

**COUPLING SEDIMENT TRANSPORT MODEL WITH  
FATE AND TRANSPORT OF TOXICANTS**

Tingting Zhu, Yafei Jia and Sam S.Y. Wang<sup>1</sup>

**ABSTRACT:** Sediments contaminated by toxicants have a long term impact on water quality and potentially on the entire ecological system through food chains. It is essential to assess these impacts and take possible mitigation measures when pollutions occurred. Because cohesive sediments compared with non-cohesive sediments, are more susceptible to pollution by toxicants, transport, erosion and deposition processes of them are critical to fully assess the environmental impacts in addition to chemical and bio-chemical processes such as absorption, desorption, volatilization, hydrolysis, photolysis and biodegradation, etc. In this study, all these physical and chemical processes related to chemical spills are investigated by integrating them into a free surface flow model, CCHE2D, which is a robust and efficient depth-averaged two-dimensional hydrodynamic model for simulating flows natural rivers, reservoirs and lakes. The integrated model was then being validated and applied to simulate sediment and water pollution of the Hudson River, NY, resulted from the release of PCBs.

**KEY TERMS:** PCBs; cohesive sediment; fate and transport, model

## 1. INTRODUCTION

Toxicants released into rivers have negative environmental and ecological impacts. The polluted water can directly do harm to human health. Toxicants such as PCBs, heavy metals etc. are often found to be attached with cohesive sediments through sorption/desorption. To better understand the fate and transport of toxicants, it is necessary to study the cohesive sediment transport and interactions between cohesive sediments and toxicants.

The physical, chemical and biochemical processes involved in the toxicant fate and transport include advection, dispersion, settling and erosion of sediments, partition between dissolved and particulate phases of toxicants, mass transfer between the water column and sediment bed, and toxicant decay through volatilization, photolysis, hydrolysis, and biodegradation. An integrated model framework of hydrodynamic model, cohesive and non-cohesive sediment transport model, toxicant fate and transport model would be necessary to assess the complex contamination problems of toxicants effectively.

Chemical spills due to accidents have been studied by numerical models by numerous researchers. Many of these studies have simplified the estimation of sediment transport and interactions between the water column and the sediment bed. For example, the study of the chemical spill on the Rhine River in November 1986 was conducted by assuming constant suspended sediment concentrations and settling velocity (Mossman et al., 1988). The error thus resulted from the short-term simulations of this case may be acceptable. However, long-term assessment of impacts of heavy metals or PCBs requires coupling of more accurate cohesive sediment transport simulation with the toxicant fate and transport simulation.

Many researchers have simulated the long-term impacts of heavy metals or PCB in both fresh water and coastal regions. Thomann et al. (1993) simulated cadmium concentrations in the Hudson River for a long term. QEA et al. (2000) simulated PCB in upper Hudson River using a series of models including a hydrodynamic model, a sediment transport model and a chemical fate and transport model. However, these models are not in the same framework, which are in different dimensions, and spatial interpolation was necessary to pass information from model to model. Recently, Ji et al. (2002) studied heavy metals in the Blackstone River using 1-D EFDC models, which coupled hydrodynamic, sediment transport and chemical fate and transport models together.

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<sup>1</sup> Respectively, Research Scientist, Research Professor, F.A.P Barnard Distinguished Professor & Director, National Center for Computational Hydrosience and Engineering, the University of Mississippi, 102 Carrier Hall, University, MS 38677, Phone: (662) 915-7783, Fax: (662) 915-7796, E-Mail: [tzhu@ncche.olemiss.edu](mailto:tzhu@ncche.olemiss.edu).

In this study, the integrated comprehensive model framework comprising of hydrodynamic model, cohesive and non-cohesive sediment transport model and toxicant fate and transport model was developed and applied. It is based on existing CCHE2D hydrodynamic and sediment transport model (Jia et al., 2002). The model's capability to simulate the fate and transport of toxicants was demonstrated through the study of PCBs in Thompson Island Pool (TIP) of Upper Hudson River. Both USEPA and General Electric (GE) had consulting companies to conduct the study on Upper Hudson River PCBs using numerical models. The results were reported by TAMS et al. (2000) and QEA (1999). In both studies PCB<sub>3+</sub> (sum of trichloro through decachloro homologue groups) was selected as simulation surrogate.

## 2. MODEL FRAMEWORK

CCHE2D is a depth-integrated two-dimensional model, (Jia et al., 2002). It has been developed for simulating free surface flows, sediment/pollutant transport and channel morphological changes. The model has been verified and validated vigorously using physical model data, which shows that it is capable of reproducing realistic physical mechanism. The model has been proven to be robust by many applications to natural channels with complex flow conditions, topography and hydraulic structures (Jia and Alonso 1994, Jia and Wang 1999, Jia et al., 2002). The details about the hydrodynamic and non-cohesive transport model can be found in these references, and will not be reported in this paper.

The comprehensive model framework was completed by integrating two newly developed models: cohesive sediment transport model and toxicant fate and transport model.

### 2.1 Cohesive Sediment Transport Model

The cohesive sediment transport model simulates the processes of sediment deposition, erosion and consolidation. The effects of turbulence on flocculation, settling of flocs and the effects of consolidation on erosion were taken into account. The model represents the bed sediments in a three-dimensional way with multiple vertical layers based on the consolidation time. The erosion and deposition processes were simulated using empirical formulae (Burban et al. 1990, and Gailani et al. 1991). The general two-dimensional depth-averaged transport equation is given as follows:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) + \frac{\partial}{\partial y}(vC) = \frac{\partial}{\partial x}\left(E_{xx} \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_{yy} \frac{\partial C}{\partial y}\right) + S \quad (1)$$

where  $C$  = depth-averaged toxicant concentration ( $\text{kg}/\text{m}^3$ );  $u, v$  = depth-averaged velocities in  $x$  and  $y$  direction ( $\text{m}/\text{s}$ ), respectively;  $E_{xx}$  and  $E_{yy}$  = components of dispersion tensor  $E$  ( $\text{m}^2/\text{s}$ ); and  $S$  = source term ( $\text{kg}/\text{m}^3/\text{s}$ ).

For cohesive sediment transport, the source term is calculated as:

$$S = \frac{D_b - E_b}{h} \quad (2)$$

where  $h$  = water depth ( $\text{m}$ );  $D_b$  = sediment deposition rate ( $\text{kg}/\text{m}^2/\text{s}$ ); and  $E_b$  = sediment erosion rate ( $\text{kg}/\text{m}^2/\text{s}$ ).

The bed elevation change due to sediment deposition or erosion is calculated as:

$$\frac{\partial z_b}{\partial t} = \frac{D_b - E_b}{\rho_d} \quad (3)$$

where  $z_b$  = bed elevation ( $\text{m}$ ).

The change of bed material thickness due to sediment consolidation is calculated as:

$$\frac{d}{dt}(H\bar{\rho}_d) = 0 \quad (4)$$

where  $H$  = thickness of bed material ( $\text{m}$ );  $\bar{\rho}_d$  = depth averaged dry density of bed material over  $H$  ( $\text{kg}/\text{m}^3$ ).

The erosion rate (Eq. 5), floc size (Eq.6), settling velocity (Eq. 7) and deposition rate (Eq. 8) are computed using empirical formulae (Burban et al. 1990, Gailani et al. 1991), which are listed as follows:

$$E_b = \frac{a_0}{t_d^m} \left( \frac{\tau_b - \tau_e}{\tau_e} \right)^n \quad (5)$$

where  $a_0$  = site-specific coefficient;  $t_d$  = time after deposition (day);  $m$  = coefficient ( $\approx 2$ ).

$$d_m = \left( \frac{\alpha_0}{CG} \right)^{1/2} \quad (6)$$

where  $d_m$  = median diameter of flocs (cm);  $G$  = fluid shear stress (dynes/cm<sup>2</sup>);  $\alpha_0$  = experimental coefficient =  $10^{-8}$  g<sup>2</sup>m/cm<sup>3</sup>/s<sup>2</sup>.

$$\omega_f = a d_m^b \quad (7)$$

where  $a = B_1 (CG)^{-0.85}$ ,  $b = -[0.8 + 0.5 \log(CG - B_2)]$ ,  $B_1 = 9.6 \times 10^{-4}$ ,  $B_2 = 7.5 \times 10^{-6}$ , and  $\omega_f$  = settling velocity (cm/s).

$$D_b = \begin{cases} 0 & \text{for } \tau_b > \tau_{d,\min} \\ \alpha_m \omega_f C & \text{for } \tau_b \leq \tau_{d,\min} \end{cases} \quad (8)$$

where  $\alpha_m = 1 - \tau_b / \tau_{d,\min}$ ,  $\tau_b$  = bed shear stress (N/m<sup>2</sup>);  $\tau_{d,\min}$  = critical bed shear stress (N/m<sup>2</sup>) below which all sediments are deposited on the bed.

More details about the cohesive sediment transport model and its verifications using lab data can be found in Zhu (2006).

## 2.2 Toxicant Fate and Transport Model

The general governing equation of two-dimensional depth-averaged toxicant fate and transport is the same as Eq. 1. The source terms comprise of external loading, exchange between sediment and water column and decay processes. In the water column, the source term is shown as Eq. 9:

$$S = S_{load} + S_{sed} + S_{v-diff} + S_{decay} \quad (9)$$

where  $S_{load}$  = external chemical load (kg/m<sup>3</sup>/s);  $S_{sed}$  = chemical source/sink due to net settling or eroded sediment flux (kg/m<sup>3</sup>/s);  $S_{v-diff}$  = vertical diffusion flux at the water-sediment interface (kg/m<sup>3</sup>/s);  $S_{decay}$  = chemical decay term (kg/m<sup>3</sup>/s).

The toxicant source/sink term due to the net settling or net eroded sediment flux is formulated based on mass balance (Wu, 2006). Both dissolved and particulate phases were considered. In case of net erosion, not only the toxicants sorbed on the bed sediment were released into the water column, but also those in the porous water. Similarly, in case of net deposition, toxicants sorbed on suspended sediments settle on the bed surface layer and the dissolved toxicants fill the porous volume as well. This source term is formulated as follows:

$$S_{sed} = \frac{J_{sed}}{h} = \frac{J_{erosion} + J_{deposition}}{h} \quad (10)$$

$$J_{erosion} = \max(E_b - D_b, 0) \frac{s_{T1}}{\rho_s (1 - \phi)} \quad (11)$$

$$J_{deposition} = \min(E_b - D_b, 0) \left( \frac{f_{p,w}}{m} + \frac{f_{d,w}\phi}{\rho_s(1-\phi)} \right) \quad (12)$$

where  $s_{T1}$  = toxicant concentration in surface sediment bed ( $\text{kg/m}^3$ );  $\rho_s$  = pure sediment density ( $\text{kg/m}^3$ )  $\phi$  = porosity, dimensionless;  $f_{p,w}$  = toxicant particulate fraction in the water column;  $f_{d,w}$  = toxicant dissolved fraction in the water column;  $m$  = sediment concentration ( $\text{kg/m}^3$ ).

The mass transfer due to vertical diffusion flux at the water-sediment interface is determined by Fick's Law:

$$S_{v-diff} = \frac{k_f}{h}(s_{d,1} - c_d) = \frac{k_f}{h}(f_{d,s1}s_{T1} - f_{d,w}c_T) \quad (13)$$

where  $k_f$  = overall mass diffusion coefficient, in m/s;  $f_{d,s1}$  = dissolved chemical fraction in surface sediment layer;  $c_T$  = total toxicant concentration in the water column ( $\text{kg/m}^3$ ).

It is assumed that the lateral convection and dispersion in sediment layer are negligible and only vertical mass transfer was considered. The governing equation for the surface sediment layer ( $i=1$ ) in conservative form is:

$$\frac{\partial(s_{T1} \times D_{sed1})}{\partial t} = S_{load} - S_{sed} + S_{v-diff,1} + S_{decay} \quad (14)$$

$$S_{v-diff,1} = k_f(f_{d,s1}s_{T,1} - f_{d,w}c_T) + k_{f,s}(f_{d,s2}s_{T,2} - f_{d,s1}s_{T1}) \quad (15)$$

where  $D_{sed1}$  = depth of surface sediment layer (m).

For a subsequent sediment layer  $i$  ( $i>1$ ), which has adjacent layers Layer ( $i-1$ ), and Layer ( $i+1$ ), the governing equation is:

$$\frac{\partial(s_{Ti} \times D_{sedi})}{\partial t} = S_{load} + S_{v-diff,i} + S_{decay} \quad (16)$$

$$S_{v-diff,i} = k_{f,s}(f_{d,si+1}s_{T,i+1} - f_{d,si}s_{T,i}) + k_{f,s}(f_{d,si}s_{T,i} - f_{d,si-1}s_{T,i-1}) \quad (17)$$

where  $D_{sedi}$  = depth of sediment layer  $i$ , in m.

The bottom layer boundary condition is assumed as constant.

$$s_{T,bottom} = \text{const.} \quad (18)$$

Details about the decay processes of toxicants include volatilization, hydrolysis, photolysis, and biodegradation, etc. can be found in Zhu (2006).

### 3. CASE STUDY OF TIP PCBS

#### 3.1 PCBs Pollution in Upper Hudson River

For about three decades, contaminated water with Polychlorinated biphenyls (PCBs) had been discharged from two capacitor factories of General Electric (GE) near the upstream of the Hudson River until 1977. In 1973, PCBs contaminated sediments were carried to downstream by the river flow after the removal of the former Fort Edward Dam which locates upstream of the contamination site. In late 1991, it was found that there was a collapse of a wooden gate structure within an abandoned paper mill which was located adjacent to one of the capacitor plant. The structure failure caused the seepage of the polluted groundwater into the surface water. The pollution was isolated and the polluted PCBs were removed in 1995.

Thompson Island Pool (TIP) is immediate downstream of the Fort Edward Dam extending from River Mile (RM) 194.6 to RM 188.5. It became the biggest PCBs reservoir due to its location and the deposition of PCB-contaminated sediments. The highest PCBs concentrations were also found in TIP (Upper Hudson River PCBs Database). In this study, for the purposes of validation and demonstration, PCB<sub>3+</sub> was simulated from 1991 through 1997 in TIP which was most polluted.

Many agencies including USGS, USEPA, NYDOT, and GE etc. have collected data on bathymetry, flow, sediment samples, surface water quality, PCBs in water column and bed since 1977. All these data and related reports have been organized by USEPA into a database (TAMS consultants and Gradient cooperation, 1995), which can be downloaded from USEPA's website: <http://www.epa.gov/hudson/reports.htm>.

### 3.2 Numerical Simulations Of TIP PCBs

In order to simulate the fate and transport of PCB in TIP, flow field, bed shear stress, suspended sediment concentrations, sediment settling and erosion rate need to be obtained using the integrated model framework. Long term simulations hydrodynamic, cohesive and non-cohesive sediment transport, and PCB<sub>3+</sub> fate and transport were conducted from 1991 through 1997 in TIP.

The computational domain of TIP was discretized by a  $23 \times 160$  mesh, which was used through out the simulations of flow, sediments and PCBs. The bed elevation was obtained based on bathymetry survey by GE in 1991. Data for boundary conditions, initial conditions and measurement data for model calibration for all flow, sediment and PCB<sub>3+</sub> simulations are available and found in the USEPA Upper Hudson PCB Database (referred as "the Database" in the following sections).

#### 3.2.1 Flow Simulations

Flow field from 1991 to 1997 was simulated after the model was calibrated and validated. No parameter was changed from the validation cases. The simulation results of upstream water surface elevation were compared with the measured values as shown in Figure 1. For the period from January 1991 to September during which there were measured data of surface elevation, good agreement between the simulation and measurement was resulted.

#### 3.2.2 Suspended Sediments Simulations

It was assumed that only suspended load is important for the study of PCBs in TIP and bed load transport of non-cohesive materials was neglected (QEA, 1999, TAMS et al, 2000).

The sediment transport was simulated using the integrated cohesive and non-cohesive sediment model. The simulation time step was 30 seconds. Three sediment classes were used to represent the bed materials: 1) cohesive material, mean diameter of 20  $\mu\text{m}$ ; 2) fine sand, mean diameter of 0.2 mm; and 3) coarse gravel, mean diameter of 9 mm.

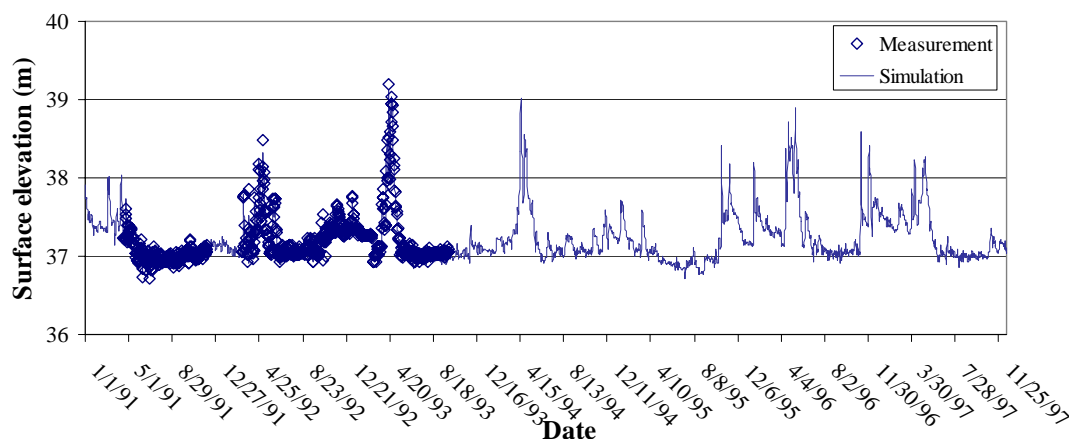


Figure 1 Simulated and Measured Upstream Surface Elevation of TIP (1991-1997)

The parameters in Eq. 5 for cohesive sediment erosion rate are given following values:  $a_0 = 0.00035 \text{ kg-day}^{1/2}/\text{m}^2$ ;

$m=0.5$ ;  $n= 2.94$ ; and critical shear stress for erosion  $\tau_e = 0.15$  Pa for layers newer than 7 days. The critical shear stress for deposition was set as 0.01 Pa. The settling velocity was calculated in a similar form as in Eq. 7, which is given as follows:

$$\omega_f = \frac{2.5}{86400} (C_1 \times G \times 1000)^{0.12} \quad (19)$$

where  $C_1$  = concentration of sediment class 1 ( $\text{kg}/\text{m}^3$ ).

Figure 2 shows the simulation results compared with the weekly measured suspended sediment concentration by GE. Although GE's measurement data was continuous during the simulation period, the peak values are missing compared with the USEPA's measurement dataset (QEA, 1999). The general trend of sedimentation from 1991 to 1997 is depositional. The simulated average deposition depth in TIP is about 1.6cm over seven years, which is consistent with observations (TAMS et al, 2000).

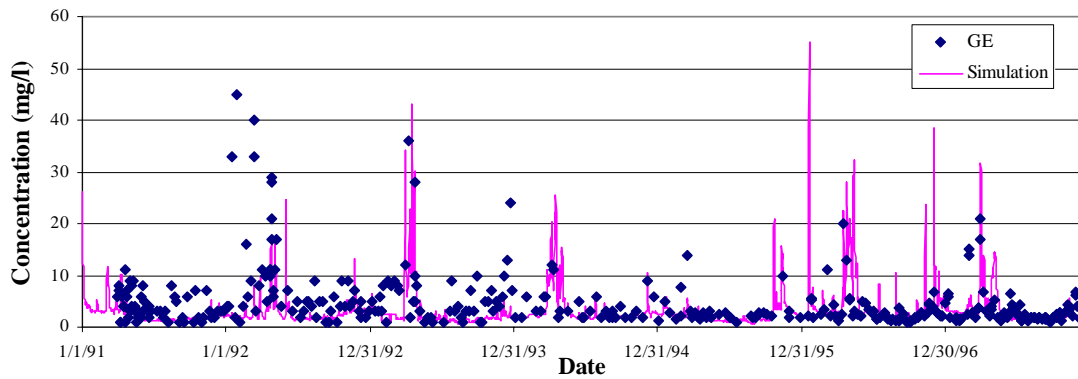


Figure 2 Simulated and Measured Suspended Sediment Concentrations in TIP

### 3.2.3 PCB Simulations

The general chemical fate and transport equation was extended from the two-phase partition to the three-phase partition. The total chemical concentration comprises of freely dissolved phase, dissolved organic carbon (DOC) bounded dissolved phase and particulate phase. The concentrations in each phase are represented by following equations (Eq. 20-23):

$$c_T = c_{fd} + c_{dd} + c_p \quad (20)$$

$$c_{fd} = f_{fd} c_T = \frac{\phi}{\phi + K_P m + K_{DOC} m_{DOC}} c_T \quad (21)$$

$$c_{dd} = f_{dd} c_T = \frac{K_{DOC} m_{DOC}}{\phi + K_P m + K_{DOC} m_{DOC}} c_T \quad (22)$$

$$c_p = f_p c_T = \frac{K_P m}{\phi + K_P m + K_{DOC} m_{DOC}} c_T \quad (23)$$

where  $c_{fd}$  = freely dissolved  $\text{PCB}_{3+}$  concentration ( $\text{kg}/\text{m}^3$ );  $c_{dd}$  = DOC-bound dissolved  $\text{PCB}_{3+}$  concentration ( $\text{kg}/\text{m}^3$ );  $c_p$  = sorbed PCBs concentration ( $\text{kg}/\text{m}^3$ );  $f_{fd}$  = fraction of freely dissolved  $\text{PCB}_{3+}$ ;  $f_{dd}$  = fraction of DOC-bound dissolved  $\text{PCB}_{3+}$ ;  $f_p$  = fraction of sorbed  $\text{PCB}_{3+}$ ;  $K_P$  = sediment partition coefficient;  $K_{DOC}$  = dissolved organic carbon partition coefficient; and  $m_{DOC}$  = DOC mass concentration ( $\text{kg}/\text{m}^3$ ).

All parameters related to physical, chemical and biochemical processes of PCB<sub>3+</sub> were obtained from the Database and studies conducted by QEA (1999) and TAMS et al. (2000). The initial bed concentration distribution of PCB<sub>3+</sub> was derived from the Database.

The PCB<sub>3+</sub> calibration was conducted in 1994 spring. The nonlinearity of PCB partition was examined. It is found that in the case of TIP, PCB transport linear partition was sufficient to represent the sorption/desorption process. The details about parameters and calibration simulations can be found in Zhu (2006).

The simulation results from 1991 to 1997 are shown in Figure 3. The simulated PCB<sub>3+</sub> concentrations in the water column agree well with the measured concentrations. Most of peaks are matched and the similar long-term pattern is obtained.

Surface bed sediment is a major source contributing to the PCB<sub>3+</sub> concentration in the water column. The releasing of PCB<sub>3+</sub> from the bed is controlled by the PCB<sub>3+</sub> concentration in the surface bed sediment. The simulation results of PCB<sub>3+</sub> concentration in the surface bed sediment from 1991 to 1997 are shown in Figure 4. The simulated PCB<sub>3+</sub> concentrations agree well with the measured concentrations.

The declining of PCB<sub>3+</sub> concentration in the water column and bed sediment complies with the observations and other modeling studies by USEPA and GE.

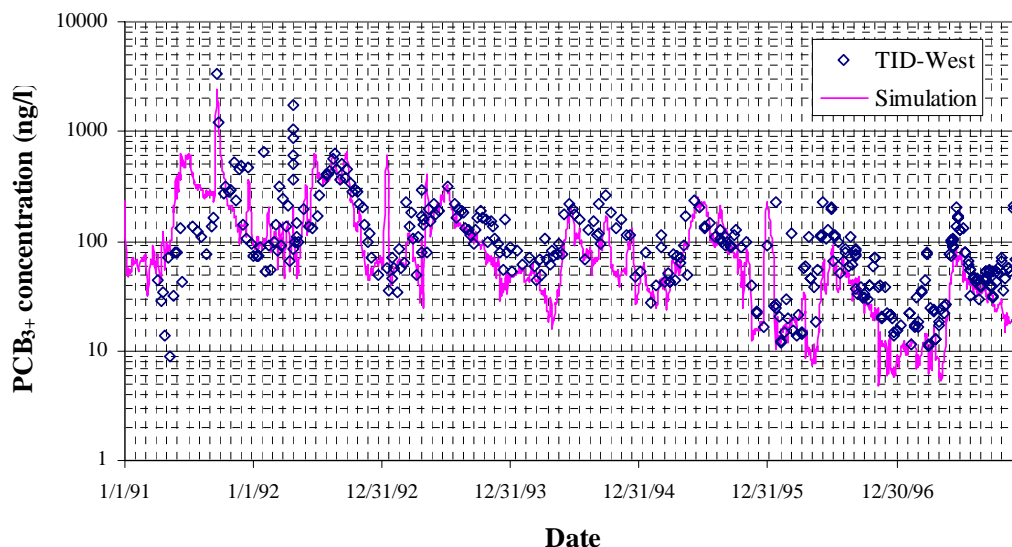


Figure 3 Simulated and Measured Water Column PCB<sub>3+</sub> Concentrations in TIP

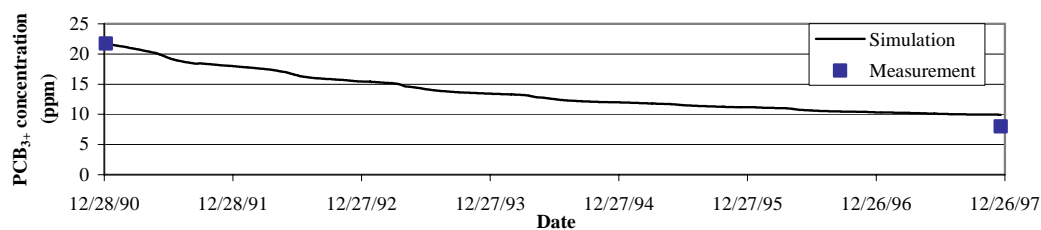


Figure 4 Simulated and Measured Surface Bed PCB<sub>3+</sub> Concentrations in TIP

#### 4. CONCLUSIONS

The coupled cohesive sediment transport model and toxicant fate and transport model is capable of simulating the major physical, chemical, biochemical processes and their interactions in freshwater systems for sediment related environmental problems.

The integrated flow, cohesive and non-cohesive sediment transport model, toxicant fate and transport model was applied to the study of Upper Hudson River PCBs. The sediment transport model gave satisfactory predictions of suspended sediment

concentrations and bed shear stress distributions. The general long-term deposition trend in TIP agrees with field observations. The PCB<sub>3+</sub> simulation from 1991 to 1997 shows good agreement with the measurement data. The declining of PCB<sub>3+</sub> concentration in the water column and bed sediment also complies with the observations and other modeling studies by USEPA and GE. It can be seen from this demonstration case that the developed models can make reliable long-term predictions and can be used to assess the real-world problems associated with sediments.

The limitations of the comprehensive model come from the empirical formulae which approximate the mechanisms of physical, chemical and bio-chemical processes. In case needed, they could be tailored to specific problems without big changes. In addition, they could be improved with the advancement of knowledge so that its capabilities can be enhanced with time.

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