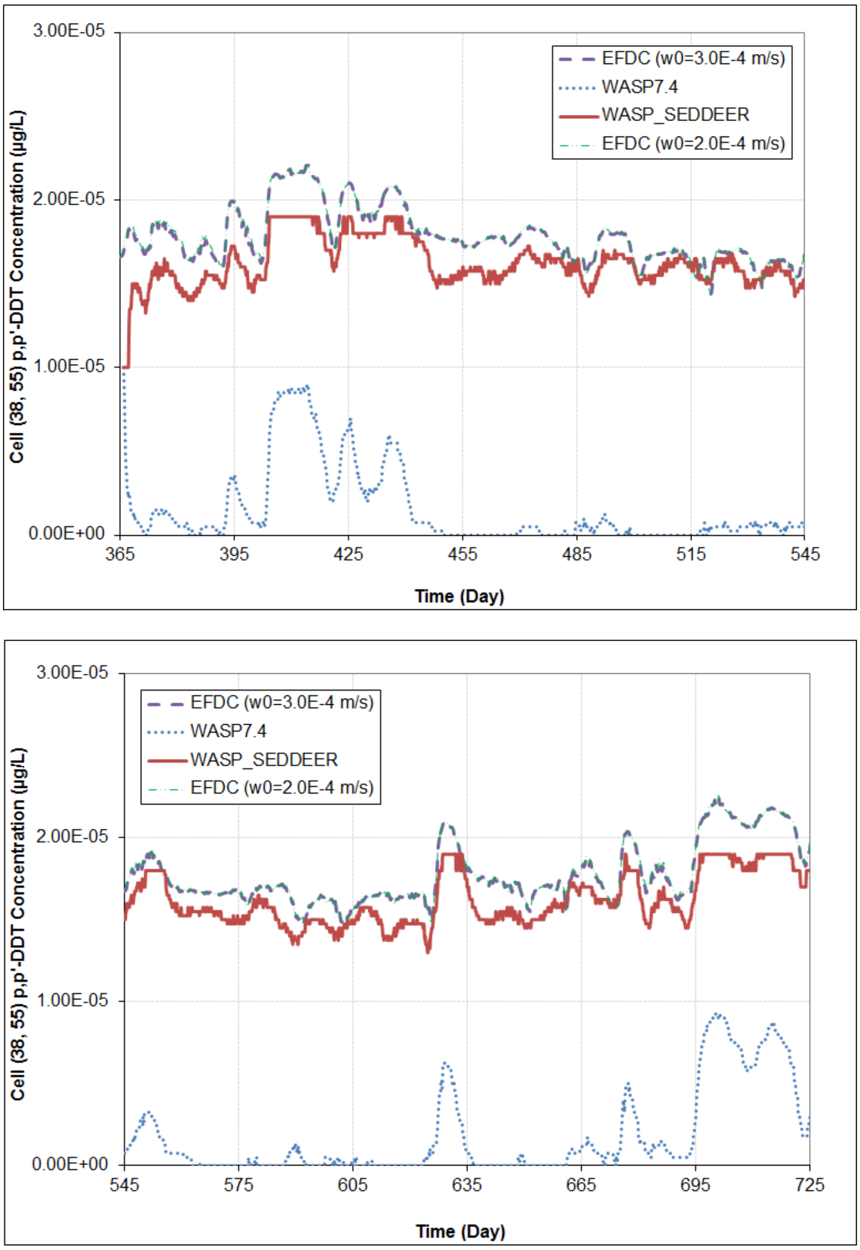


Figure 20. Simulated p,p’-DDT Concentration at Navigation Channel Cell (38, 55)

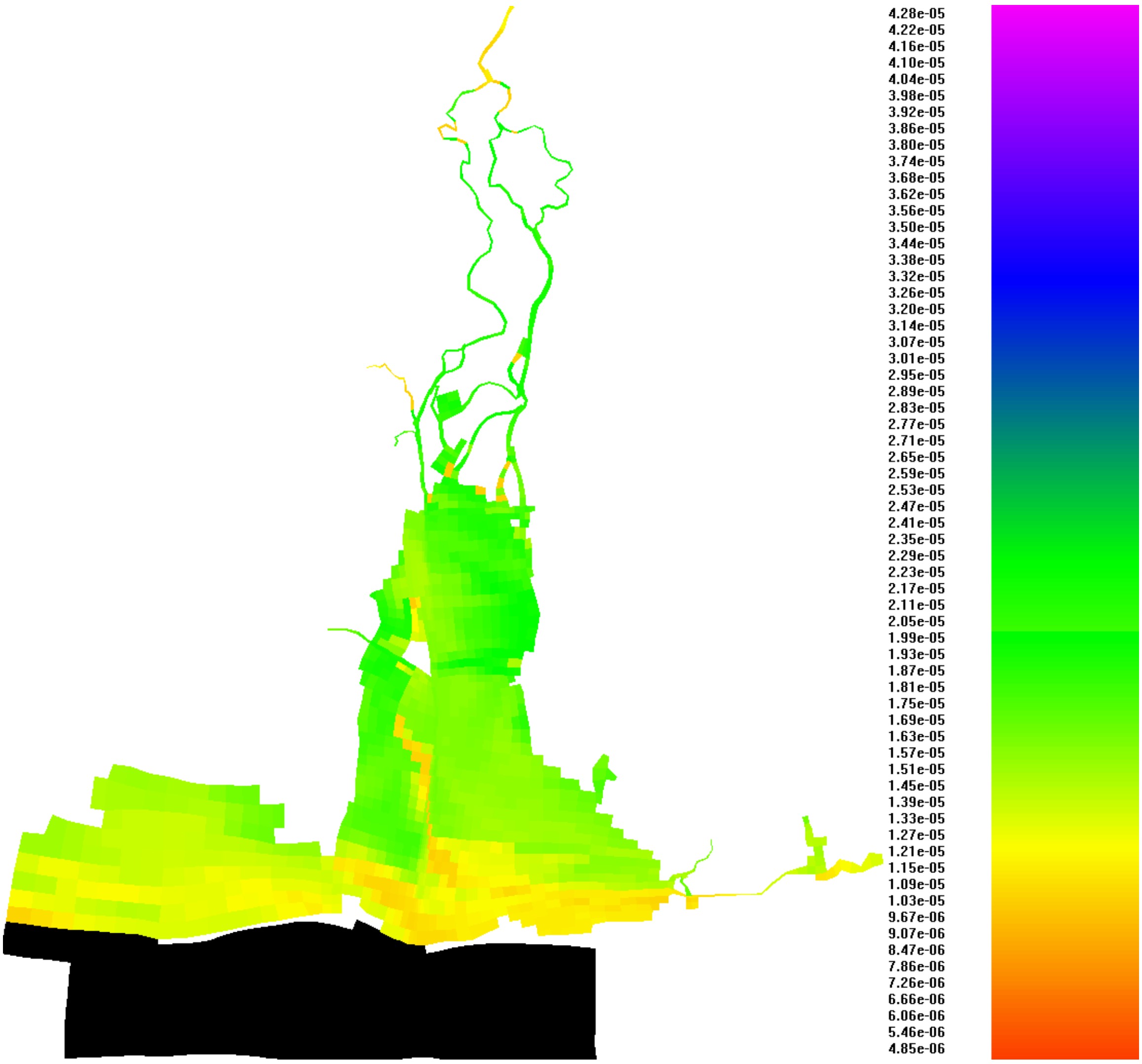


Figure 21. WASP7.4 Simulated Surface Layer p,p'-DDT Distribution at the beginning of the simulation period (January 2004)

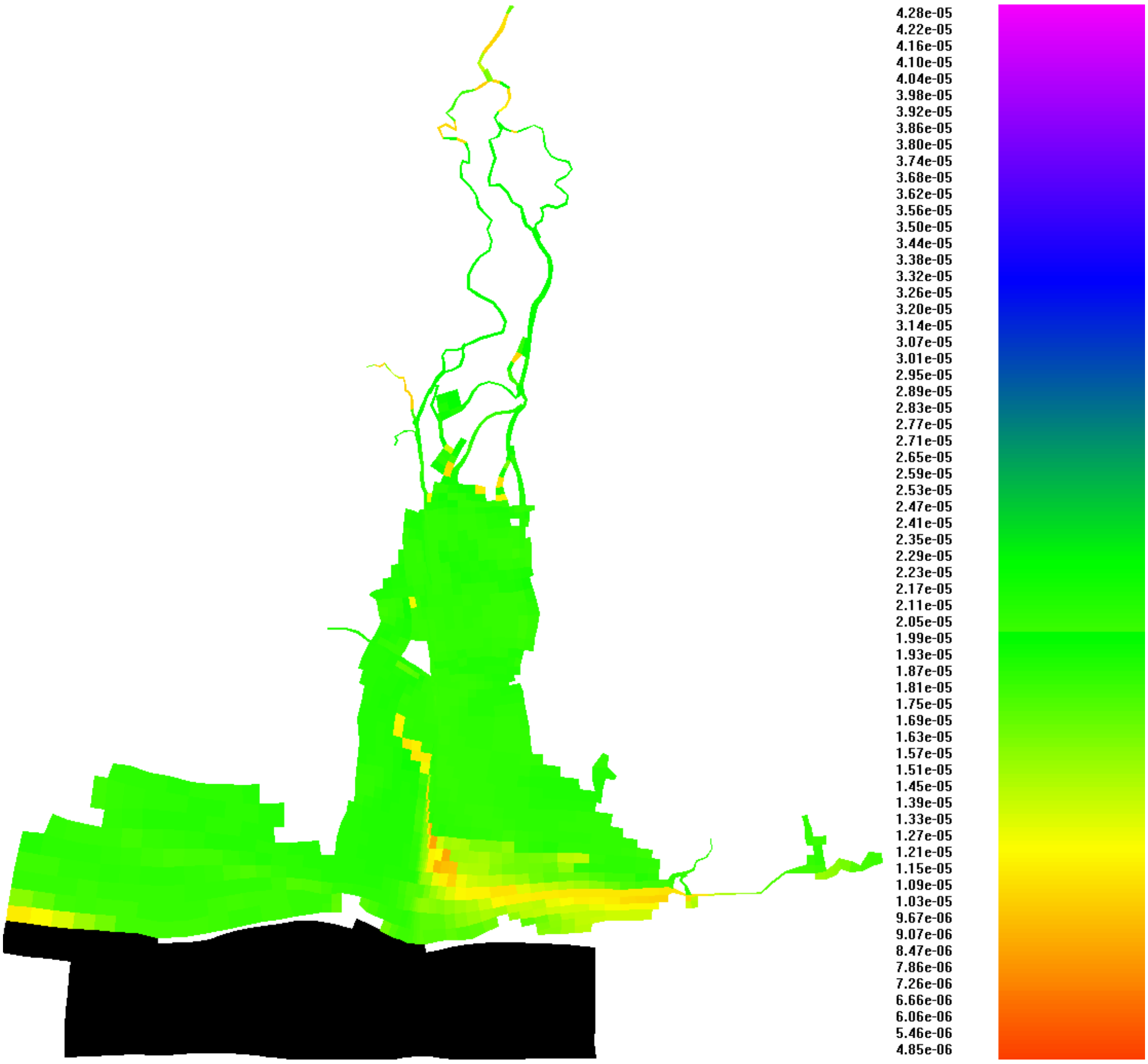


Figure 22. WASP7.4 Simulated Surface Layer p,p'-DDT Distribution at the end of the simulation period (December 2004)

4. Conclusions

The test results demonstrate that WASP_SEDDEER and SEDDEER generate the same output, indicating that the incorporation of sediment into WASP TOXI7 has been performed correctly for sediment deposition and resuspension. Similar conclusions can be drawn for diffusion across the sediment-water interface. With regards to bioturbation diffusion across the sediment-water interface WASP_SEDDEER and SEDDEER solutions are also identical, showing that the incorporation of diffusion algorithms into WASP TOXI7was successful. Comparisons for two-vertical boxes showed that simulation results from EFDC and WASP_SEDDEER are very similar, evidenced by high R^2 values.

WASP_SEDDEER output for suspended sediment concentrations (calculated at the navigation channel cells) are generally lower than those estimated by EFDC and higher than those of WASP 7.4. These results are reasonable because flocculated sediments tend to settle and not remain suspended as EFDC predicts. Similarly, WASP 7.4 does not model sediment resuspension, bioturbation, or flocculation. Therefore, it is expected that WASP_SEDDEER would predict suspended sediment concentrations higher than WASP's.

Isomer p,p'-DDT concentrations follow a similar trend to suspended sediment concentrations. Isomer concentration values simulated by WASP_SEDDEER were found to be consistently lower than those estimated by EFDC, and greater than those simulated by WASP. Surface layers for p,p'-DDT using WASP_SEDDEER captured at the beginning and the end of a one-year simulation show its capabilities for estimating contaminant and sediment concentrations throughout the computational domain.

References

Ambrose, R. B., Wool, T. A., & Martin, J. L. (1993). *WASP5, The Water Quality Analysis Simulation Program - Part A: Model Documentation.* Retrieved from http://sdi.odu.edu/mbin/wasp/dos/wasp5_model.pdf

Chapra, S. C. (1997). *Surface Water-Quality Modeling*. New York, NY: McGraw-Hill.

Clay Minerals Society, University of California, Berkeley, National Research Council U.S., & Committee on Clay Minerals (1966). *Clays and Clay Minerals*. Oxford, NY: Pergamon Press.

Collins, K. (2007). *Mobile Basin: A Review of Basin Hydrology and Bay Hydraulics*. Unpublished manuscript, Mississippi State University Department of Civil and Environmental Engineering (May 2007).

Hearn, C. J. (2008). *The Dynamics of Coastal Models*. Cambridge, UK: Cambridge University Press.

Kim, C. (2009). *A Modeling Study of Oyster Larval Transport in Mobile Bay and Eastern Mississippi Sound, Alabama* (Doctoral dissertation). Available from Dissertation Express database. (UMI No. 3353449)

Lung, W. (2001). *Water Quality Modeling for Wasteload Allocation and TMDLs*. Hoboken, NJ: John Wiley & Sons, Inc.

Martin, J. L., Evans, D. W., McAnally, W. H., McNeal, K. S., & Horton, M. (2009). *Evaluation of the Factors Affecting the Fate and Transport of Mercury in Coastal Estuaries with a Focus on Mobile Bay*. Northern Gulf Institute, Stennis Space Center, MS.

May, E. B. (1973). Extensive Oxygen Depletion in Mobile Bay, Alabama. *Limnology and Oceanography*. *18* (3). 353-366. http://dx.doi.org/10.4319/lo.1973.18.3.0353

Raines, B. (2003). *Press-Register: Scientists suspect that DDT, Mercury contamination may be to blame. Special Report*. Retrieved from http://www.al.com/specialreport/mobileregister/index.ssf?merc45.html

Stout, J. P. (1998). Preliminary Characterization of Habitat Loss: Mobile Bay National Estuary Program. Retrieved from: http://www.outdooralabama.com/images/File/Weeks_Bay/Preliminary_Character_of_Habitat_Loss_Mobile_Bay_NEP.pdf

Summersell, S. G. (2008). *Mobile Bay Sub-Estuary Monitoring Program Report*. Retrieved from Mobile Bay National Estuary Program website: http://www.mobilebaynep.com/images/uploads/library/BonSecourFINAL_2008.pdf

Wool, T. A., Ambrose, R. B., Martin, J. L., & Comer, E. A. (2002). *Water Quality Analysis Simulation Program (WASP), Version 6.0 Draft: User's Manual.* Retrieved from http://eng.odu.edu/cee/resources/model/mbin/wasp/win/wasp6_manual.pdf

Wool, T. A., Davie, S. R., Plis, Y. M., & Hamrick, J. (2003). The Development of a Hydrodynamic and Water Quality Model to Support TMDL Determinations and Water Quality Management of a Stratified Shallow Estuary: Mobile Bay, Alabama. *Proceedings of the Water Environment Federation, National TMDL Science and Policy*, *USA, 15*, 378-392. Retrieved from http://coe.uncc.edu/~jdbowen/LCFR/reports_papers/WEF%20Mobile %20Bay%20Paper%20-%20TWOOL.pdf

Xiong, Y. (2010). *Coupling Sediment Transport and Water Quality Models* (Doctoral dissertation). Available from Dissertation Express database. (UMI No. 3432283)

Xiong, Y., Martin, J. L., & McAnally, W. H. (2010). *SEDDEER for VBA (SEDDEER_VBA): A Sediment Transport Model for Water Quality Modeling: Users Guide and Documentation*. Retrieved from Mississippi State University, Starkville website: http://www.msstate.edu/~vja1/SEDDEER/seddeer_user_guide.doc