

## MODELING THE FATE AND TRANSPORT OF ORGANIC CONTAMINANTS IN LAKE ST. CLAIR

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**ABSTRACT.** Despite the rapid hydraulic turnover time of Lake St. Clair, inputs of organic contaminants to the lake are a cause for concern because of their potential long-term storage in the lake's surficial sediments. In order to understand and predict the transport and fate of organic contaminants in Lake St. Clair, a multisegment, contaminant mass balance model was developed. The model was calibrated and tested against four data sets that describe the behavior of the conservative chloride ion, and against two data sets that describe the fate and distribution of sediment-bound cesium-137. Model applications included simulations of octachlorostyrene (OCS) and polychlorinated biphenyl (PCB) dynamics in the lake. The model predicted that during 1971-83, 3.8 MT of OCS entered the lake, 2.8 MT were flushed from the system, 0.8 MT were lost due to biological degradation and volatilization, and 0.2 MT remained in the system. The model also predicted that during 1970-74, 3.4 MT of PCB entered the lake, 2.1 MT were flushed from the system, 2.2 MT were lost due to biological degradation and volatilization, and the system mass of PCB decreased from 1.9 to 1.0 MT.

**INDEX WORDS:** Mathematical models, cesium, polychlorinated biphenyls, Lake St. Clair, fate of pollutants, model studies.

### INTRODUCTION

Lake St. Clair has been described as simply a wide part of the river system that extends from the mouth of Lake Huron to the head of Lake Erie. The lake differs from the Great Lakes in that its average depth is only about 3.5 m (the next most shallow lake is Lake Erie at 19 m), and its mean hydraulic retention time is only about 8 days (the next quickest flushing lake is Lake Erie at about 2.5 years). Except for Lang *et al.* (1988) and the UGLCCS Management Committee (1988), Great Lakes mass budget calculations have generally overlooked the dynamics of nutrient and contaminant transport into and through Lake St. Clair. Despite the rapid hydraulic turnover time of the lake, documented storages of polychlorinated biphenyl (Frank *et al.* 1977, Pugsley *et al.* 1985, Oliver and Bourbonniere 1985), octachlorostyrene

(Pugsley *et al.* 1985, Oliver and Bourbonniere 1985), and heavy metals such as lead and cadmium (Munawar *et al.* 1985, Pugsley *et al.* 1988) in the lake's sediments indicate the need to understand contaminant fate and transport in Lake St. Clair. Zones of high chemical concentration that generally correspond to the distribution of fine-grain, organic-rich solids indicate the ability of the lake's sediments to retain significant amounts of particle-associated radionuclides, metals, and organic contaminants.

Retention of contaminants in the lake's sediments has potential ramifications, particularly for sediment-based foodwebs. Of particular concern is the length of time that toxic metals and organic contaminants remain in the system, and the extent to which different portions of the lake are exposed to them. The residence time and spatial distribution of these compounds in water and surficial sediments are controlled by the physical, biological, and chemical characteristics of the ecosystem and by the chemical characteristics of the compound.

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Because hydrophobic contaminants are strongly associated with particulate matter, suspended and settled sediments play a key role in determining their fate and distribution.

In order to understand and predict the transport and fate of organic contaminants in Lake St. Clair, a multisegment, contaminant mass balance model was developed, based on the Environmental Protection Agency's TOXIWASP model (Ambrose *et al.* 1983). The model was calibrated and tested against chloride data (Bell 1980) and cesium-137 data (Robbins *et al.* 1990). It was then used to understand polychlorinated biphenyl and octachlorostyrene dynamics in the lake. Here, we describe the model processes, the segmentation scheme, the physical characteristics of the lake, tracer and contaminant input data, and simulation results.

### MODEL DESCRIPTION

TOXIWASP combines the kinetic formulations in the EXposure Analysis Modeling System (EXAMS) developed by Burns *et al.* (1982), and the transport processes in the Water Analysis Simulation Program (WASP) developed by DiToro *et al.* (1983). TOXIWASP balances the difference between the mass flux into and out of a model segment or compartment with the change in mass storage within that segment or compartment, thus conserving mass over time and space. The one-dimensional mass flux approximation of the advection-dispersion equation for calculating the change in chemical mass over time is written as:

water column

$$\frac{\Delta(V_j C_j)}{\Delta t} = W_j - \Sigma \left[ -Q_{ij} C_{ij} - E_{ij} A_{ij} \left( \frac{\Delta C}{\Delta x} \right)_{ij} \right] - k_j V_j C_j + S_j \quad (1)$$

sediment layer

$$\frac{\Delta(V_j C_j)}{\Delta t} = -k_j V_j C_j - B_j A_{ij} C_j - S_j \quad (2)$$

where  $C$  is chemical concentration,  $V$  is segment volume,  $W$  is mass loading,  $Q$  is advective flow,  $E$  is the horizontal dispersion coefficient,  $A$  is cross-sectional area,  $k$  is the kinetic degradation or transformation rate,  $S$  is the net exchange of chemical from the sediment layer to the water column,  $B$  is the rate of chemical burial to the deep sediment layer,  $j$  denotes the segment number,  $i$  denotes adjacent segment numbers, and  $ij$  is the interface

between segments  $i$  and  $j$ . The exchange of chemical between the water column and sediment layer includes settling and resuspension of bound chemical and pore water diffusion of dissolved chemical.

Two state variables are included in the model: total chemical and total sediment. Sediment concentrations are controlled by advection, dispersion, mass loading, settling, and resuspension. Chemical concentrations are affected by these same processes, plus degradation, sediment-water diffusion, and burial to deep sediments. Chemical degradation includes hydrolysis, biolysis, photolysis, oxidation, and volatilization. Chemical sorption onto sediments and biota is calculated via equilibrium kinetics, using chemical-specific partition coefficients and organic carbon fractions of the sediments and biota. The transport and transformation processes are fully detailed in Ambrose *et al.* (1983), Burns *et al.* (1982), and DiToro *et al.* (1983). The complete set of differential, mass-balance equations describing contaminant and sediment dynamics were solved numerically using a forward difference Euler scheme with a time step of 2.4 h.

### Physical Parameters

Lake St. Clair has a surface area of 1,063 km<sup>2</sup> and a volume of 3.8 km<sup>3</sup>. As a result of the lake's shallowness and resident high wave energy, thermal stratification does not occur. In the model, the study area was segmented into 126 well-mixed segments: 42 water segments, 42 active sediment layer segments situated directly below the water column segments, and 42 deep sediment segments. The average segment size was about 5 km per side. The segments of the active sediment layer are characterized by continuous and event-related physical and biological mixing resulting in vertically homogeneous chemical concentrations. The segmentation scheme was based on the results of a cluster analysis performed on the available chemical, physical, biological, and contaminant data in the water column and sediments of Lake St. Clair (Rybczyk 1986). The resultant 42-segment grid (Fig. 1) was overlaid onto the 1.2-km grid of the Lake St. Clair Rigid Lid Hydrodynamic Model (Schwab and Liu 1987), which was used to generate the wind-driven, vertically averaged flow field. The hydrodynamic model flows were then summed along the larger segment interfaces of the contaminant model, yielding 75 net interface flows.

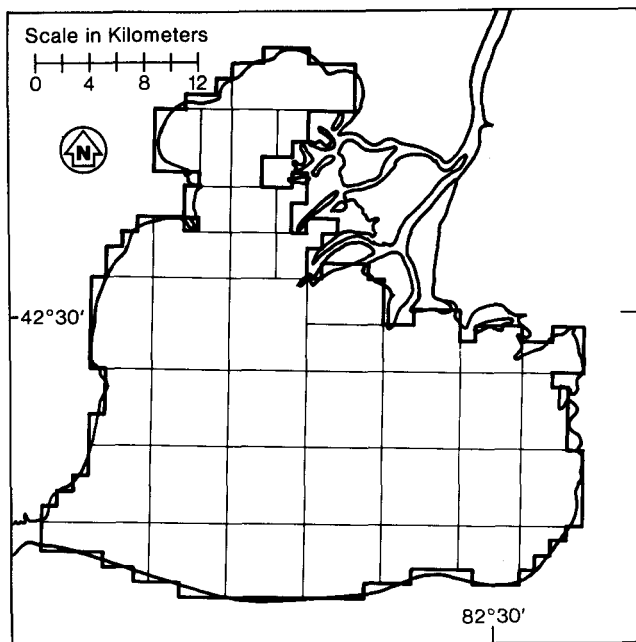


FIG. 1. Numerical grid used in Lake St. Clair contaminant fate and transport model. Average segment size is 5 km per side.

The volumetric inflow rate to the model was held constant at  $5,700 \text{ m}^3 \text{ s}^{-1}$  (Schwab and Liu 1987), entering the lake through the St. Clair River. The lake's outflow was through the Detroit River. The depth of the water column segments ranged from 2 to 5.2 m (areal mean = 3.5 m). The depth of the active sediment layer was set equal to 2 cm throughout the lake. The depth of the deep sediment layer equaled the total depth of the recent (postglacial) sediments minus the active sediment layer depth, and it ranged from 1 to 28 cm.

The spatial distribution of the horizontal dispersion coefficient in the water column was estimated through a calibration exercise that will be presented in a later section. Vertical pore water diffusion of dissolved contaminants between the water column and the active sediment layer was set equal to  $10^{-5} \text{ cm}^2 \text{ s}^{-1}$  (Bowie *et al.* 1985). An average wind speed of  $6 \text{ m s}^{-1}$  from the southwest was used in all long-term simulations. In the chloride calibration exercises, however, actual winds were used. Wind frequency data from meteorological sampling stations in the St. Clair region during the period 1951–80 show a predominantly moderate wind speed ( $5\text{--}8 \text{ m s}^{-1}$ ) with a southwesterly flow in all seasons (Great Lakes Institute 1986). Table 1 con-

tains the values of physical parameters used in the Lake St. Clair simulations.

### Solids Parameters

The suspended solids loading from the St. Clair, Clinton, Sydenham, and Thames rivers was calculated from average tributary concentrations and flows reported by the Great Lakes Institute (1986). The total load equaled  $2,700 \text{ MT d}^{-1}$  and was held constant throughout the simulations. The settling velocity of solids was set equal to  $3 \text{ m d}^{-1}$  (Simons and Schertzer 1986).

The model treats sediment as a single size fraction. This could be a particular concern when simultaneously modeling nearshore and offshore concentrations of organic, hydrophobic contaminants because the organic content and sorptive capacity of sediment types differ. Limno-Tech, Inc. (1985) characterized the lake's sediments as approximately 50% sand and gravel, 33% silt, and 17% clay. The percentage of clay is greatest in the deeper water regions and decreases toward the shallower areas.

Although the model does not distinguish among different sediment size fractions, it does permit the user to define the spatial distribution of the organic carbon content of suspended and settled sediments. Bell (1980) measured organic carbon in Lake St. Clair sediments during two cruises in 1974. The spatial distribution of the organic carbon in 1974 generally matched the observed grain size distribution reported by Limno Tech, Inc. (1985). Therefore, the distribution of organic carbon was assumed to approximate the distribution and sorptive characteristics of the different sediment types (e.g., coarse sand has a low organic carbon content and a low affinity for organic contaminants, the clay-sized fraction has a high organic carbon content and a high affinity for organic contaminants, etc.). However, the two 1974 data sets reported by Bell (1980) covered  $< 65\%$  and  $< 45\%$  of the lake's sediments, respectively, and there were differences between the two data sets. For these reasons, the spatial distribution and magnitude of the organic carbon content of suspended and settled sediments was estimated through a calibration exercise that will be explained in a section below. It was assumed that the average organic carbon content of each segment would be maintained over time. This is a reasonable assumption, given the nature and size

TABLE 1. Physical and solids parameters of Lake St. Clair required by the TOXIWASP model.

Property	Units	Value	Reference
Segment temperature	°C	13.0	STORET
Segment depth			
Water	m	2.0–5.2	Schwab and Liu (1987)
Active sediments	m	0.02	Robbins <i>et al.</i> (1990)
Deep sediments	m	0.01–0.28	Robbins <i>et al.</i> (1990)
Segment surface area	km <sup>2</sup>	5.76–43.2	Schwab and Liu (1987)
Water velocity	m s <sup>-1</sup>	0.15	Schwab and Liu (1987)
Wind velocity	m s <sup>-1</sup>	6.0	Great Lakes Institute (1986)
Bacterial density			
Water	cells mL <sup>-1</sup>	10 <sup>6</sup>	Ibrahim (1986)
Sediments	cells 100 g <sup>-1</sup>	10 <sup>7</sup> –10 <sup>8</sup>	Ibrahim (1986)
Total segment biomass			
Water	mg L <sup>-1</sup>	10	Ibrahim (1986)
Sediments	g m <sup>-2</sup>	1–50	Ibrahim (1986)
Horizontal dispersion	m <sup>2</sup> s <sup>-1</sup>	1.5–300	Present study
Pore water diffusion	cm <sup>2</sup> s <sup>-1</sup>	10 <sup>-5</sup>	Bowie <i>et al.</i> (1985)
Sediment organic carbon	%	0.14–5.0	Present study
Solids concentration			
Water	mg L <sup>-1</sup>	4.7–10.0	Present study
Sediments	mg L <sup>-1</sup>	10 <sup>6</sup>	Robbins (1987, pers. comm.)
Settling rate	m d <sup>-1</sup>	3.0	Simons and Schertzer (1986)
Resuspension rate	cm yr <sup>-1</sup>	0.51–1.1	Present study
Contaminant burial rate	cm yr <sup>-1</sup>	0.1	Robbins <i>et al.</i> (1990)
pH	pH units	8.1	STORET
Light extinction	m <sup>-1</sup>	2.0	STORET

of the system and the time scale of the simulations.

The concentration of solids in the active and deep sediment layers was set equal to 1.0 kg L<sup>-1</sup>, based on the sandy nature of the Lake St. Clair sediments and on data from sediment cores collected in 1985 (Robbins 1987, Great Lakes Environmental Research Laboratory, personal communication). Table 1 contains the values of these and other solids parameters used in the Lake St. Clair simulations.

#### Concentrations and Resuspension Rates

Knowledge of the dynamics of suspended solids is necessary for accurately predicting the fate of particle-bound contaminants. Using the solids parameters and loads presented above, and assuming zero net particle sedimentation, we conducted preliminary model runs to determine the spatial distribution of suspended solids in Lake St. Clair. Zero net sedimentation was assumed for our time

scale of interest because only 30 cm of sediment, at most, has accumulated in the lake in postglacial times (Limno-Tech, Inc. 1985, Robbins *et al.* 1990). With constant external solid loads and constant wind conditions (6 m s<sup>-1</sup> southwest), simulated suspended solids concentrations quickly reached steady state concentrations. The simulated spatial distribution of suspended solids concentrations ranged from 4.7 to 10.0 mg L<sup>-1</sup> (volumetric mean = 6.0 mg L<sup>-1</sup>). These values are in the range of those measured by Bukata *et al.* (1987) along ship transects during three separate Lake St. Clair cruises in September, 1985. They reported a range of 2.5–16 mg L<sup>-1</sup> ( $\bar{x}$  = 6.2 mg L<sup>-1</sup>). The simulated suspended solids concentrations are also in the range of those measured by Bell (1980) during four lake-wide cruises in 1974. Bell reported a range of 1.0–16.2 mg L<sup>-1</sup> ( $\bar{x}$  = 5.3 mg L<sup>-1</sup>).

The resuspension velocity in each segment was calculated such that the settling and resuspension fluxes of the particulate solids across the sediment/water interface were equal (i.e., zero net sedimen-

tation). The resulting distribution of resuspension rates calculated by the model ranged from 0.5 to 1.1 cm  $y^{-1}$ . These values are equivalent to fluxes of 0.6–1.3 g  $m^{-2} h^{-1}$ , and compare reasonably well with measured fluxes of 0.5–4 g  $m^{-2} hr^{-1}$  in summer 1985 (Charlton and Oliver 1986).

### Chemical Parameters

The modeled chemical was loaded into the system from atmospheric, land runoff, and tributary sources, as appropriate. The model assumed a local equilibrium between the dissolved, sorbed, and biologically bound chemical as defined by the organic carbon and octanol/water partition coefficients,  $K_{oc}$  and  $K_{ow}$ , respectively. The chemical-specific  $K_{oc}$  was multiplied by the spatially varying organic carbon content of suspended and settled sediments, resulting in vertical and horizontal distributions of the sediment/water partition coefficient,  $K_p$ .  $K_{ow}$  was multiplied by the organic carbon content of the biomass to yield an overall biota/water partition coefficient,  $K_b$ . The fraction of the total chemical concentration present in each of the three physical phases was calculated from the partition coefficients, the concentrations of solids and biota in the water and sediments, and the porosity of the sediments.

Two fundamental processes that affect chemical fate are settling and resuspension of sediment-sorbed chemical. These processes were controlled by the spatially varying settling and resuspension velocities. Horizontal mixing of total chemical in the water column was a function of the spatially varying dispersion coefficient, the horizontal chemical concentration gradient, the segment interface area, and the characteristic mixing length. The rate of pore water diffusion was controlled by the vertical concentration gradient of dissolved chemical, the vertical diffusion coefficient, the sediment/water interface area, the mixing length, and the porosity of the active sediment layer.

The kinetic transformation term in equation (1) includes hydrolysis, microbial degradation, photolysis, oxidation, and volatilization. The chemical under consideration may be affected by any or all of these processes. The overall transformation rate was calculated as the sum of the pseudo-first-order rate constants for each of these processes. These processes are detailed in Ambrose *et al.* (1983) and Burns *et al.* (1982).

Vertical distributions of excess lead-210, mea-

sured from a set of diver-collected sediment cores from Lake St. Clair in 1985, possessed a zone of constant activity extending down to about 2 or 3 cm, with exponential falloff below that depth (Robbins *et al.* 1990). Analyses of these distributions plus those of cesium-137 indicate a rate of net downward transport of chemical in the range of 0–0.2 cm  $yr^{-1}$ . This rate is comparable to the range of burial velocities in the Great Lakes, from 0.063 cm  $yr^{-1}$  for Lake Superior up to 0.35 cm  $yr^{-1}$  for Lake Erie (Chapra and Reckhow 1983). Although the individual processes contributing to this downward transport are not well defined, biological mixing (UGLCCS Management Committee 1988) and particle accumulation (Robbins *et al.* 1990) are favored. Because there is no mechanism for biological mixing in TOXIWASP and because of our assumption of zero net sedimentation, the model was modified to empirically account for a constant net burial of total chemical from the active sediment layer to the deep sediments. This rate was set equal to 0.1 cm  $yr^{-1}$  throughout the lake.

### Model Output vs. Measured Data: Testing Goodness of Fit

In the simulations discussed below, it was necessary to determine how closely the model results matched the measured data, particularly during the calibration exercises. While visual comparisons of modeled and observed distributions could be considered adequate, a statistical approach was desired. The available data were grouped and averaged within segments that correspond directly to the segmentation in the model. The goodness of model fit to the data was tested using two techniques. First, we performed regressions of model output versus measured data for all segments that contained data. For a perfect model fit, the regression coefficient,  $r^2$ , should equal one, and the slope and intercept of the regression line should equal one and zero, respectively. Second, we used a two-sided t-test to test whether the mean difference between pairs of model output and measured data is significantly different from zero. These techniques are simplistic, but their results plus visual comparisons of model output and measured data gave a general indication of goodness of fit.

### MODEL CALIBRATION

Two calibration exercises were performed. Simulations of chloride ion transport was used to calibrate the spatial distribution of horizontal disper-

sion coefficients in the water column. Simulation of cesium-137 fate was used to calibrate the spatial distribution of the organic carbon content of suspended and settled sediments. Descriptions of simulation conditions, data for calibration, loading functions, and chemical coefficients required for these simulations follow.

### Chloride

Bell (1980) documented chloride and meteorological data collected during a series of cruises in Lake St. Clair during the summer of 1974. The data included wind speeds and directions, and chloride concentrations throughout the lake and near the mouth of the major tributaries. Cruises 3 (19–29 June), 5 (15–24 July), 6 (5–15 August), and 8 (16–25 September) were the most complete and were thus selected for this study. At least 30 stations were monitored during each cruise. The root-mean-square wind speed and prevailing direction for cruises 3, 5, 6, and 8 were  $4 \text{ m s}^{-1}$  from the northeast,  $5 \text{ m s}^{-1}$  from the north,  $5 \text{ m s}^{-1}$  from the east, and  $6 \text{ m s}^{-1}$  from the west, respectively. The extensive data set corresponding to these four cruises provided an opportunity to estimate, through model calibration, the spatial distribution of the horizontal dispersion coefficients in the water column.

The chloride load to the lake was calculated for each cruise as the product of the flow and chloride concentration measured near the mouth of each tributary. The total chloride loads to Lake St. Clair during the four cruise periods were calculated to be  $3,700 \text{ MT d}^{-1}$ ,  $3,400 \text{ MT d}^{-1}$ ,  $3,200 \text{ MT d}^{-1}$ , and  $3,300 \text{ MT d}^{-1}$ , respectively. These values compare well with an independent estimate of the chloride load of  $4,000 \text{ MT d}^{-1}$  in 1984 (Johnson and Kauss 1987). The majority of the chloride load (more than 95%) entered the lake through the St. Clair River; the remainder entered through Chenal Ecarte and the Clinton and Thames rivers. Chloride loads from the Thames and Clinton rivers were only available for cruise 5; consequently, loads from the Clinton and Thames rivers for cruises 3, 6, and 8 were estimated from the cruise 5 load. This approach seemed reasonable since less than 5% of the total cruise 5 load entered the lake through the Thames and Clinton rivers.

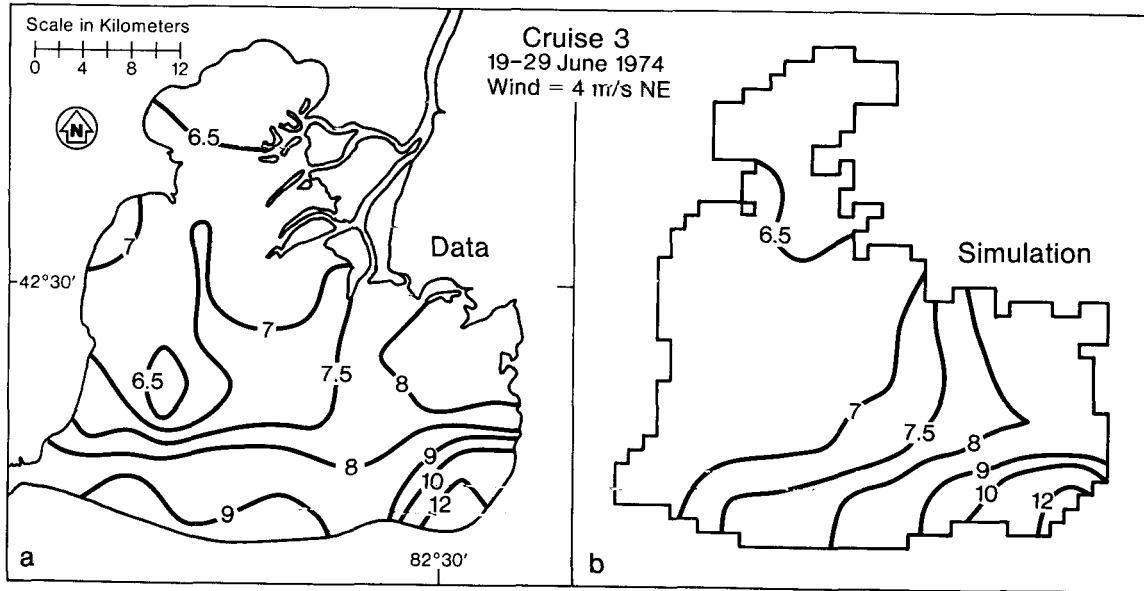
Four simulations were performed, corresponding to the four cruises; each simulation had a different chloride load and wind-induced flow field. The flow fields during each cruise were generated

with the Lake St. Clair Rigid Lid Hydrodynamic Model (Schwab and Liu 1987) using the observed, cruise-averaged wind conditions. Initial chloride concentrations were set equal to  $7 \text{ mg L}^{-1}$  throughout the lake, and the chloride load was held constant. The model was run for 14 days and steady state values were reached in all four simulations. Because chloride is a dissolved conservative substance, partitioning, settling, resuspension, and degradation were not included in these simulations.

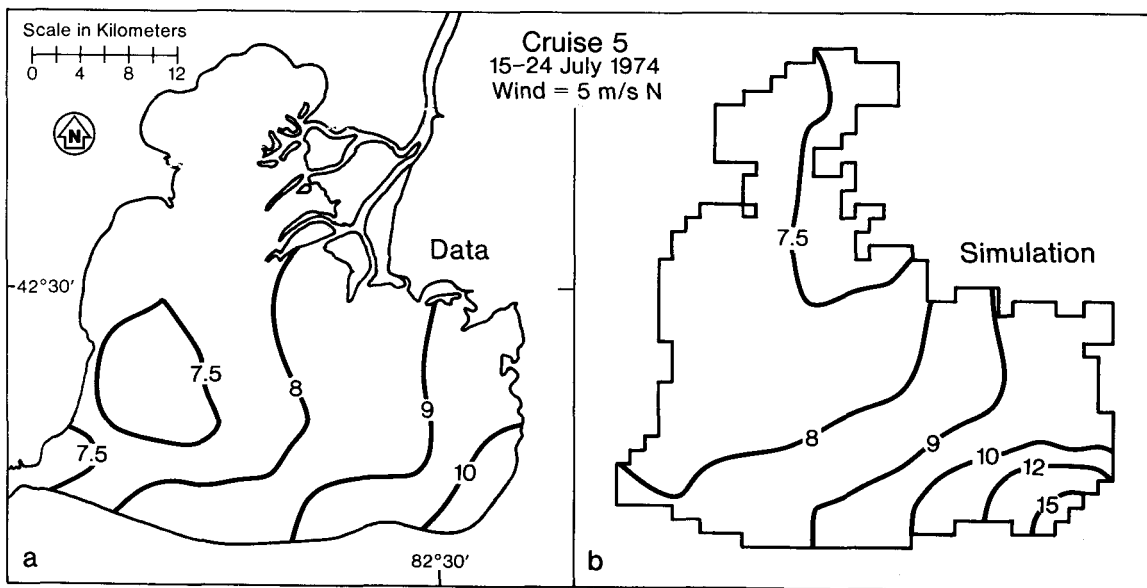
The horizontal dispersion coefficients for each segment interface were adjusted within the range of literature values (Bowie *et al.* 1985) until the observed and modeled chloride distributions most closely matched each other for all four cruises. The simulations corresponding to the calibrated dispersion coefficients are presented in Figures 2 through 5. The range of observed chloride concentrations for cruises 3, 5, 6, and 8 were  $5.9\text{--}14.6 \text{ mg L}^{-1}$  ( $\bar{x} = 7.7 \text{ mg L}^{-1}$ ),  $7.1\text{--}15.0 \text{ mg L}^{-1}$  ( $\bar{x} = 8.2 \text{ mg L}^{-1}$ ),  $6.9\text{--}19.9 \text{ mg L}^{-1}$  ( $\bar{x} = 8.2 \text{ mg L}^{-1}$ ), and  $6.7\text{--}12.7 \text{ mg L}^{-1}$  ( $\bar{x} = 7.4 \text{ mg L}^{-1}$ ), respectively. These compare to the range of the simulated chloride concentrations for the four cruises:  $6.2\text{--}12.7 \text{ mg L}^{-1}$  ( $\bar{x} = 7.3 \text{ mg L}^{-1}$ ),  $7.3\text{--}15.8 \text{ mg L}^{-1}$  ( $\bar{x} = 8.4 \text{ mg L}^{-1}$ ),  $6.8\text{--}11.8 \text{ mg L}^{-1}$  ( $\bar{x} = 7.7 \text{ mg L}^{-1}$ ), and  $6.6\text{--}10.9 \text{ mg L}^{-1}$  ( $\bar{x} = 7.4 \text{ mg L}^{-1}$ ), respectively.

The spatial agreement between the observed and simulated chloride concentrations was quite good. Regressions of model output versus observations for the four simulations are presented in Table 2. The regressions are all highly significant ( $p = 0.0001$ ). Note that by removing one particularly poor segment prediction, the slope and intercept for cruises 5 and 8 can be greatly improved. In this case, for cruise 5:  $m = 0.96$  and  $b = 0.43$ , and for cruise 8:  $m = 0.99$  and  $b = 0.01$ . In addition, the mean difference between pairs of model output and data was not significantly different from zero for the simulations corresponding to cruises 3, 5, and 8 ( $p = 0.2396$ ,  $p = 0.1679$ ,  $p = 0.3161$ , respectively).

The calibration yielded minimum and maximum horizontal dispersion coefficient values of  $2 \times 10^4$  and  $3 \times 10^6 \text{ cm}^2 \text{ s}^{-1}$ , respectively. Throughout much of the lake, the transport and distribution of chloride was controlled to a great extent by the advective flows, and by the magnitude and location of the chloride loads. The model was relatively insensitive to changes in the horizontal dispersion coefficient at 60 of the 75 segment interfaces, and the dispersion coefficients were subsequently set



**FIG. 2.** Comparison of observed (a) and model-simulated (b) water column concentrations ( $\text{mg L}^{-1}$ ) of chloride in Lake St. Clair during cruise 3, 19-29 June 1974. Wind speed:  $4 \text{ m s}^{-1}$  NE. Isopleths represent interpolation of measured and simulated concentrations.



**FIG. 3.** Comparison of observed (a) and model-simulated (b) water column concentrations ( $\text{mg L}^{-1}$ ) of chloride in Lake St. Clair during cruise 5, 15-24 July 1974. Wind speed:  $5 \text{ m s}^{-1}$  N. Isopleths represent interpolation of measured and simulated concentrations.

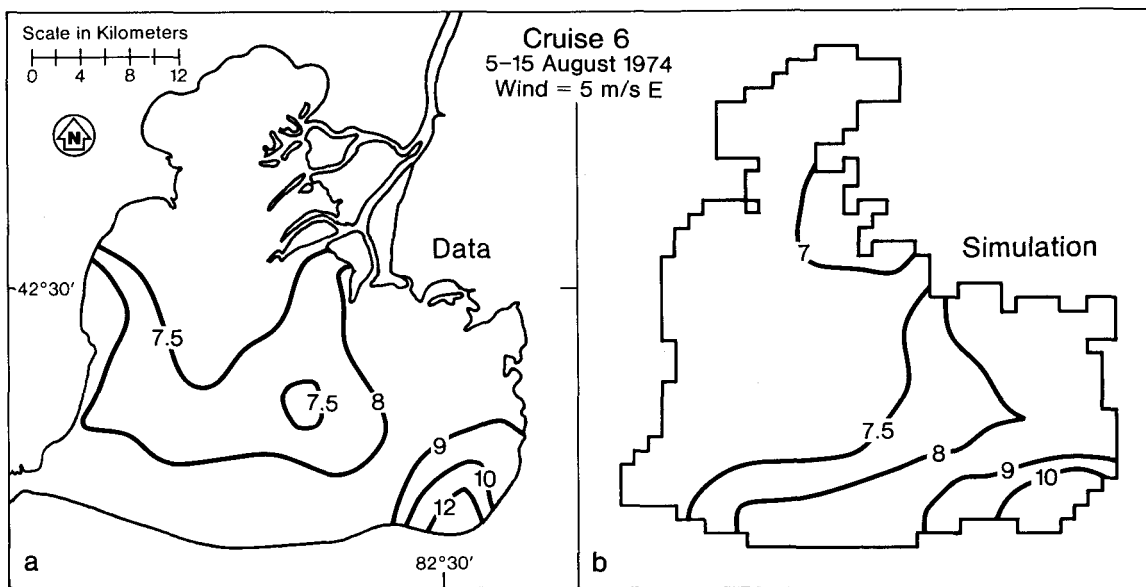


FIG. 4. Comparison of observed (a) and model-simulated (b) water column concentrations ( $\text{mg L}^{-1}$ ) of chloride in Lake St. Clair during cruise 6, 5-15 August 1974. Wind speed:  $5 \text{ m s}^{-1}$  E. Isopleths represent interpolation of measured and simulated concentrations.

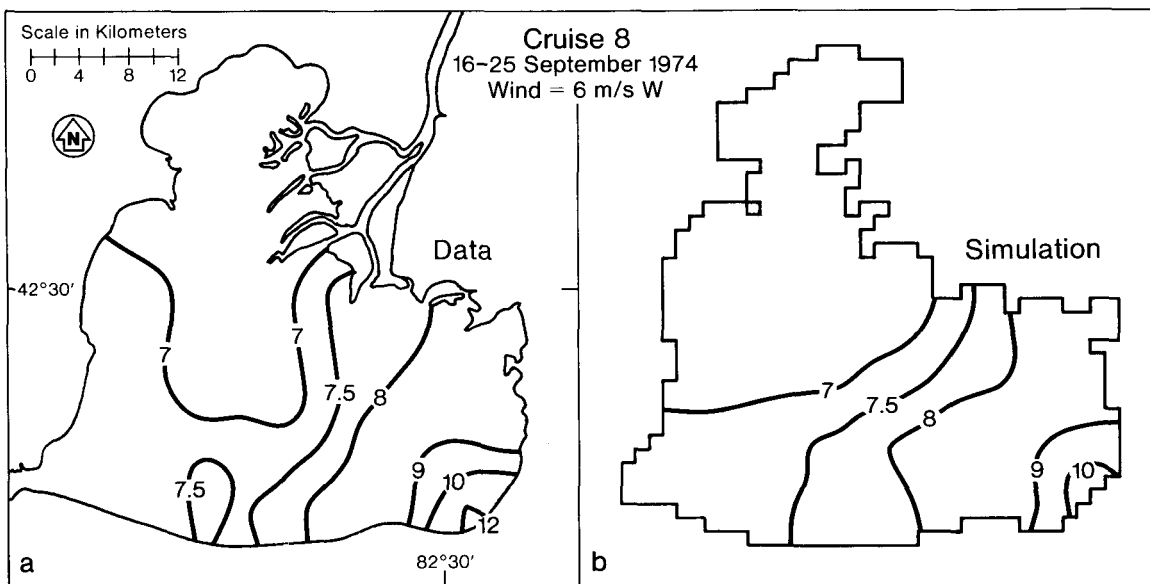


FIG. 5. Comparison of observed (a) and model-simulated (b) water column concentrations ( $\text{mg L}^{-1}$ ) of chloride in Lake St. Clair during cruise 8, 16-25 September 1974. Wind speed:  $6 \text{ m s}^{-1}$  W. Isopleths represent interpolation of measured and simulated concentrations.



TABLE 2. Regression of model output versus data for chloride simulations corresponding to four Lake St. Clair cruises in 1974.

Cruise	Dates	n	y = mx + b			
			m	b	r <sup>2</sup>	p
3	19–29 June	23	1.04	-0.52	0.64	0.0001
5	15–24 July	23	1.57	-4.34	0.73	0.0001
6	5–15 Aug.	24	0.82	1.05	0.78	0.0001
8	16–25 Sep.	22	0.76	1.75	0.87	0.0001

equal to  $3 \times 10^5 \text{ cm}^2 \text{ s}^{-1}$  at those interfaces. The higher and lower values were located in the eastern part of the lake where the advective flows were greatly reduced and wind-induced circulation gyres were often found. Because the calibration was performed to achieve the best fit for all four cruises, the spatial distribution of calibrated horizontal dispersion coefficients was assumed to be representative of various wind speeds and directions, and it was therefore used in all subsequent simulations.

### Cesium-137

Cesium-137, a surrogate for many hydrophobic, organic contaminants because of its sorptive characteristics, was used to calibrate and examine the relative importance of the processes associated with sediment-bound contaminant movement. The 35-year history (1950–85) of cesium-137 loading to Lake St. Clair (Fig. 6) was well documented by Robbins *et al.* (1990). During this period, the largest portion of the load was inflow from Lake Huron (55% in 1950 up to 75% in 1985). The contribution from the atmosphere decreased from about 40% of the total load in 1950 to about 20% of the total load in 1985. The remainder of the load (about 5%) originated from land runoff sources.

Cesium concentrations in the upper 2 cm of bottom sediment were reported for 1976 and 1985 by Robbins *et al.* (1990). In both years, concentrations were closely related to the thickness of the recent sediments, with the highest concentrations located in the corridor between the mouth of the St. Clair River and the head of the Detroit River. Robbins *et al.* (1990) also estimated the total accumulation of cesium-137 over the entire depth of sediments in 1985. The extensive cesium data set and well-documented loading function provided an opportunity to estimate, through model calibration, the spatial distribution of the organic carbon content of suspended and settled sediments.

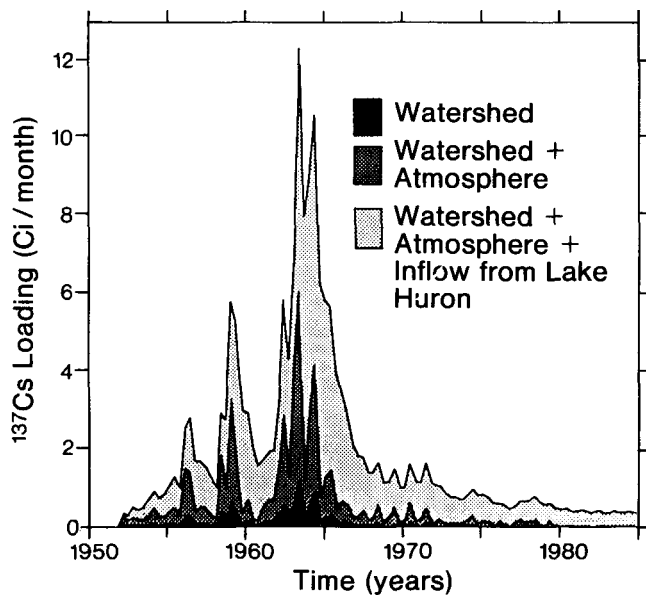


FIG. 6. Loading of cesium-137 to Lake St. Clair during the period 1950–85 from three principal sources: inflow from Lake Huron, direct atmospheric fallout, and land runoff from the watershed (Robbins *et al.* 1990).

Cesium-137 has a half-life of 30.2 years and a sediment/water partition coefficient of about  $29,000 L_w \text{ kg}^{-1}$ . This partition coefficient was calculated from the mean suspended solids concentration in Lake St. Clair ( $6.0 \text{ mg L}^{-1}$ ) and the fraction of dissolved cesium-137 (about 0.85) in the open-lake waters of the Great Lakes (Robbins 1985). With an average organic carbon content of open-lake sediments in Lake St. Clair equal to about 2.5%,  $K_{oc}$  was calculated to be  $1.16 \times 10^6 L_w \text{ kg org C}^{-1}$ . Since cesium-137 does not actually associate with organic carbon (Robbins 1989, Great Lakes Environmental Research Laboratory, personal communication), the  $K_{oc}$  used here is an apparent  $K_{oc}$ .

The model was run for 9,700 days, corresponding to the early-1950 to mid-1976 period, with a constant flow field generated by a  $6 \text{ m s}^{-1}$  wind from the southwest. Initial 1950 cesium-137 concentrations were set equal to zero in all segments. The organic carbon content of each segment was adjusted within the measured range of 0–8% (Bell 1980) until the model results most closely matched the magnitude and distribution of sediment-bound cesium-137 concentrations in the active sediment

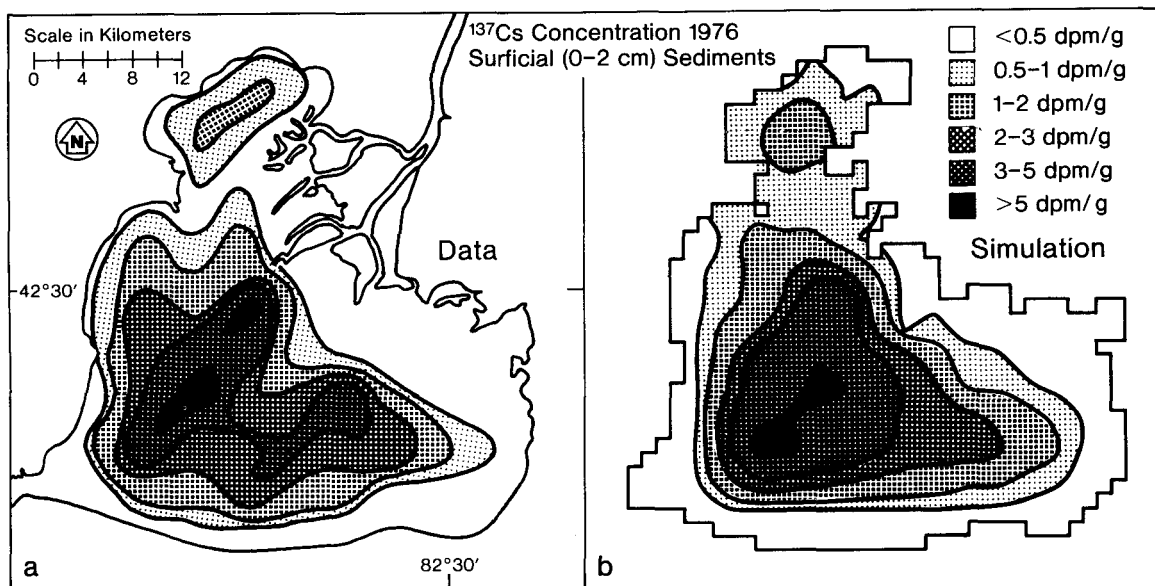


FIG. 7. Comparison of observed (a) and model-simulated (b) concentrations ( $\text{dpm g}^{-1}$ ) of cesium-137 in surface (0–2 cm) sediments in 1976. Isopleths represent interpolation of measured and simulated concentrations.

layer (0–2 cm) throughout the lake in 1976 (Fig. 7). The regression line of model output versus data had a slope of 1.07, an intercept of 0.023, and was highly significant ( $r^2 = 0.70$ ,  $p = 0.0001$ ,  $n = 31$ ). In addition, the mean difference between pairs of model output and data was not significantly different from zero ( $p = 0.4929$ ). The observed mean and maximum concentrations for 1976 were 1.5 and 6.7  $\text{dpm g}^{-1}$ , respectively. These compare with calibrated values of 1.6 and 5.7  $\text{dpm g}^{-1}$ , respectively.

The calibrated distribution of the organic carbon content of the sediments can be summarized as follows: 55% of the lake's sediments contained less than 0.5% organic carbon, 27% contained between 0.5% and 2% organic carbon, and 18% contained more than 2% organic carbon. The highest organic carbon values were located in the deepwater, high clay content regions of the lake, and the lowest values were located in the sandy, near-shore regions of high wave energy. The calibrated distribution of organic carbon closely matched the pattern of observed grain size reported by Limno-Tech, Inc. (1985), and the pattern of observed organic carbon reported by Bell (1980).

The magnitude of the calibrated organic carbon

values ranged from 0.1 to 5% (areal mean = 1.3%) for the 0–2 cm depth. These calibrated values generally fall within the range of literature values for the St. Clair corridor. Bell (1980) reported 0.7–6.0% ( $\bar{x} = 2.5\%$ ) and 0.6–8.0% ( $\bar{x} = 2.9\%$ ) in Lake St. Clair sediments. Maguire *et al.* (1985) reported 1–4% in St. Clair River sediments (0–2 cm) and 1–14% in Detroit River sediments (0–2 cm). Kaiser *et al.* (1985) reported 1–6% in Detroit River sediments (0–5 cm). Ibrahim (1986) and the Great Lakes Institute (1986) used values of 5% for their simulations of contaminant fate in Lake St. Clair. In addition, the sediments of Lakes Huron and Erie have mean organic carbon contents of 2.1 and 1.6% respectively (Thomas *et al.* 1976).

To test the reasonableness of the calibrated sediment organic carbon contents, the cesium simulation was extended for an additional 3,300 days (out to 1985) using the known cesium-137 loads from 1976 to 1985, without changing any of the sediment organic carbon values. The resulting magnitude and distribution of predicted sediment-bound cesium-137 in the active sediment layer compared well with the observed 1985 values (Fig. 8). The regression line of model output versus data had a slope of 1.05, an intercept of  $-0.13$ , and was highly significant ( $r^2 = 0.56$ ,  $p = 0.0001$ ,  $n = 20$ ). In

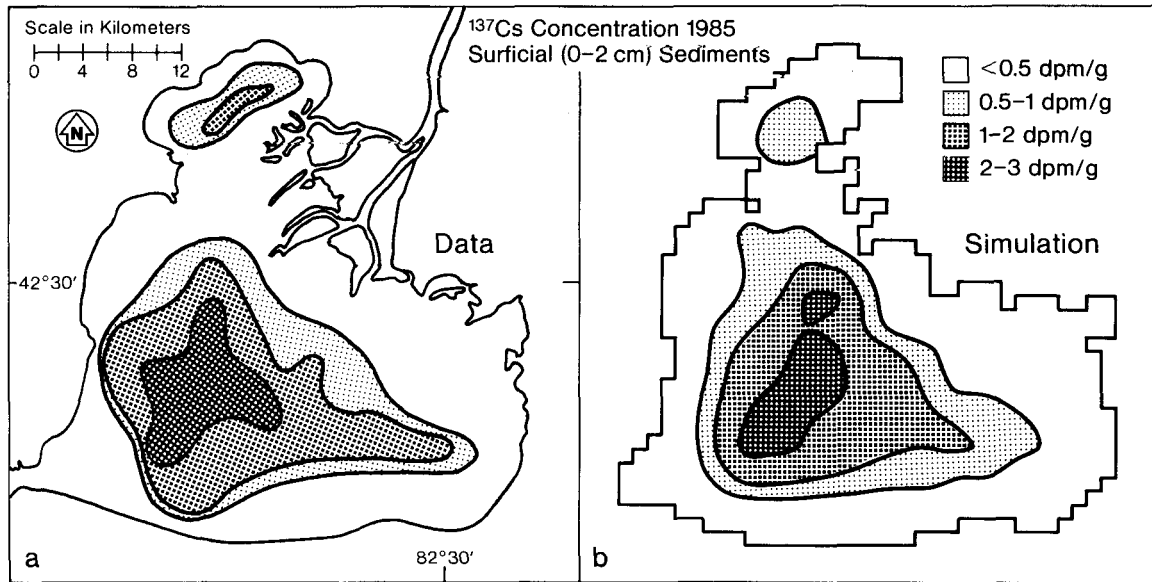


FIG. 8. Comparison of observed (a) and model-simulated (b) concentrations ( $\text{dpm g}^{-1}$ ) of cesium-137 in surface (0–2 cm) sediments in 1985. Isopleths represent interpolation of measured and simulated concentrations.

addition, the mean difference between pairs of model output and data was not significantly different from zero ( $p = 0.5550$ ). The observed mean and maximum values in 1985 were 1.1 and 2.5  $\text{dpm g}^{-1}$ , respectively. The corresponding values predicted by the model were 0.7 and 2.4  $\text{dpm g}^{-1}$ , respectively. During the 9-year period from 1976 to 1985, the decline in cesium-137 concentrations in the active sediment layer was due to decreased loading, radioactive decay, cesium-associated particle resuspension and subsequent flushing, and burial to the deep sediments. The model predicted that the lake-wide mass storage of cesium-137 in the active and deep sediments was 35 Ci in 1985. This value is in close agreement with the measured 1985 value of 37 Ci (Robbins *et al.* 1990).

During the 35 years of simulation, the total cesium-137 loading to the system was 800 Ci. Of the total load, the model predicted that 730 Ci (92%) exited through the Detroit River, 33 Ci (4%) were lost due to radioactive decay, and 35 Ci (4%) remained in the system. Of the 4% that remained after 35 years, the model estimated that more than 99% of it was located in the active and deep sediments. Robbins *et al.* (1990) performed similar calculations that were normalized for radioactive decay. They concluded that a maximum of 470 Ci

of the 800 Ci of cesium loaded into the system during the 35 years could remain in 1985 if radioactive decay were the only loss mechanism. Thus, their calculated retention equaled about 7.9% (37/470). If calculated this way, retention in our model would be 7.5% (35/470).

The chloride and cesium-137 calibration exercises provided estimates of the magnitude and distribution of the horizontal dispersion coefficient in the water column, and of the organic carbon content of suspended and settled solids. These values, which are key components of the hydrodynamic and sediment transport processes, were assumed to be representative of average lake conditions and not dependent on the chemical being modeled. They were thus used, unaltered, in the following model applications.

### MODEL APPLICATIONS

Additional simulations were performed to help understand the fate of two organic contaminants (octachlorostyrene, OCS, and polychlorinated biphenyl, PCB) that have been input to the lake. Descriptions of simulation conditions, published data, loading functions, and chemical coefficients required for these simulations follow.

## OCS

OCS is a by-product of several industrial processes including PVC incineration, and chlorine and solvent production. OCS was first reported in the lower Great Lakes in 1980 (Kuehl *et al.* 1980). The occurrence of an OCS discharge to the St. Clair River and subsequent input to Lake St. Clair from the Sarnia industrial complex located along the northeastern shore of the St. Clair River has been documented (Bonner and Meresz 1981, Oliver and Bourbonniere 1985, Great Lakes Institute 1986). However, the historical, time-varying loading of OCS to Lake St. Clair is unknown. Limno-Tech, Inc. (1985) speculated that OCS was introduced to the lower Great Lakes beginning in the early 1970s as chlorine-manufacturing industries converted from a process using mercury to one which produced OCS as a by-product. Concern about OCS exists because it is a chlorinated hydrocarbon and tends to bioconcentrate.

Pugsley *et al.* (1985) found that OCS concentrations in surficial (0–10 cm) sediments ranged from nondetectable to  $26.2 \mu\text{g kg}^{-1}$  in 1983. Concentrations of OCS were highest in the corridor between the mouth of the South Channel (of the St. Clair River) and the head of the Detroit River. A tongue of lower concentrations extended from there toward the eastern part of the lake. The total load of OCS to Lake St. Clair was estimated to be about  $1.9 \text{ lb d}^{-1}$  (Great Lakes Institute 1986), based on model results in which the load was adjusted until predicted sediment concentrations matched observed values. We also used  $1.9 \text{ lb d}^{-1}$  and assumed that most of the load entered the lake through the South Channel outflow because of its origin along the eastern shore of the St. Clair River.

Assuming OCS first entered Lake St. Clair in mid-1971, the model was run for 12 years (4,380 days) to give predictions for mid-1983, corresponding to the time of the observations reported by Pugsley *et al.* (1985). Initial conditions of OCS were set equal to zero in all segments, based on the assumption that background levels of OCS in Lake St. Clair prior to the 1970s were negligible. The constant flow field used in the model simulation was generated by  $6 \text{ m s}^{-1}$  wind from the southwest.  $K_{ow}$  and  $K_{oc}$  were set equal to  $1.9 \times 10^6 L_w L_{oc}^{-1}$  and  $9.1 \times 10^5 L_w \text{ kg org C}^{-1}$ , respectively (Pugsley *et al.* 1985). The chemical properties and transformation rates used in the OCS simulation, as required by TOXIWASP, are presented in Table 3.

The model predicted that sediment-bound OCS concentrations in the active sediment layer (0–2 cm) ranged from 0 to  $40.5 \mu\text{g kg}^{-1}$  (areal mean =  $6.9 \mu\text{g kg}^{-1}$ ). In order to compare simulated with observed OCS concentrations, profiles of sediment OCS concentrations down to 10 cm were estimated from predicted active sediment layer concentrations using the method described in Chapra and Reckhow (1983). The method calculates the chemical concentration profile below the active sediment layer as a function of depth, decay rate, and chemical burial rate. We used the average sediment OCS decay rate of  $10^{-4} \text{ d}^{-1}$  predicted by the model. Average OCS concentrations down to 10 cm were then calculated from the profiles (Fig. 9).

There was good agreement between the observed (Pugsley *et al.* 1985) and predicted OCS concentrations (1–10 cm). The regression line of model output versus data had a slope of 1.10, an intercept of 0.37, and was highly significant ( $r^2 = 0.47$ ,  $p = 0.0001$ ,  $n = 42$ ). In addition, the mean difference between pairs of model output and data was not significantly different from zero ( $p = 0.2536$ ). The model was able to adequately reproduce the observed 1983 OCS pattern in the sediments: a concentrated plume of OCS extending from the mouth of the South Channel to the head of the Detroit River. The model predicted that the mean and maximum OCS concentrations in the top 10 cm of sediment in 1983 were  $3.1$  and  $18.4 \mu\text{g kg}^{-1}$ , respectively. These values compare with values measured in 1983 by Pugsley *et al.* (1985) ( $\bar{x} = 2.7 \mu\text{g kg}^{-1}$ ,  $\text{max} = 26.2 \mu\text{g kg}^{-1}$ ,  $n = 70$ , 0–10 cm) and by Oliver and Bourbonniere (1985) ( $\bar{x} = 8.1 \mu\text{g kg}^{-1}$ ,  $\text{max} = 11 \mu\text{g kg}^{-1}$ ,  $n = 2$ , 0–3 cm). In addition, observed OCS concentrations in sediment trap samples from nine stations in 1985 ranged from  $<1$  to  $10 \mu\text{g kg}^{-1}$  ( $\bar{x} = 3 \mu\text{g kg}^{-1}$ ) (Charlton and Oliver 1986). These values are in the range of OCS concentrations on suspended sediment predicted by the model for 1983: 0–50  $\mu\text{g kg}^{-1}$  ( $\bar{x} = 8 \mu\text{g kg}^{-1}$ ).

For 1983, the model predicted biologically bound OCS levels of 0–215  $\mu\text{g kg}^{-1}$  dry wt. ( $\bar{x} = 46 \mu\text{g kg}^{-1}$  dry wt.) in the water column and 0–167  $\mu\text{g kg}^{-1}$  dry wt. ( $\bar{x} = 35 \mu\text{g kg}^{-1}$  dry wt.) in the active sediment layer. These results compare reasonably well with observed concentrations. Suns *et al.* (1985) found mean OCS levels of 3–5  $\mu\text{g kg}^{-1}$  wet wt. in Lake St. Clair young-of-the-year spottail shiners in 1982 and 1983. Assuming a wet to dry weight ratio of 5, this range corresponds to 15–25  $\mu\text{g kg}^{-1}$  dry wt. Pugsley *et al.* (1985) reported levels

**TABLE 3.** Chemical properties of octachlorostyrene and polychlorinated biphenyl required by the TOXIWASP model. From Ibrahim (1986), Pugsley et al. (1985), and Mabey et al. (1982).

Property	Units	OCS Value	PCB Value <sup>1</sup>
Octanol/water partition coefficient	$L_w L_{oct}^{-1}$	$1.9 \times 10^6$	$6.0 \times 10^5$
Organic carbon partition coefficient	$L_w \text{ kg org C}^{-1}$	$9.1 \times 10^5$	$2.9 \times 10^5$
Bacterial transformation rate	$\text{mL cell}^{-1} \text{ hr}^{-1}$	$10^{-9}-10^{-11}$	$10^{-9}-10^{-11}$
Hydrolysis rate constant	$\text{M}^{-1} \text{ hr}^{-1}$	0	0
Molecular weight	$\text{g mol}^{-1}$	300	328
Henry's Law constant	$\text{Atm m}^3 \text{ mol}^{-1}$	$10^{-4}$	$2.6 \times 10^{-3}$
Vapor pressure	torr	$4 \times 10^{-5}$	$7.7 \times 10^{-5}$
Aqueous solubility	$\text{mg L}^{-1}$	0.02	0.031

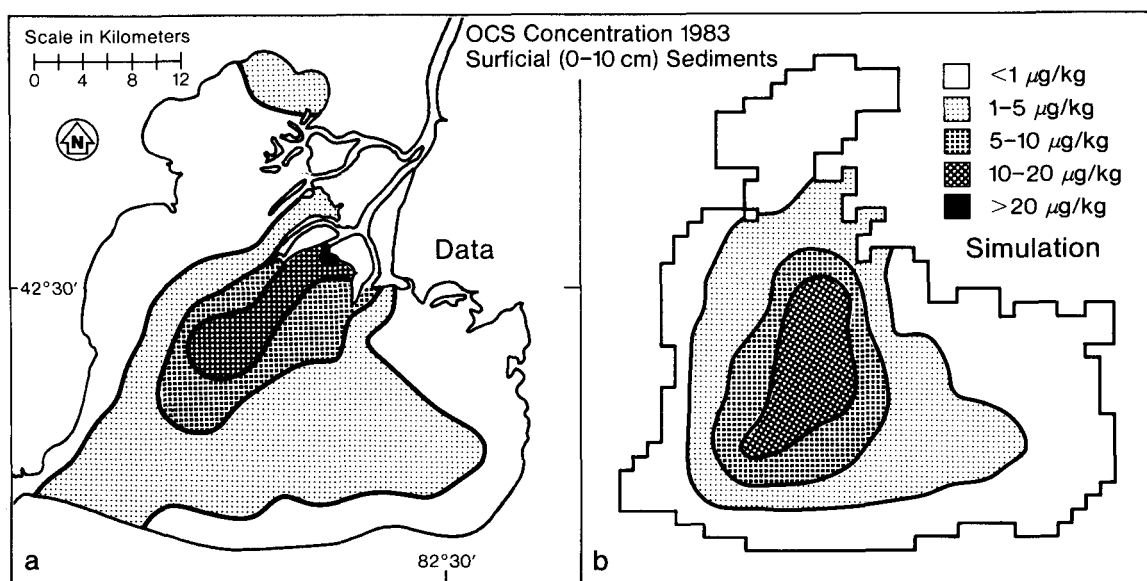
<sup>1</sup>Within range of values for Aroclors 1242, 1248, 1254, and 1260. They most closely resemble values for Aroclor 1254.

of 2–154  $\mu\text{g kg}^{-1}$  dry wt. ( $\bar{x} = 43 \mu\text{g kg}^{-1}$  dry wt.) in whole clam tissue (*Lampsilis radiata siliquoidea*) collected in Lake St. Clair during 1983. As expected, the predicted and observed distributions of biologically bound OCS in the sediment layer resembled the distribution of sediment-bound OCS.

During the 12-year simulation period, the model predicted that 3.8 MT of OCS entered Lake St. Clair. Of this total load, 2.8 MT (73%) were flushed from the system through the Detroit River,

0.83 MT (22%) were lost due to biological degradation and volatilization, and 0.18 MT (5%) remained in the system. As with cesium, the model estimated that in 1983 more than 97% of the OCS mass in the system was located in the active and deep sediments.

From depth-integrated samples, the UGLCCS Management Committee (1988) estimated that, as of 1985, Lake St. Clair received about 4.3 MT of OCS and retained about 0.21 MT. Extending the simulation for an additional 2 years, the model



**FIG. 9.** Comparison of observed (a) and model-simulated (b) concentrations ( $\mu\text{g kg}^{-1}$ ) of OCS in surface (0–10 cm) sediments in 1983. Isopleths represent interpolation of measured and simulated concentrations.

predicted that, as of 1985, 4.4 MT of OCS were loaded into the lake and 0.19 MT remained in the system. These values compare well with those estimated by the UGLCCS Management Committee.

### PCB

As a final application, the model was used to simulate the fate and distribution of total PCB in Lake St. Clair. PCBs are of particular concern because of their known toxicity to biota, low solubility in water, bioaccumulation, and extreme environmental persistence. Frank *et al.* (1977) measured PCB concentrations of surficial (0–2 cm) sediments collected from Lake St. Clair in 1970 and 1974. They found that the distribution of PCB in 1970 showed regions of higher concentrations that originated near the mouths of the St. Clair and Thames rivers. As with the OCS simulation, the loading function of PCB was unknown during the 1970–74 period. However, the load has been estimated to be 5.1 lb d<sup>-1</sup> (Great Lakes Institute 1986), based on model simulations in which the load was adjusted to reach the best comparison between model predictions and measured values in 1974. This load is comparable to an estimated load of 1–4 lb d<sup>-1</sup> based on PCB fluxes to Lakes Erie and Huron during the late 1970s (Thomann and Mueller 1983). The Great Lakes Institute (1986) estimated that 66% of the total PCB load entered the lake through the St. Clair River, 18% through the Thames River, and 16% through the Clinton River. In the present study, we used the 5.1 lb d<sup>-1</sup> estimate and the stated load distribution.

Because PCB concentrations were measured in 1970 and 1974 (Frank *et al.* 1977), initial concentrations of PCB were set equal to the 1970 values and the model was run for 4 years to 1974. The flow field was held constant and corresponded to a 6 m s<sup>-1</sup> wind from the southwest.  $K_{ow}$  and  $K_{oc}$  were set equal to  $6.0 \times 10^5 L_w L_{oc}^{-1}$  and  $2.9 \times 10^5 L_w \text{ kg org C}^{-1}$ , respectively (Mabey *et al.* 1982). The partition coefficients, chemical properties, and transformation rates were within the range of values for Aroclors 1242, 1248, 1254, and 1260 presented in Mabey *et al.* (1982); however, they most closely resemble values for Aroclor 1254. The chemical properties and transformation rates used in the PCB simulation are presented in Table 3.

The model was able to reproduce the observed sediment PCB distribution in 1974 fairly well (Fig. 10). Model predictions were best for PCB concentrations in Anchor Bay and the open-lake sedi-

ments. However, the model tended to underpredict the PCB values in some segments along the eastern and western shores of the main lake. This may indicate additional or increased PCB sources in these areas. The data indicate a decline in mean sediment (0–2 cm) concentration of total PCB from 19  $\mu\text{g kg}^{-1}$  in 1970 to 10  $\mu\text{g kg}^{-1}$  in 1974, and a decline in maximum sediment concentration from 40  $\mu\text{g kg}^{-1}$  in 1970 to 28  $\mu\text{g kg}^{-1}$  in 1974 (Frank *et al.* 1977). The model simulated a similar 4-year decline in mean active sediment layer concentration from 19.4  $\mu\text{g kg}^{-1}$  to 9.6  $\mu\text{g kg}^{-1}$  and in maximum sediment concentration from 38.0  $\mu\text{g kg}^{-1}$  to 27.7  $\mu\text{g kg}^{-1}$ .

For 1974, the model predicted biologically bound PCB levels of 3–217  $\mu\text{g kg}^{-1}$  dry wt. ( $\bar{x} = 70 \mu\text{g kg}^{-1}$  dry wt.) in the water column and 30–297  $\mu\text{g kg}^{-1}$  dry wt. ( $\bar{x} = 124 \mu\text{g kg}^{-1}$  dry wt.) in the active sediment layer. Scant information exists on the levels of biologically bound PCB in the early 1970s. However, these model results seem reasonable, given that from 1979 to 1983 mean levels of total PCB in young-of-the-year spottail shiners from three sites in Lake St. Clair ranged from 29 to 114  $\mu\text{g kg}^{-1}$  wet wt. (Suns *et al.* 1981, 1985). Assuming a wet to dry weight ratio of 5, this range corresponds to 145–570  $\mu\text{g kg}^{-1}$  dry wt. In addition, Pugsley *et al.* (1985) reported mean values of 90.6 and 44.2  $\mu\text{g kg}^{-1}$  dry wt. in whole clam tissue (*Lampsilis radiata siliquoidea*) for Aroclors 1254 and 1260, respectively, in Lake St. Clair during 1983. Direct comparison between the model results and the data is difficult because of the differences in years (1974, 1979, 1983) and units (dry wt., wet wt.). However, the general agreement between the model and the data is encouraging.

From 1970 to 1974, the model predicted that the total system mass of PCB decreased from 1.9 MT to 1.0 MT. During this time period, 3.4 MT of PCB were loaded into the system, 2.1 MT were flushed from the lake through the Detroit River, and 2.2 MT were lost due to biological degradation and volatilization. The model predicted that, in 1974, more than 98% of the PCB mass in the system was located in the active and deep sediments.

### CONCLUSIONS

The multisegment, contaminant mass balance model presented here has improved our understanding of processes and parameters that are important for accurate simulation of contaminant fate and transport in Lake St. Clair. Through four

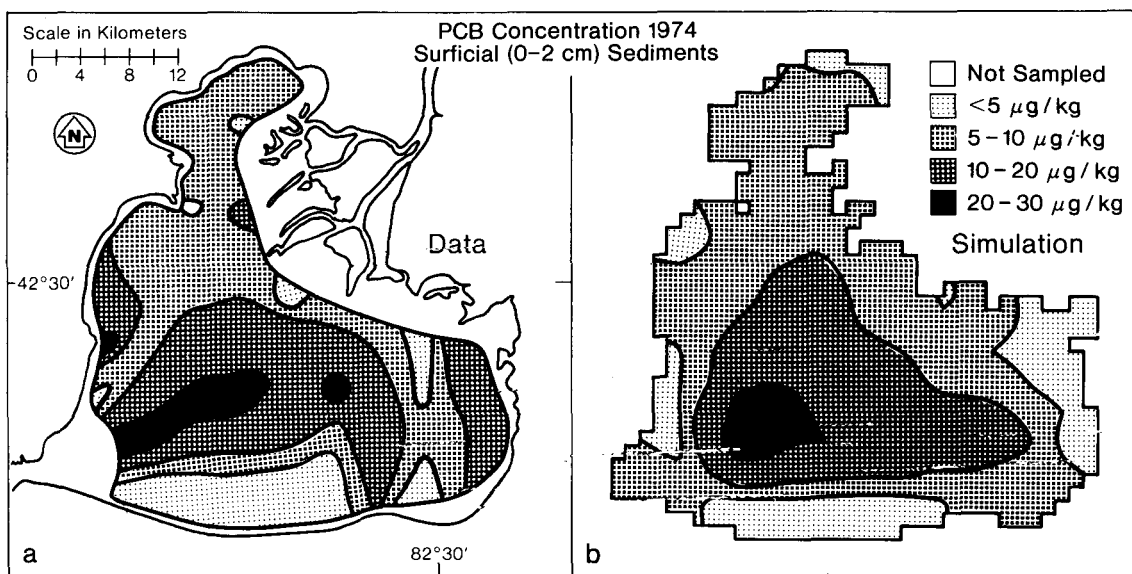


FIG. 10. Comparison of observed (a) and model-simulated (b) concentrations ( $\mu\text{g kg}^{-1}$ ) of total PCBs in surface (0–2 cm) sediments in 1974. Isopleths represent interpolation of measured and simulated concentrations.

simulations of chloride in Lake St. Clair in 1974, we calibrated the spatial distribution of the horizontal dispersion coefficient in the water column. The magnitude and distribution of these dispersion coefficients were then used in all subsequent simulations. The unique, documented loading history of cesium-137 and the extensive records of cesium-137 concentration in the sediments of Lake St. Clair in 1976 and 1985 provided an opportunity, through model calibration, to estimate the spatial distribution of the organic carbon content of suspended and settled sediments in the lake. This was an important modeling step for later simulations of the fate of organic contaminants since their partitioning depended heavily on the organic carbon content of the sediments.

Simulations of OCS and PCB fates were intended as applications of the model. Although the OCS and PCB loads were estimated from independent modeling exercises (Great Lakes Institute 1986) and not measured, they seem consistent with total historical loading estimates of OCS (UGLCCS Management Committee 1988) and with estimates of PCB fluxes to Lakes Erie and Huron (Thomann and Mueller 1983). Using known initial conditions, estimated loads, and the specific chemical properties of OCS and PCB,

measured distributions of OCS in 1983 and PCB in 1974 were adequately reproduced by the model.

Although the 12-year OCS simulation and the 4-year PCB simulation (both using constant loads) generated contaminant distributions that agreed reasonably well with the data, other time-varying load combinations could have produced similar results. It is unlikely that both loads remained constant over the entire simulation period. In fact, a more recent estimate of the OCS load to Lake St. Clair in 1984 ( $0.5 \text{ lb d}^{-1}$ , Johnson and Kauss 1987) is lower than that used in our OCS simulation ( $1.9 \text{ lb d}^{-1}$ ). Since OCS was first introduced to Lake St. Clair in the early 1970s, it is likely that the actual loading started out low in 1971, increased above  $1.9 \text{ lb d}^{-1}$  during the 1970s and early 1980s, and then decreased to  $<1 \text{ lb d}^{-1}$  in the mid-1980s once the load origin was identified. The same argument is probably true for PCB loads to Lake St. Clair. Given the voluntary ban on PCB production, which began in 1971, the actual PCB loading history probably started out higher in 1970 than that used in our PCB simulation ( $5.1 \text{ lb d}^{-1}$ ), and then decreased somewhat during the 4 years.

The modeling exercises presented here demonstrate the need for both spatially and temporally complete data sets, and for detailed historical load

estimates in terms of magnitude, duration, and temporal variability so that model calibration and application are as meaningful as possible. A model such as the one described here could be used to predict how the magnitude and distribution of contaminants in Lake St. Clair would be affected by future load reductions or additions, by significant changes in lake biomass, or by storm-related resuspension events.

Ongoing applications of the model include exploring the relative effects of load origin, wind direction, and partition coefficient on the distribution and residence times of generic contaminants in Lake St. Clair. Future versions of the model could be improved by including a more detailed biotic component, thereby enabling the study of the contaminant interactions between the physical transport mechanisms and food web dynamics.

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