
An integrated geochemical and hydrodynamic model for tidal coastal environments

Jian Peng and Eddy Y. Zeng¹

ABSTRACT

In this paper, the design, calibration, and application of an integrated geochemical-hydrodynamic model are described. The model is comprised of three parts: a hydrodynamic submodel that was adopted from a depth-averaged, semi-implicit hydrodynamic model, a geochemical submodel based on equilibrium partitioning of chemicals between aqueous and particulate phases, and a particle dynamic submodel that simulates the resuspension, transport and settling of suspended particulate matter (SPM). The integrated model was implemented in San Diego Bay (SDB), a heavily urbanized, semi-closed mesotidal embayment. A series of model calibrations were carried out based on the observations on salinity, polychlorinated biphenyls (PCBs) and SPM. Salinity calibrations indicated that only 15% of the precipitation in the drainage area of SDB could reach the bay, presumably due to dams in tributary rivers. Steady-state calibrations of PCBs based on fixed concentrations at known 'hot spots' have reproduced PCB concentrations observed in both dissolved and particulate phases. SPM calibrations showed that shipping-induced resuspension produce more SPM than natural processes. Based on the calibrated model, the annual transport of PCBs out of SDB was estimated to be 3.85 kg (3.5 kg and 0.35 kg in dissolved and particulate phases), much higher than the previous estimates based on steady-state assumptions. It was also found that only a small portion of the fine sediment exported from SDB was derived from riverine input. This model can be applied to studies of the transport and fate of other chemical species, and it is applicable other coastal areas. The integrated model offers a novel framework in which geochemical processes in coastal environments can be investigated on a truly dynamic basis.

INTRODUCTION

In shallow coastal seas, many biogeochemical processes are controlled directly or indirectly by

hydrodynamics. These processes include diffusion, dispersion, and transport of solutes; sediment-water interaction; and adsorption-desorption of chemicals to and from suspended particulate matter (SPM). Processes within the sediment column, though of much longer time scales, can be affected indirectly by hydrodynamics in the overlying water column through sediment-water interactions. If the water column hydrodynamics is quantitatively defined, these related processes may be studied dynamically and quantitatively in both temporal and spatial domains. For example, in a study area where hydrodynamic parameters such as velocity, turbulence, water surface elevation and density are defined in each time step at every computational grid, it is possible to quantitatively study the behavior and environmental fate of the chemical species of concern by defining processes such as diffusion and advection, adsorption and desorption, chemical and biological transformation, among others (Christiansen *et al.* 2000, James 2002, Karickhoff 1979, Lumborg and Windelin 2003, Martin and McCutcheon 1999, McDonald and Cheng 1994).

Recent advances in the numerical modeling techniques have enabled simulations of coastal ocean physical processes in great detail and with high accuracy, allowing forecasting and nowcasting of oceanic conditions such as tides, currents and waves (Cheng *et al.* 1993, Wang *et al.* 1998). However, application of these hydrodynamic models on the transport and fate of environmentally significant chemical species remains limited, especially for those chemicals that are associated with particulate matter. The difficulties originate from the fact that particle dynamic modeling itself is a nontrivial task. Equations describing particle resuspension and settling, two key processes in particle dynamics, are still largely empirical and rigid. Applying these equations to a new study areas requires a considerable amount of measurement and calibration to select optimal values for a large number of empirical constants (Christiansen *et al.* 2000, McDonald and Cheng

¹Guangzhou Institute of Geochemistry, State Key Laboratory of Organic Geochemistry, Chinese Academy of Sciences, Guangzhou, China

1994, Taki 2001). Consequently, the difficulty propagates to the modeling of particle-reactive chemical species, in which a reliable simulation of particle dynamics is a prerequisite.

Moreover, the difficulty of establishing an integrated geochemical and hydrodynamic model lies in the demanding task of calibration and verification of the geochemical model. In order to calibrate a geochemical model, a large number of chemical analyses with sufficient temporal and spatial coverage as well as frequency is needed. For chemical species of very low concentrations (e.g., such as many trace organic contaminants), time-series measurements are often costly or unattainable. As a result, as long as the hydrodynamic model is properly calibrated and verified, a compromise is often needed in terms of calibration and verification of the chemical model. For example, the sampling for ppb-level chemicals may not necessarily represent a 'snapshot' because the sampling time can be as long as a few days.

To address the above issues and establish a novel approach to studying transport and geochemical processes of non-conservative chemicals in coastal oceans, an integrated geochemical and hydrodynamic model is needed. To this end, an existing depth-averaged hydrodynamic model was adopted and integrated with particle dynamic and geochemical submodels. The integrated model was calibrated and applied in a study of the long-term transport and fate of particle-associated contaminants, and polychlorinated biphenyls (PCBs) were used as an example of non-conservative, particle-reactive chemicals. The capability of simulating these chemicals implies that the integrated model can be used to study a wide range of chemicals of natural or anthropogenic origins.

MODEL FORMULATION AND INTEGRATION

There are a number of available hydrodynamic and water quality models that can be applied to shallow coastal oceans (Cheng and Casulli 2001, Cheng *et al.* 1993, Martin and McCutcheon 1999, Sheng *et al.* 1992, Sheng 1996). For shallow coastal oceans and estuaries, it is essential that the residual currents and baroclinic forcing be reproduced in order to achieve satisfactory accuracy. At the same time, due to strong influence of tides, the model should also be able to simulate the tidal forcing and drying-wetting of shallow intertidal zones during flooding and ebbing tides.

Based on the above considerations, a numerical hydrodynamic model (the Tidal, Residual, Intertidal Mudflat Model; TRIM) was selected for this study because it allows an efficient and accurate simulation of tidal-influenced shallow estuarine environment and has been fully calibrated and verified in San Francisco Bay and San Diego Bay (Cheng *et al.* 1993, Wang *et al.* 1998). The model uses a semi-implicit, time-stepping finite-difference numerical method to solve the nonlinear, depth averaged (2-D) shallow water equations. An Eulerian-Lagrangian method (ELM) was used to treat advection terms in the momentum equations such that the numerical method is unconditionally stable if the baroclinic forcing is weak. For many shallow seas, a depth-averaged model is sufficient to simulate the hydrodynamics of shallow water circulation accurately and efficiently. The model also keeps track of the drying and wetting of shallow water cells during flooding and ebbing tides, making it an ideal choice for hydrodynamic modeling of tidal shallow coastal environments.

The integrated model was formulated by combining the newly designed geochemical and particle dynamic modules with the original TRIM model. The additional modules provide functionalities such as sediment resuspension, partitioning of chemicals between aqueous and particle phases, particle settling, storm events, river input of freshwater, and evaporation. These functionalities were implemented in the form of individual subroutines in the computer program of the original TRIM model. The so-called geochemical and particle dynamic submodels were in effect conceptualized units consisting of one or more of the above subroutines. The geochemical submodel was embedded in the partitioning subroutine, and particle dynamic submodel consisted of subroutines that simulate tidal resuspension, particle settling, and some random processes (storms, shipping activities, etc.) that affect SPM concentrations. Details of the integrated model are given below.

Hydrodynamic submodel

The hydrodynamic submodel performs the simulations of tides (i.e. variations in water surface elevation) and tidal/residual circulations. The governing equations include the conservation equations of mass, momentum, conservative scalar variables, and an equation of state (Cheng *et al.* 1993). In Cartesian coordinates, the depth averaged continu-

ity equation (i.e., conservation of mass) is given by

$$\frac{\partial \zeta}{\partial t} = \frac{\partial[(h + \zeta)U]}{\partial x} + \frac{\partial[(h + \zeta)V]}{\partial y} = 0 \quad (1)$$

the x-momentum equation (conservation of momentum at x-direction) by

$$\frac{DU}{Dt} - fV = -g \frac{\partial \zeta}{\partial x} + \frac{1}{\rho_0(h + \zeta)} (\tau_x^w - \tau_x^b) + A_h \nabla^2 U - \frac{g}{2\rho_0} (h + \zeta) \frac{\partial \rho}{\partial x} \quad (2)$$

the y-momentum equation (conservation of momentum at y-direction) by

$$\frac{DV}{Dt} - fU = -g \frac{\partial \zeta}{\partial y} + \frac{1}{\rho_0(h + \zeta)} (\tau_y^w - \tau_y^b) + A_h \nabla^2 V - \frac{g}{2\rho_0} (h + \zeta) \frac{\partial \rho}{\partial y} \quad (3)$$

the scalar transport equation by

$$\frac{DC_i}{Dt} = \frac{1}{(h + \zeta)} \nabla [K_h(h + \zeta) \nabla C_i] + \Sigma(I_i) + \Sigma(O_i) \quad (4)$$

and the equation of state,

$$\rho = \rho_0 [1 + (0.78C_o - 0.75)/1000] \quad (5)$$

Density is treated as a function of salinity (C_o) only. In temperature range of 10-20°C, the temperature dependence of water density can be neglected (Cheng *et al.* 1993). For the definitions of the symbols, please refer to Table 1.

In Equations 2 and 3, the terms starting from the left are the substantial derivatives of U and V, the momentum flux due to Coriolis acceleration, the difference in water surface elevation (propagation of gravity waves), wind and bottom shear stress, the turbulent dispersion of momentum, and the baroclinic change of momentum flux. The salt transport equation, Equation 4, is needed only if $\frac{\partial \rho}{\partial x}$ and $\frac{\partial \rho}{\partial y}$ are not zero in Equations 2 and 3, i.e., the baroclinic condition exists. The conventional Manning-Chezy type of formulation is used for the bottom shear stresses such that

$$\tau_x^b = \frac{\rho_0 g U \sqrt{U^2 + V^2}}{C_z^2}, \quad \tau_y^b = \frac{\rho_0 g V \sqrt{U^2 + V^2}}{C_z^2} \quad (6)$$

where C_z is the Chezy coefficient relating to a Manning's constant n by (Cheng *et al.* 1993)

$$C_z = \frac{(h + \zeta)^{1/6}}{n} \quad (7)$$

Table 1. Definition of Symbols

Symbol	Definition
A	atmospheric input
A_h	horizontal eddy viscosity coefficient
C_i	general representation of the concentration of a chemical of interest
C_{oc}	organic carbon normalized concentration of particulate phase PCB in ng/kg
C_p	particle phase PCB concentration in ng/kg
C_w	dissolved phase PCB concentration in ng/L
C_{we}	equilibrium dissolved phase PCB concentration in ng/L
C_z	Chezy coefficient used in calculation of bottom shear stress
D	diameter of the particulate matter in μm in Sternberg's scheme
$\frac{D}{Dt}$	$\frac{D}{Dt} = \frac{\partial}{\partial t} + U \frac{\partial}{\partial x} + V \frac{\partial}{\partial y}$ is the substantial derivative in the x-y plane, which is the time rate of change of a property following a fluid particle (i.e. a Lagrangian concept) in an Eulerian coordinate system.
f	Coriolis parameter
f_{oc}	fraction of organic carbon in the particulate phase
g	gravitational acceleration
h	reference water depth at mean lower low water
H	total water depth ($h + \zeta$)
K_h	horizontal diffusivity coefficient
K_{oc}	organic carbon normalized particle-water partition coefficient
K_{ow}	octanol-water partition coefficient
M	empirical constant used in sediment resuspension calculation
n	Manning's constant used in Manning-Chezy equation
OC	percentage of organic carbon in SPM
R	river input of PCB
S_d	amount of SPM settling in mg/L
S_d'	loss of particulate PCB due to settling
U, V	depth averaged velocity components at x, y directions
\vec{U}	vector linear velocity of the water mass
W_s	settling speed in mm/sec calculated following Sternberg's scheme
(x, y, z)	Cartesian coordinates
Δt	length of the time step
Δ_{w-p}	amount of PCB adsorption in ng/L
Φ	overall mass discharge across a designated cross section
ε	amount of resuspension in mg/L
ε'	addition of particulate PCB due to sediment resuspension
λ	biodegradation/chemical transformation rate constant (s^{-1})
ρ	depth averaged water density
ρ_0	reference density of water
τ_{cc}	critical shear stress for sediment resuspension
τ_d	critical bottom shear stress for sediment settling
τ_x^w, τ_y^w	specific wind stress
τ_x^b, τ_y^b	bottom shear stresses
ξ	free-surface above a reference horizontal plane (MLLW)
∇	$\nabla = i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y}$ is a vector operator in x-y plane

In the model, a series of n values were assigned for computation cells of different depth (Wang *et al.* 1998). With appropriate boundary and initial conditions, Equations 1 - 6 constitute a well-posed initial-boundary value problem whose solution describes the depth-averaged circulation in a tidal basin.

Particle dynamics submodel

The particle dynamic submodel in the integrated model simulates processes of resuspension and settling of SPM. In the water column, SPM was treated as an aqueous chemical species. For SPM, the source and sink terms in Equation 4 became resuspension and settling, respectively:

$$\Sigma(l_i) = \varepsilon_i \quad (8a)$$

$$\Sigma(O_i) = S_{d,i} \quad (8b)$$

where the subscript i denotes the particle size group, ε is the amount of particles resuspended during each time period Dt in mg/L; S_d is the amount of settled particles during Dt in mg/L (Table 1). In most cases, SPM concentrations were generally low enough (<10 mg/L) that their effect on the water density ($<10^{-5}$) can be neglected. As the computation of terms other than ε and S_d is carried out by the hydrodynamic model, particle dynamics simulation is simplified to modeling sediment resuspension and settling. Following the scheme proposed by Partheniades (1965), sediment resuspension for the i -th group can be determined by the relationship between the bottom shear stress τ_b and critical shear stress for erosion τ_{ce} :

$$\varepsilon_i = \frac{M}{(h + \zeta)} \left(\frac{\tau_b}{\tau_{ce,i}} - 1 \right) \quad \text{if } \tau_b > \tau_{ce,i} \quad (9a)$$

$$\varepsilon_i = 0 \quad \text{if } \tau_b < \tau_{ce,i} \quad (9b)$$

where M is an empirical constant (1.0×10^{-4} mg/L), ζ is an empirical parameter for particle species i . The determination of values of $\tau_{ce,i}$ can only be carried out in the model calibration. The particle settling parameter, S_d , is calculated using McDonald and Cheng (1994):

$$S_{d,i} = -\frac{2W_{s,i}}{h + \xi} C_i \left(1 - \frac{\tau_b}{\tau_{cd,i}} \right) \quad \text{if } \tau_b < \tau_{cd,i} \quad (10a)$$

$$S_{d,i} = 0 \quad \text{if } \tau_b > \tau_{cd,i} \quad (10b)$$

where $\tau_{cd,i}$ is the critical bottom shear stress for deposition for the i th particle species, which is a

threshold bottom shear stress allowing sediment to deposit on bed. Like $\tau_{ce,i}$, $\tau_{cd,i}$ will also be determined in model calibration; $W_{s,i}$ is the settling velocity (mm/s) calculated following the method of Sternberg *et al.* (1999) as follows:

$$W_{s,i} = 0.0002 D_i^{1.54} \quad (11)$$

where D_i is the diameter of the i -th particle species in μm .

The success of the integrated modeling is dependent heavily on the simulation of particle dynamics, which is the crucial link between hydrodynamic model and geochemical model. This is also a complicated issue in that it requires quantification of many empirical constants through testing and calibration. As stated above, the equations for resuspension and settling of particles are for two specific particle sizes only. If a more robust particle dynamic modeling is desired, additional particle sizes should be integrated into the model. However, the calibration of such model would be challenging due to the requirement of a large amount of observational data on particle sizes as well as characterizations of each size group (e.g., total organic carbon, density, etc.). At the same time, the empirical parameters in Equations 9, 10 and 11 may need to be calibrated individually for each size group. As a result, a balance needs to be struck between model performance and simplicity.

Geochemical submodel

The geochemical submodel simulates the transport and fate of chemical species with hydrodynamic and particle dynamic processes. It was designed to simulate the transport and geochemical behavior of non-conservative, hydrophobic chemicals. Following the general form of the transport equation (Equation 4), the source and sink terms for the chemical species in dissolved and particulate phases are (see table 1 for definitions of symbols):

Dissolved phase:

$$\Sigma(I_{w,i}) + \Sigma(O_{w,i}) = -\lambda C_{w,i} - \Delta_{w-p} + A_{w,i} \quad (12)$$

Particulate phase:

$$\Sigma(I_{p,i}) + \Sigma(O_{p,i}) = -\lambda C_{p,i} + \Delta_{w-p} + A_{p,i} + \varepsilon' - S_d' \quad (13)$$

Equations 12 and 13 indicate that the capabilities of the chemical submodel include, but are not limited to, the following processes: biodegradation/chemical transformation, adsorption/desorption, atmospheric input, and input and output due to particle resuspension and settling. Obviously, more source and sink terms could be added to accommodate chemicals that are subject to corresponding processes; for conservative chemicals there will be no source and sink terms.

Finally, the net flux of the i -th chemical species Φ_i across any given cross section in the model domain can be calculated using Equation 14.

$$\Phi_i = \sum_{j=1}^N \left\{ \left[\sum_{k=1}^M \bar{U}(k) * dy * H(k) * C_i(k) \right] * \Delta t_j \right\} \quad (14)$$

APPLICATION OF THE INTEGRATED MODEL IN SAN DIEGO BAY

The integrated geochemical and hydrodynamic model was applied in a study of polychlorinated biphenyls (PCBs) in San Diego Bay (SDB), California, a semi-closed embayment on the southwestern corner of California near the US-Mexican border (Figure 1). It covers an area of about 4.1×10^7 m² at mean lower low water with an average depth of about 6.5 m (Chadwick *et al.* 1999). In general, north SDB is narrow and deep, and south SDB is broad and shallow with a large stretch of intertidal mudflat at the southern end. It is a typical low-inflow estuary with an annual precipitation of approximately 25 cm and excess evaporation of up to 160 cm in dry season. The semidiurnal tides in the bay have an average range of 1.7 m with maximum tidal amplitudes of about 3 m (Chadwick *et al.* 1999). Bordered by four cities, including the City of San Diego with an estimated total population of 1.2 million, SDB is used by a large number of recreational, commercial, and naval facilities. Heavy commercial and military shipping activities, as well as surface runoff draining densely populated areas, have resulted in highly elevated levels of organic contaminants and metals in sediments and biota (Chadwick *et al.* 1999, Chadwick *et al.* 2004, Zeng *et al.* 2002). Of particular concern to the environmental management community is the widespread distribution of PCBs in sediments and biota within SDB. These studies implicate the sediments of historical ‘hot spots’ as the main source of PCBs in the water column of SDB (Chadwick *et al.* 1999, Fairey *et al.* 1998, McCain *et al.* 1992, Noblet 2002, SDBI-

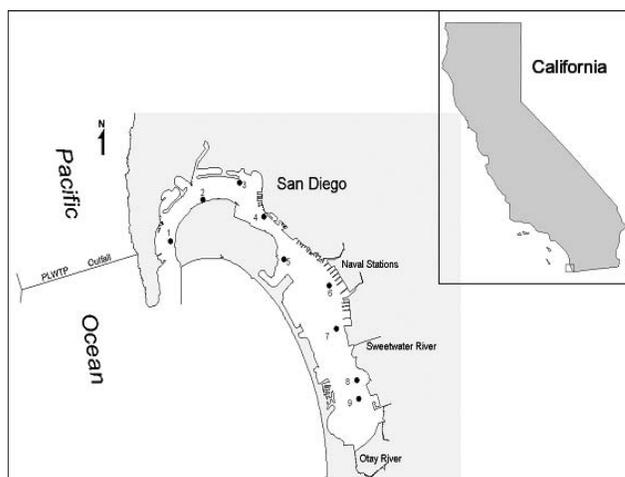


Figure 1. Map of San Diego Bay indicating sampling locations.

WQP 1994, Zeng *et al.* 2002). Sediment-bound PCBs can be released to the water column through sediment-water interaction and during sediment resuspension. Subsequently, PCBs in the water column are then transported to the open ocean through tidal exchange, which also brings cleaner water from the open ocean. We measured concentrations of individual PCB congeners at stations 1 - 9 (Figure 1) during summer 1999 and winter 2000 (Zeng *et al.* 2002; data are presented in Table 2).

Due to tidal exchange, the average residence time for waters within SDB is estimated to be only 11 days and as short as 1 day at the bay mouth (Chadwick *et al.* 2004, Largier 1995). There are large variations in hydrographical conditions, as well as in the concentrations of many environmentally significant chemicals due to vigorous tidal exchange. As a result, it is not sufficient to merely obtain information about these chemicals, spatial distributions, or ‘snap shots’. On the other hand, comprehensive investigations involving time-series observations and measurements throughout the study area are often too costly to be practicable. For example, tidal variations in SDB consist of semidiurnal, biweekly, and six-month components. As a result, the observation data need extrapolation and interpolation for both spatial and temporal scales. However, lack of observational data in some areas makes extrapolation or interpolation difficult.

Based on the above considerations, the previously described integrated model was used. The hydrodynamic submodel had been calibrated and verified in SDB (Wang *et al.* 1998). In order to run the model efficiently using personal computers for long-

Table 2. Observed concentrations of PCB congeners (ng/L) in SDB during summer 1999 sampling season.

Congener	logKow*	1-1m	1-5m	2-1m	3-1m	3-5m	4-1m	4-5m	5-1m	5-5m	6-1m	6-5m	8-1m	8-5m	9-1m	average
18	5.24	0.0076	nd	0.0111	0.0174	0.0257	0.0136	0.0175	0.0107	0.0113	0.0142	0.0121	nd	0.0119	nd	0.0139
50	5.63	nd	nd	nd	nd	0.0182	nd	0								
28	5.67	0.0152	nd	0.0288	0.0412	0.049	0.0295	0.0428	0.0266	0.0257	0.0209	0.0288	0.025	0.022	0.0294	0.0296
52	5.84	0.0136	0.0544	0.0237	0.0423	0.065	0.0425	0.0432	0.0367	0.0388	0.0347	0.0435	0.0316	0.0334	0.0272	0.0379
44	5.75	nd	nd	0.0124	0.0222	0.0328	0.0196	0.0165	0.0178	0.0169	0.0136	0.0171	0.0133	0.0153	nd	0.018
66	6.2	0.0094	nd	0.0172	0.028	0.0368	0.0261	0.0239	0.0255	0.0234	0.0185	0.0271	0.0151	0.015	nd	0.0222
101	6.38	0.0115	nd	0.0195	0.0329	0.043	0.035	0.0278	0.0325	0.0321	0.0311	0.042	0.0254	0.0221	0.0162	0.0285
87	6.29	nd	nd	0.0055	0.0103	nd	0.0115	nd	0.0093	0.0081	0.0084	0.0112			nd	0.0092
118	6.74	nd	nd	0.0154	0.0208	0.0272	0.0231	0.0176	0.0207	0.0161	0.0155	0.0219	0.015	0.0119	nd	0.0187
153	6.92	0.0078	nd	0.0145	0.0205	0.0195	0.0229	0.0191	0.0218	0.0156	0.0172	0.0229	0.0143	0.0145	nd	0.0175
105	6.65	nd	nd	0.0079	nd	nd	0.008	nd	0.0066	nd	nd	nd	nd	nd	nd	0.0075
138	6.83	nd	nd	0.0149	0.0121	0.0142	0.0134	0.012	0.0149	0.0096	0.0105	0.0169	nd	nd	nd	0.0132
187	7.17	nd	0.0052	nd	nd	nd	nd	nd	nd	0.0052						
180	7.36	nd	0.005	nd	nd	nd	nd	nd	nd	0.005						
total	0.065	0.054	0.171	0.248	0.331	0.245	0.22	0.233	0.198	0.184	0.244	0.14	0.146	0.14		
SPM(mg/L)	4.49		3.26	3.05	3.69	3.46		1.28	1.66	1.36	1.9	5.1	5.35	8.44		
TOC	2.34		3.9	5.03	5.75	3.22		3.87	4.18	5.16	4.01	2.7	2.85	2.89		

nd: not detected

*: Based on Hawker and Connell (1988)

term simulations (>100 days), the grid size was changed to 150'200 m from the original 50'50 m. The length of time step was also optimized to 3 minutes per step to achieve the most efficient simulations for the revised grid size without affecting the numerical stability of the model. An evaporation function was added to the original model to extract freshwater from SDB at an average rate of 160 cm/yr (Chadwick *et al.* 1999). The salinity values and other chemical species in the water column were adjusted accordingly due to evaporation.

In the particle dynamic submodel for SDB, two particle sizes of 2 and 20 μm were used to represent clay and fine silt, respectively. Due to the lack of a complete dataset of sediment sizes, this simplified treatment of suspended particles was necessary to achieve a realistic calibration of the modeling of particle dynamics. The use of only fine particles also corresponds to Equations 9 and 10, which were based on the investigations of cohesive muddy sediments in shallow environments (Christiansen *et al.* 2000, Lumborg and Windelin 2003, Martin and McCutcheon 1999, Partheniades 1965, Taki 2001). Lastly, compared to coarse particles, fine particles are more closely associated with organic carbon in both water column (Chadwick *et al.* 1999), as well as surface sediments (K. Richter, personal communications). Because PCBs interact only with organic portion of the fine particles, the simplified treatment of particle sizes is not expected to significantly affect model performance.

Because the time scale of the simulation (within one year) is considerably shorter than that of PCB biodegradation, the λC terms in Equations 12 and 13 were neglected in the present study. In addition, the river and atmospheric inputs of PCBs are deemed negligible (Chadwick *et al.* 1999). The governing equations for geochemical submodel (Equations 12 and 13) can be simplified to:

Dissolved Phase

$$\Sigma(I_{w,i}) + \Sigma(O_{w,i}) = -\Delta_{w-p} \quad (15)$$

Particulate Phase

$$\Sigma(I_{p,i}) + \Sigma(O_{p,i}) = \Delta_{w-p} + e' - S'_d \quad (16)$$

The central part of the simulation was the term Δ_{w-p} , i.e., the partitioning of the chemicals between

dissolved and particulate phases. If the partitioning of PCBs between the dissolved and particulate phases is assumed to be at equilibrium, C_w and C_p are related to each other by the organic carbon normalized particle-water partition coefficient (K_{oc}):

$$K_{oc} = \frac{C_p}{C_{w,e} \times OC} = \frac{C_{oc}}{C_{w,e}} \quad (17)$$

where $C_{w,e}$ is the dissolved PCB concentration at equilibrium with the particulate phase (Table 2); C_{oc} ($= C_p/OC$) is the organic carbon normalized PCB concentration in the particulate phase; and OC is the content of organic carbon in the particulate phase. Equation 17 indicates that if the TSS concentration changes due to resuspension/settling, the concentrations of PCBs in both the dissolved and particulate phases will change accordingly to maintain a constant K_{oc} . At the same time, the total amounts of PCBs are conserved before and after the re-partitioning.

Practically, K_{oc} is not readily available, but it can be associated with the commonly available octanol-water partition coefficient, K_{ow} by

$$\log K_{oc} = a \log K_{ow} + b \quad (18)$$

with a and b determined experimentally.

Boundary and initial conditions

The hydrodynamic submodel is driven by tides defined by a tidal function on the open boundaries (north, west, and south) of the model domain (Cheng *et al.* 1993, Wang *et al.* 1998). The values of the harmonic constants defining the boundary conditions were determined through an extensive calibration and verification using data collected in 1983 and 1992 to 1996 (Wang *et al.* 1998).

In the particle dynamics submodel, the SPM concentrations at the open boundaries are set to 1 mg/L, which essentially represents the background values observed previously (Chadwick *et al.* 1999). The initial SPM concentrations for non-boundary cells are assumed to be zero. Of the two particle sizes considered in the present study, only the 2-mm particles are assumed to be present at the open boundaries. The initial salinity value is set to 33.5 throughout the model domain based on field measurements (Chadwick *et al.* 1999, Peng 2004). This value is always maintained at the open boundaries. After the model spin-up, salinity varies with the mass balance of water and salt, and SPM is produced

dynamically until a quasi-equilibrium state is eventually reached. These aspects will be discussed in the following section. Initial PCB concentrations are set to zero at open boundaries and at all water cells except for those ‘hot spots’, which were assumed to have fixed concentrations of PCBs.

Random inputs of freshwater and particulate matter

As an urban ocean environment, SDB is heavily influenced by anthropogenic sources, including shipping activities and storm water runoff that input large amounts of particulate matter into the water column. Runoff also brings a fair amount of freshwater into the bay. The quantitative levels and randomness of these inputs will need to be modeled adequately in the simulation.

To simulate the effects of shipping activities, the data from a two-month survey of the suspended particles revoked by US Navy warships were used (Chadwick *et al.* 1999). The randomness of these shipping events was controlled by a series of random numbers generated in each time step. River inputs of particulate matter and freshwater were simulated for two major rivers, Sweetwater River and Otay River (Figure 1). Based on SDB’s drainage area (970 km²), average rainfall (25 cm/yr), and an assumed average land retention factor (70%), the amount of freshwater flow into SDB could be estimated. Computer-generated random numbers were used to simulate major, average, and minor rainfalls with 5, 2.5, and 1 cm of precipitation, respectively. The frequency of these precipitation events was prescribed by the random numbers such that on average 25 cm of precipitation was produced each year. The duration of each precipitation event was assumed to be 12 hours. Finally, the SPM content of river inflow was 60 mg/L, a number consistent with a previous measurement (Chadwick *et al.* 1999).

MODEL CALIBRATION

The calibration and validation of the hydrodynamic model in SDB were already carried out with satisfactory results (Cheng *et al.* 1993, Wang *et al.* 1998), so they are not repeated here. The calibration and validation of the geochemical and particle dynamics sub-model were based on long-term simulation that lasted 104 days and ended in mid June of 1999 when the first field sampling was conducted. The concentrations of the chemical species were found to have reached dynamic equilibrium within 15 days.

Freshwater input calibration

Salinity is an excellent indicator for the model calibration because it is a conservative chemical tracer. It provides a strong constraint upon the amount of freshwater input from rivers, thus ensuring a good simulation of the dilution or accumulation of other chemicals in the water column in SDB. Without proper calibration of the freshwater input, the model would produce severe ‘pumping’ effects for some man-made chemicals in south SDB, such as sustained high concentrations of PCBs that were inconsistent with previous observation (Zeng *et al.* 2002).

Freshwater inputs from Sweetwater River and Otay River (Figure 1) were difficult to estimate because of sporadic surface flow and constraints exerted by dams during wet weather season (Figure 2). On the other hand, initial model calibrations indicated that the actual amount of freshwater input was a crucial parameter for the integrated model, especially in the simulation of chemical species. In SDB, low salinity and slightly hypersaline conditions are typical during the wet and dry weather seasons, respectively (Chadwick *et al.* 1999, Largier *et al.* 1997). During two sampling cruises in summer 1999 (dry weather season) and winter 2000 (wet weather season), the measured salinities were in a narrow range of 32 - 35. Higher (up to 37) and lower (~25) salinity values have also been reported during a prolonged dry period and after major precipitation, respectively (Chadwick *et al.* 1999, Largier *et al.* 1997). The calibration of the model in terms of freshwater inflow and salinity pattern requires long-term (at least 3 months) simulations due to the slow evaporation rate compared to the

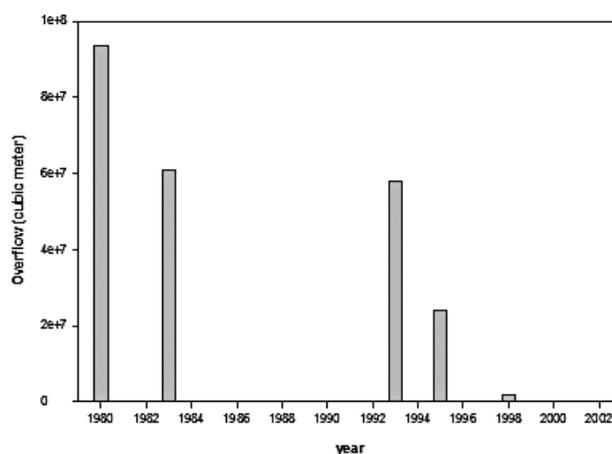


Figure 2. Records of flow in acre-feet over Sweetwater Dam since 1980 (courtesy of Michael Garrod, Sweetwater Authority).

volume of SDB. The results consistently showed that the amount of freshwater input to SDB was much smaller than the assumed retention factor of 70%. The difference reflects the restriction of freshwater inflow by dams. Simulations employing a retention factor of 70% yielded lower salinity values in south SDB than other parts of SDB (Figure 3), inconsistent with observed patterns (Chadwick *et al.* 1999, Largier *et al.* 1997, Peng 2004). In contrast, calibrations with a retention factor of 85% resulted in salinity values compatible with the observation, as shown in Figure 4.

SPM calibration

As stated previously, the amount of sediment resuspended in the water column due to tidal currents can be predicted via the particle dynamics submodel. The critical bottom shear stress for erosion, τ_{ce} , and critical shear stress for deposition, τ_{cd} , are two important empirical parameters used to describe resuspension and settling of particles, respectively (Equations 9 and 10). Previous studies on environments similar to SDB obtained τ_{ce} in the range of 0.1 - 0.5 N/m². Typically, the τ_{cd} value is approximately 0.01N/m² (Christiansen *et al.* 2000, Krone 1962, Lumborg and Windelin 2003, Partheniades 1965, Sternberg *et al.* 1999, Torfs *et al.* 2001, van Rijn 1989).

Human-induced sediment resuspension complicated the calibration process in SDB. If shipping-induced resuspension were not considered, calibration runs showed that tidal currents would

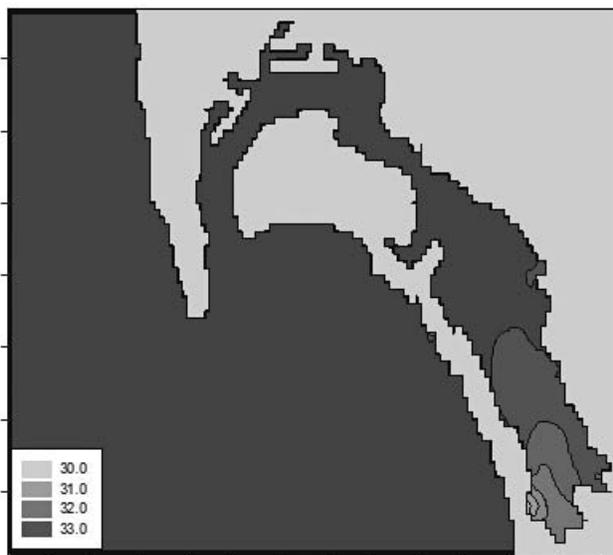


Figure 3. Simulated salinity distribution in SDB with a retention ratio of 70%.

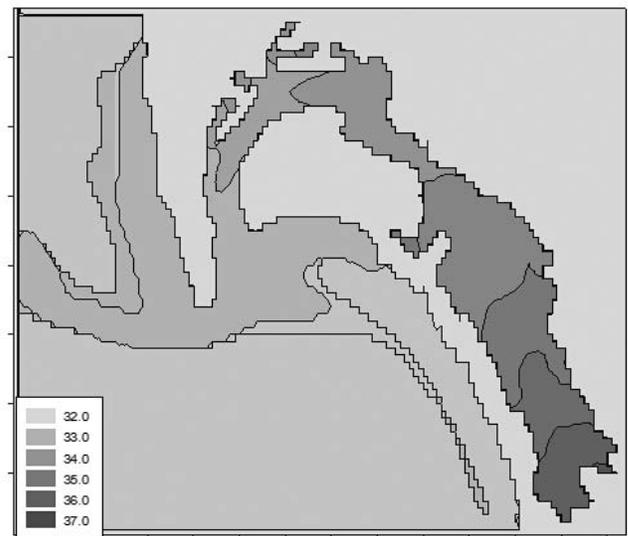


Figure 4. Simulated salinity distribution in SDB using a retention ratio of 85%.

produce less than one-half of the observed SPM concentrations in the water column. Therefore, the impact of shipping events had to be adequately simulated in order to reproduce the observed SPM patterns. The optimal values of τ_{ce} determined from fitting the predicted and observed TSS values were 0.1 and 0.12 N/m² for the particle sizes of 2 and 20 μ m, respectively. Similarly, the optimal values of τ_{cd} for the particle sizes of 2 and 20 μ m were 0.02 and 0.05 N/m², respectively.

The model predicted SPM concentrations in general agreement with the measured values (Figure 5). There is a large range for observed values, presumably due to patchiness of suspended sediment distribution. The simulated SPM levels generally fall within the range of the observed values, with a small (5.9%) difference between the average values. Hence, the simulation of the TSS distribution in the water column of SDB by the model was deemed satisfactory.

PCB calibration

Previous studies by US Navy and other agencies of sediment PCB contamination around SDB showed that highest contamination levels are centered at the submarine base near the eastern end of Coronado Bridge, and near the Cruise Ship Terminals (Chadwick *et al.* 1999, SDSC 2004), indicating that they are probably the chief sources of PCBs in SDB. Sediment PCB concentrations at other locations within SDB were all near or below detection limit. There

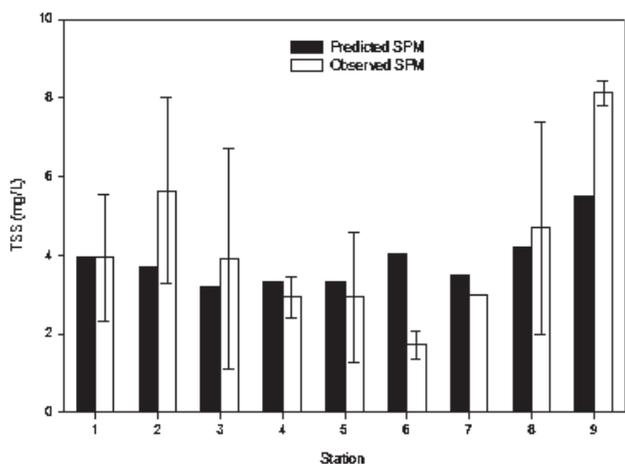


Figure 5. Comparison between predicted and observed concentrations of SPM (mg/L); vertical bars indicate uncertainties in field data.

has been evidence that persistent organic contaminants can diffuse into the water column, thus becoming the chief source of the contaminants when the sediment concentration of this contaminant is high (Zeng *et al.* 1999). This could probably be the case in SDB, where sediments at some ‘hot spots’ with very high concentrations (>1500 ppb) of PCBs provide a continuous source of PCB into the overlying water column. Figure 6 shows a close resemblance between the ‘fingerprints’ of PCB congeners concentration in water column and sediment associated with ‘hot spots’. More heavily chlorinated PCB congeners (those with higher K_{ow} values) tend to bind to sediment, as shown by a slight difference in the trend lines in Figure 6. Therefore, it is reasonable to assume that these ‘hot spots’ are the sources of dissolved phase PCBs in SDB waters. In the model, the input of PCBs is simulated by defining boundary conditions at certain locations that are known to have high PCB concentrations in sediments. Because the sediment-water exchange of PCBs should be a slow process, PCB concentrations in the water column at ‘hot spots’ should be relatively constant, warranting fixed value boundary conditions for the model.

The initial conditions of PCB concentrations in the particulate phase are not set. Rather, they are simulated dynamically based on SPM levels, TOC and dissolved phase PCBs in the scheme described by Equations 15 - 18. The simulation of PCBs (especially the ratio between PCB concentrations in the dissolved and particulate phases) will be affected by the choice of parameters related to the PCB-particle interactions, or a and b in Equation 18. Empirical

relationship given by Karickhoff *et al.* (1979; $a = 1.0$, $b = -0.21$) was found to fit the observation data better, but significant adjustment was needed in order to fit predictions with observation in terms of the dissolved and particulate phase at the same time. The best result was obtained when $b = -0.51$ was used. On the other hand, the empirical relationship given by Schwarzenbach and Westall (1981; $a = 0.72$, $b = 0.49$) was apparently not supported by our model. Using the latter scheme, there are significant overestimates for the concentrations of dissolved phase PCBs, and underestimates for the particulate phase. There have been reports (Cornelissen and Gustafsson 2005, Cornelissen *et al.* 2005a, Cornelissen *et al.* 2005b, Sobek *et al.* 2004) that elemental carbon (black carbon, char, soot, etc.) in sediment could affect the sorption property such that the linear relationship between K_{oc} and K_{ow} could be altered significantly. However, our previous study (Zeng *et al.* 2002) did not find effects of elemental carbon on the sorption characteristics of PCBs; thus, elemental carbon was not considered in the model. It is cautioned that when this model is applied to other regions, effects of elemental carbon on hydrophobic chemicals need to be carefully evaluated.

When $a = 1.0$ and $b = -0.51$ were used in the long-term calibration (~100 days), optimal results were obtained for both dissolved and particulate PCBs (Figures 7a and 7b). The predicted spatial distributions of PCBs in the dissolved and particulate phases are shown in Figure 8a and 8b. On average, the differences between predicted and observed concentrations are within 10% and 50% for the dissolved and particulate phase, respectively. If averaged over all stations, the differences between the concentrations of

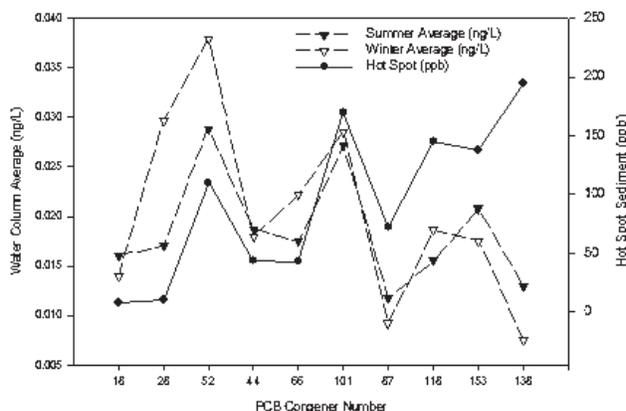


Figure 6. Comparison between concentrations of dissolved PCB congeners in water columns and sediments.

the predicted and observed PCBs in both phases are within 5%. Larger discrepancies for particle phase PCBs were probably due to transient changes in SPM concentrations caused by natural and man-made sediment resuspension. Freshly resuspended particles may not reach equilibrium with the ambient seawater due to insufficient time allotment. Relatively large analytical uncertainties for PCB concentrations, especially for the particulate phase due to their low concentrations, may also have played a role. Uncertainties of the exact locations of the PCB ‘hot spots’ can also contribute to the differences. For example, the predicted PCB concentrations for south SDB in both phases tend to be lower than observed values, suggesting that there might be additional ‘hot spots’ in the south bay that were not fully accounted for in the model. Overall, the calibration of PCBs in both phases is deemed satisfactory and will be applied in the subsequent investigations.

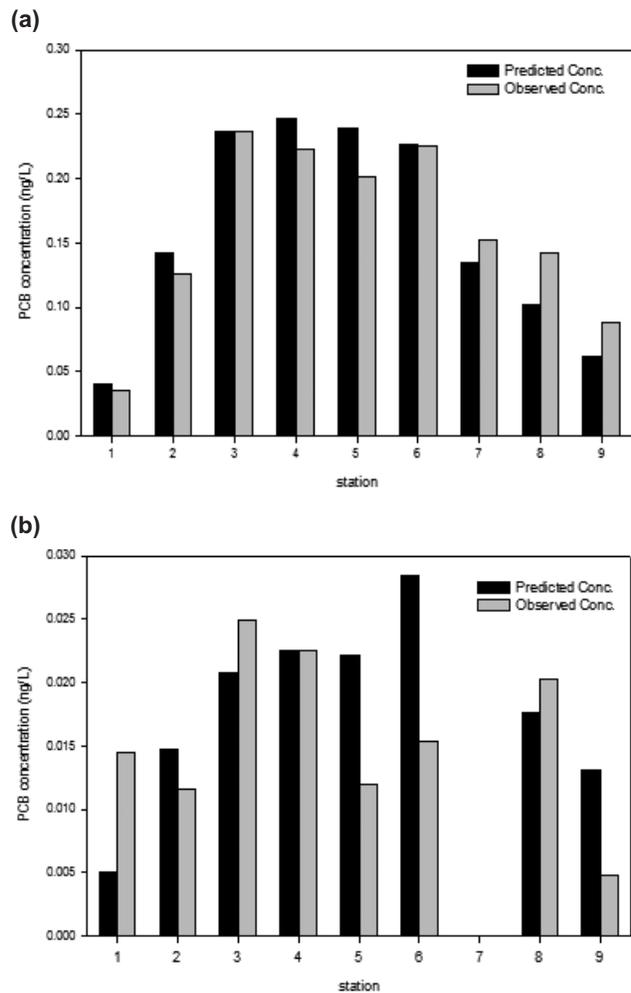


Figure 7. Comparison between predicted (two-day average) and measured PCB concentrations for dissolved phase(a) and particulate phase (b).

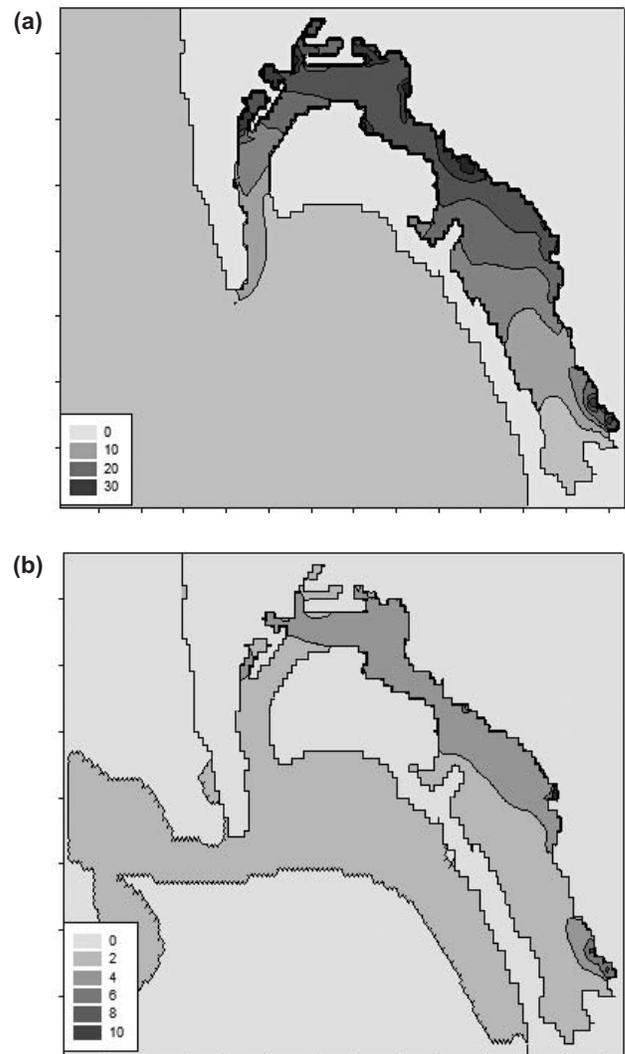


Figure 8. Simulated steady-state distributions of PCBs for dissolved phase (a) and particulate phase (b).

MODEL APPLICATIONS

Sediment transport simulation

As stated above, SPM was treated as a chemical species once its sources and sinks were properly defined by particle dynamics. Therefore, Equation 14 can be used to calculate the export of sediment out of SDB when the cross section is set at the bay mouth. The result (Figure 9) shows that the annual net transport of sediment (a combination of particle sizes of 2 and 20 μm) from SDB to the ocean is 4.72×10^7 kg/yr. It is interesting to note that the amount of sediment input from rivers is only 2.25×10^7 kg/yr. The discrepancy is a clear indication that river input contributes only part of the suspended fine particles in SDB. A large amount of fine particles are either input from non-point sources such as storm runoff, or produced in situ from sediment

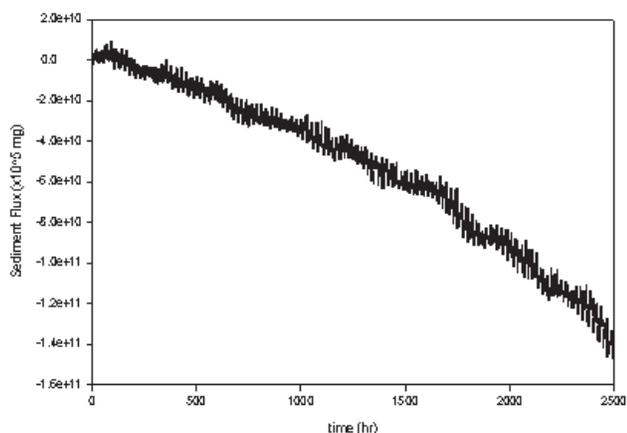


Figure 9. Simulated mass discharge of suspended sediments (including both the 2- and 20- μm particle sizes) out of SDB.

resuspension due to human activities and tidal currents. The excess sediment loss over input to SDB does not necessarily suggest that SDB is no longer accumulating sediment as only fine particles are considered in the model. Relatively large ranges in the measurement of SPM concentrations might also be a factor in the apparent sediment imbalance. The discrepancy may be compensated by coarser sediments, which are transported by rivers and storm runoff into SDB but could not be carried out to the open ocean. A comprehensive, long term sediment transport observation campaign for sediment transport is needed in order to provide better constraints for the integrated model; however, this type of comparison is beyond the scope of the current study.

Transport and fate of PCBs

Successful calibration of PCB concentrations in both the dissolved and particulate phases lent confidence to the investigation of the transport and fate of PCBs in SDB. Based on Equation 14, the losses of PCBs and particulate matter across the SDB mouth were calculated. Figures 10a and 10b show the net losses of PCBs and particulate matter, which amount to 3.50 kg of PCBs each year in the dissolved form and 0.35 kg in the particulate form. The total loss of PCBs of 3.85 kg is significantly higher than the previous estimate of ~ 1.0 kg (Zeng *et al.* 2002) which was based on a residence time of 11.8 days and about 50% reflux of bay water during flooding tides (i.e., about 50% of water flowing into SDB is ‘old’ SDB water) according to Largier (1995). The difference between these two estimates could come from the following sources: (a) overestimated residence time and reflux ratio by Largier (1995); (b) the use

of average concentration of PCBs in the previous calculation (Zeng *et al.* 2002). In reality, north-central SDB sustains more vigorous tidal exchange and has relatively higher PCB concentrations. In a dynamic modeling approach as employed in this study, the details of PCB distribution and its transient variations were included implicitly in the numerical model. Therefore, the present calculation should be a better estimate.

DISCUSSION

The present study represents an attempt to link hydrodynamics with the resuspension, transport and deposition of suspended solids, enabling an investigation of the transport and fate of environmentally significant chemicals in dynamic coastal environments. This study found quantitative investigations based on the numerical model to be superior to the semi-quantitative estimates based on steady-state assumptions. The integrated model is the first of its kind that explicitly links hydrodynamics, particle dynamics, and geochemistry to study environmental

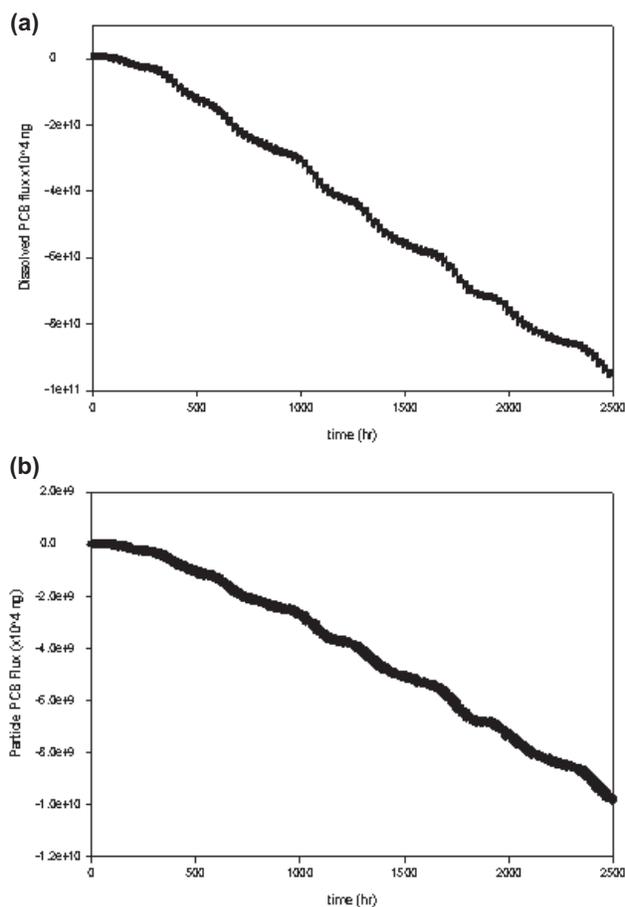


Figure 10. Simulated mass discharge of PCBs out of SDB for dissolved phase (a) and particulate phase (b).

issues. It also has the potentials to study many other chemical species of environmental significance. Notably, that the model has been applied to naturally occurring, particle reactive radionuclides ^{210}Pb and ^{234}Th in SDB (Peng 2004). The model was calibrated with observed concentrations of suspended particles and radionuclides, which provided strong constraints for the geochemical submodel because their natural occurrences are better defined than man-made contaminants. The capability of modeling a diverse range of chemicals validate the importance of the integrated model in the studies of geochemical cycles of non-conservative chemicals in dynamic coastal oceans.

A properly calibrated numerical model can help extrapolate and interpolate field data to areas not sampled, thereby facilitating the data interpretation and visualization by providing a complete and dynamic characterization of the study area. It can also derive secondary information such as the water fluxes, dissolved chemical species, and SPM, in addition to forecasting and nowcasting oceanic conditions and chemical distributions. The model can also provide important insights into ‘what-if’ scenarios. For example, what environmental consequences would be if certain events (e.g. oil spills, storm runoffs) take place.

The requirement for large quantities of observational data for model setup and calibration can be a limiting factor for application of the model. In the present study, the hydrodynamic submodel of the integrated model benefits from years of extensive work (Cheng *et al.* 1993, Wang *et al.* 1998), but some components in the sediment dynamics and geochemical submodels are limited by difficulties in obtaining large quantities of data. For example, shipping-induced sediment resuspension is difficult to quantify and predict; river input is so severely affected by reservoirs that vital correlation between precipitation and freshwater input into SDB no longer exists; the number of measurements for PCBs is limited by cost and manpower. Therefore, more observational data are desired to strengthen the geochemical submodel such that applications of the integrated model can be further explored with more confidence.

The integrated geochemical and hydrodynamic model developed in the present study can be applied to other chemicals and in other study areas. The bathymetry of the study area needs to be obtained, so are the tidal function and large-scale oceanic circula-

tion patterns, which are necessary boundary conditions for the hydrodynamic submodel. Grid dimensions and length of time step for integration need to be optimized for computation efficiency and accuracy. The particle dynamic and geochemical submodels are not as site-specific as the hydrodynamic submodel. However, careful calibrations relevant to a specific location (e.g., human-induced sediment resuspension, bottom sediment type, etc.) are indispensable. Special attention is needed to treat the interactions between chemical species and SPM for calibrations involving chemicals that are associated with SPM or components of SPM such as organic carbon or elemental carbon. Observations should also be made on SPM distribution and variation in order to determine the site-specific empirical parameters (i.e., Equations 9, 10, and 11). Long-term calibrations are needed to validate the submodels before the integrated model can be applied.

The present study has provided a framework for the study of environmental issues in tidal coastal oceans and estuaries based on an explicit link between hydrodynamics, particle dynamics, and chemistry of organic and inorganic chemicals. Despite its limitations, it represents an improvement from traditional geochemical studies that are based on steady state assumptions. Moreover, the modeling approach facilitates visualization and integration of observation results such that inventories and fluxes of chemical species (including SPM) can be quantitatively studied, making this approach a useful tool for the study of transport and fate of environmental pollutants in the coastal seas and estuaries.

LITERATURE CITED

Chadwick, B., J. Leather, K. Richter, S. Apitz, D. Lapota, D. Duckworth, C. Katz, V. Kirtay, B. Davidson, A. Patterson, P. Wang, S. Curtis, G. Key, S. Steinert, G. Rosen, M. Caballero, J. Groves, G. Koon, A. Valkirs, K. Meyers-Schulte, M. Stallard, S. Clawson, R. Streib Montee, D. Sutton, L. Skinner, J. Germano and R. Cheng. 1999. Sediment quality characterization. Final Summary Report. Space and Naval Warfare Systems Command (SPAWAR). San Diego, CA.

Chadwick, D.B., A. Zirino, I. Rivera-Duarte, C.N. Katz and A.C. Blake. 2004. Modeling the mass balance and fate of copper in San Diego Bay. *Limnology and Oceanography* 49:355-366.

- Cheng, R.T. and V. Casulli. 2001. Evaluation of the UnTRIM model for 3-D tidal circulation. pp. 628-642 in: 7th International Conference on Estuarine and Coastal Modeling Proceedings. St. Petersburg, FL.
- Cheng, R.T., V. Casulli and J.W. Gartner. 1993. Tidal, residual, intertidal mudflat (TRIM) model and its applications to San Francisco Bay, California. *Estuarine, Coastal and Shelf Science* 36:235-280.
- Christiansen, T., P.L. Wiberg and T.G. Milligan. 2000. Flow and sediment transport of a tidal salt marsh surface. *Estuarine, Coastal and Shelf Science* 50:315-331.
- Cornelissen, G. and O. Gustafsson. 2005. Importance of unburned coal carbon, black carbon, and amorphous organic carbon to phenanthrene sorption in sediments. *Environmental Sciences and Technology* 39:764-769.
- Cornelissen, G., O. Gustafsson, T.D. Bucheli, M.T.O. Jonker, A.A. Koelmans and P.C.M. van Noort. 2005a. Extensive sorption of organic compounds to black carbon, coal, and kerogen in sediments and soil: mechanisms and consequences for distribution, bioaccumulation, and biodegradation. *Environmental Sciences and Technology* 39:6881-6895.
- Cornelissen, G., J. Haftka, J. Parsons and O. Gustafsson. 2005b. Sorption to black carbon of organic compounds with varying polarity and planarity. *Environmental Sciences and Technology* 39:3688-3694.
- Fairey, R., C. Roberts, M. Jacobi, S. Lamerdin, R. Clark, J. Downing, E. Long, J. Hunt, B. Anderson, J. Newman, R. Tjeerdema, M. Stephenson and C. Wilson. 1998. Assessment of sediment toxicity and chemical concentrations in the San Diego Bay region, California, USA. *Environmental Toxicology and Chemistry* 17:1570-1581.
- James, I.D. 2002. Modeling pollution dispersion, the ecosystem and water quality in coastal waters: a review. *Environmental Modeling and Software* 17:363-385.
- Karickhoff, S.W., S. David and A. Trudy. 1979. Sorption of hydrophobic pollutants on natural sediments. *Water Research* 13:241-248.
- Krone, B.R. 1962. Flume studies of the transport of sediment in estuarial shoaling processes, Hydraulic Engineering Laboratory. University of California Press. Berkeley, CA.
- Largier, J.L. 1995. San Diego Bay circulation: a study of the circulation of water in San Diego Bay for the purpose of assessing, monitoring and managing the transport and potential accumulation of pollutants and sediment in San Diego Bay. The California State Water Resources Control Board and the California Regional Water Quality Control Board, San Diego Region. San Diego, CA.
- Largier, J.L., J.T. Hollibaugh and S.V. Smith. 1997. Seasonally hypersaline estuaries in Mediterranean-climate regions. *Estuarine, Coastal and Shelf Science* 45:789-797.
- Lumborg, U. and A. Windelin. 2003. Hydrography and cohesive sediment modeling: application to the Romo Dyb tidal area. *Journal of Marine Systems* 38:287-303.
- Martin, J.L. and S.C. McCutcheon. 1999. Hydrodynamics and transport for water quality modeling. Lewis Publishers. Boca Raton, FL.
- McCain, B.B., S.L. Chan, M.M. Krahn, D.W. Brown, M.S. Myers, J.T. Landahl, S. Pierce, R.C. Clark Jr. and U. Varanasi. 1992. Chemical contamination and associated fish diseases in San Diego Bay. *Environmental Science and Technology* 26:725-733.
- McDonald, E.T. and R.T. Cheng. 1994. Issues related to modeling the transport of suspended sediments in northern San Francisco Bay, California. pp. 1-41 in: M.L. Spaulding et al. (eds.), 3rd International Conference on Estuarine and Coastal Modeling Proceedings. Oak Brook, IL.
- Noblet, J. 2002. Sediment chemistry in the Southern California Bight: Results from the 1998 regional monitoring study. Southern California Coastal Water Research Project. Westminster, CA.
- Partheniades, E. 1965. Erosion and deposition of cohesive soils. *Journal of the Hydraulics Division (ASCE)* 91:105-139
- Peng, J. 2004. Integrated geochemical and hydrodynamic modeling of San Diego Bay, California. PhD Dissertation, University of Southern California. Los Angeles, CA.

- San Diego Bay Interagency Water Quality Panel (SDBIWQP). 1994. San Diego Bay 1992 Annual Report. Technical Report AB 158. California State Water Resources Control Board. Sacramento, CA.
- Schwarzenbach, R.P. and J. Westall. 1981. Transport of nonpolar organic compounds from surface water to groundwater: laboratory sorption studies. *Environmental Sciences and Technology* 15:1360-1367.
- San Diego Supercomputer Center (SDSC). 2004. Environmental Data Repository of the Interagency Water Quality Panel and San Diego Supercomputer Center. <http://sdbay.sdsc.edu>.
- Sheng, P.Y., D.E. Eliason and X.-J. Chen. 1992. Modeling three-dimensional circulation and sediment transport in lakes and estuaries. pp. 109-115 in: M.L. Spaulding (ed.), 2nd International Conferences on Estuarine and Coastal Modeling Proceedings. Tampa, FL.
- Sheng, Y.P. 1996. Pollutant load reduction models for estuaries. pp. 1-15 in: M.L. Spaulding, R.T. Cheng (eds.), 4th International Conference on Estuarine and Coastal Modeling. San Diego, CA.
- Sobek, A., O. Gustafsson, S. Hajdu and U.Larsson. 2004. Particle-water partitioning of PCBs in the photic zone: a 25-month study in the open Baltic Sea. *Environmental Sciences and Technology* 38:1375-1382.
- Sternberg, R.W., I. Berhane and A.S. Ogston. 1999. Measurement of size and settling velocity of suspended aggregates on the Northern California continental shelf. *Marine Geology* 154:43-53.
- Taki, K. 2001. Critical shear stress for cohesive sediment transport. pp. 53-61 in: A.J. Mehta and W.H. McAnally (eds.), Coastal and Estuarine Fine Sediment Transport. Elsevier Science BV. St. Louis, MO.
- Torfs, H., J. Jiang and A.J. Mehta. 2001. Assessment of the erodibility of fine/coarse sediment mixtures. pp. 109-123 in: A.J. Mehta, W.H. McAnally (eds.), Coastal and Estuarine Fine Sediment Processes. Elsevier Science BV. St. Louis, MO.
- Van Rijn, L.C. 1989. Handbook-Sediment transport by currents and waves. Delft Hydraulics. Delft, Netherlands.
- Wang, P.-F., R.T. Cheng, K. Richter, E.S. Gross, D. Sutton and J.W. Gartner. 1998. Modeling tidal hydrodynamics of San Diego Bay, California. *Journal of American Water Resources Association* 34:1123-1140.
- Zeng, E.Y., J. Peng, D. Tsukada and T.-L. Ku. 2002. *In-situ* measurements of polychlorinated biphenyls in the waters of San Diego Bay, California. *Environmental Sciences and Technology* 36:4975-4980.
- Zeng, E.Y., C.C. Yu and K. Tran. 1999. *In situ* measurements of chlorinated hydrocarbons in the water column off the Palos Verdes Peninsula, California. *Environmental Science and Technology* 33:392-398.

ACKNOWLEDGEMENTS

The modeling work was made possible by the author of the original TRIM model Dr. Ralph Cheng, who offered the TRIM source code and provided insightful comments on the manuscript. Dr. Teh-Lung Ku of the University of Southern California (USC) encouraged and supported the modeling effort. We thank the crew of the research vessels Metro and Monitor II (City of San Diego) for sampling assistance in San Diego Bay. Special thanks go to Dario Diehl of SCCWRP for managing all field samplings. P.-F. Wang and K. Richter of Space and Naval Warfare System Command (SPAWAR), US Navy are appreciated for their help on the modeling effort and discussions of the manuscript. This study was funded in part by the USC Sea Grant Program, National Oceanic and Atmospheric Administration (NOAA), under Grant CE-5. The USC Sea Grant Traineeship also provided financial support for Jian Peng. during 1999-2001. Support of Eddy Y. Zeng by the "Hundred Talents" Program of the Chinese Academy of Sciences is gratefully acknowledged.