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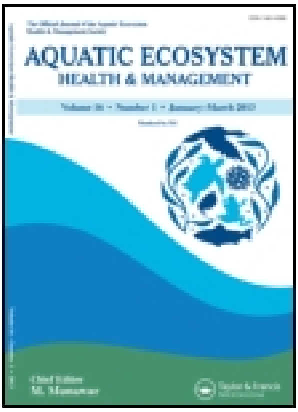

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Nilima Gandhi[a], Miriam L. Diamond[ab], Roshanak Razavi[a], Satyendra P. Bhavsar[a], Erin M. Hodge[a], Sarah B. Gewurtz[a] & George B. Arhonditsis[b]

[a] Department of Geography, University of Toronto, Toronto, Ontario M5S 3G3, Canada

[b] Department of Physical and Environmental Sciences, University of Toronto at Scarborough, Toronto, Ontario M1C 1A4, Canada

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A modeling assessment of contaminant fate in the Bay of Quinte, Lake Ontario: Part 2. Organic chemicals

Nilima Gandhi,[1] Miriam L. Diamond,[1,2,♦*] Roshanak Razavi,[1] Satyendra P. Bhavsar,[1,†] Erin M. Hodge,[1,‡] Sarah B. Gewurtz,[1,±] and George B. Arhonditsis[2]

[1]*Department of Geography, University of Toronto, Toronto, Ontario M5S 3G3, Canada*
[2]*Department of Physical and Environmental Sciences, University of Toronto at Scarborough, Toronto, Ontario M1C 1A4, Canada*
**Corresponding author: miriam.diamond@utoronto.ca*

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*A mass balance model of contaminant fate-transport was applied to 11 organic compounds in the Bay of Quinte and its foodweb. Total loadings were back-calculated from measured concentrations in sediment and/or fish for most chemicals due to limited measured concentrations in the contributing tributaries and point sources such as STPs. Total loadings decreased between 1988 and 2000 from 1–2 orders of magnitude for TCDD/F to 30% B[*a*]P and 80% for ΣPCBs. Total loadings in 2000 ranged from 10 mg day^{-1} for TCDD/TCDF to $\sim$0.01–0.5 kg year^{-1} for mirex,* p,p′-*DDT and BDE-47, to $\sim$1 kg year^{-1} for dieldrin and HCB, $\sim$10–50 kg year^{-1} for ΣPCB and B[*a*]P, and 2000 kg year^{-1} for atrazine. Despite concentration reductions, sport fish exceeded the lowest Ontario fish consumption guidelines for ΣPCB, TCDD and TCDF. Model results suggested that atmospheric deposition was the main source of lower molecular weight PCBs, TCDD/F and DDT, tributaries for higher molecular weight PCBs, and Lake Ontario for mirex, atrazine and dieldrin loadings. The main source of B[*a*]P was thought to be urban runoff, unknown for long-banned HCB and sewage treatment plants for 17β-estradiol. Results for BDE-47 were illustrative due to the lack of data. Industrial sources did not contribute to overall sediment or fish concentrations (not including "hot spots"). Organic compounds in the Bay were estimated to have a short residence time of days in the water column due to rapid export to Lake Ontario, except for HCB and 17β-estradiol which were estimated to be lost by volatilization and transformation, respectively. The response time of organic compounds in sediment varied from <1 year (atrazine) to $\sim$50 years (ΣPCB).*

Keywords: fate and transport, polychlorinated biphenyls, chlorinated organic contaminants, Laurentian Great Lakes, long-term trend, fish - foodweb

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[♦] Current address: Department of Earth Sciences, University of Toronto, Ontario M5S 3B1, Canada
[†] Current address: Environmental Monitoring and Reporting Branch, Ontario Ministry of the Environment, 125 Resources Road, Toronto, Ontario M9P 3V6, Canada
[‡] Current address: Public Health Ontario, 480 University Avenue, Suite 300, Toronto, Ontario M5A 4H8, Canada
[±] Current address: Conestoga-Rovers & Associates, 651 Colby Drive, Waterloo, Ontario N2V 1C2, Canada

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Introduction

Chemical contamination is one of the main stressors for fresh water ecosystems near populated areas. The Bay of Quinte, situated at the eastern end of Lake Ontario, suffered degradation of its water and sediment quality due to excessive loadings of toxic chemicals starting in the 1950s. Monitoring data collected during the 1980s raised concerns about elevated concentrations of several persistent organic pollutants (POPs) in addition to metals. Phenols and pentachlorophenol (PCP) exceeded Provincial Water Quality Guidelines (PWQG), polychlorinated biphenyls (PCBs) surpassed the Provincial Sediment Quality Guidelines (PSQG) at several stations throughout the Bay, and PCB and mercury were elevated in the tissue of larger fish species (Bay of Quinte RAP Coordinating Committee, unpubl., University of Toronto, Toronto, ON, 1990). One action taken by the Bay of Quinte Remedial Action Plan (RAP) Coordinating Committee in 1990 was to commission a study to answer questions regarding the sources and fate of contaminants, and the time over which concentrations would fall below PWQG and PSQG should the loadings decrease. To answer these questions, Diamond et al. (1994, 1996) assembled a mass balance model that assessed 4 metals and 13 hydrophobic organic chemicals in 5 geographic segments and the foodweb of the Bay of Quinte. The exercise was frustrated by a lack of data, but the general conclusions were that chemicals originated from the watershed (metals from the mining and mineral processing activities that took place in the past), industrial sources (PCP), non-point sources (naphthalene), urban discharges (chloroform, benzo[*a*]pyrene), Lake Ontario (tetrachlorodibenzodioxin or TCDD, DDT, mirex) and atmospheric deposition (DDT and tetrachlorodibenzofuran or TCDF) (Diamond et al., 1994, 1996; Poulton, 1992; Wong et al., 1995). Their results also pointed to the inevitably of having elevated concentrations of contaminants entering from the 18,000 km^2 watershed into the relatively small waterbody that has restricted dilution with Lake Ontario and considerable sediment–water exchange that slows reductions in concentrations in response to the reduced loadings.

In 2005, the Bay of Quinte RAP Restoration Council requested an update of the existing fate and transport model to gauge progress on reducing contaminant concentrations and to identify potential future actions that could be taken to improve the Bay's water quality. Since the first modeling effort, ecological changes in the Bay have been marked by the invasion of Zebra Mussels in 1995 that altered the foodweb structure, increased water clarity and subsequently hastened rates at which contaminants exchange between the sediment and water (Klerks et al., 1996, 1997). The second change since 1990 was the reduction of some chemical loadings due to pollution prevention and remediation actions. A third change that occurred was a reduction in monitoring efforts and institutional support with responsibility for collating relevant data in a single repository.

The goal of this study was to revisit the previous mass balance effort using updated data on contaminant loadings and measured concentrations in water, sediment and fish in order to assess progress towards restoring environmental quality. The model framework and assumptions for the abiotic fate calculations were kept similar to those of Diamond et al. (1994, 1996). This model has been widely used to explore chemical loadings, fate and transport (Mackay and Hickie, 2000; Gandhi et al., 2007; Sommerfreund et al., 2010a,b). The foodweb was revised to accommodate changes in its structure, such as including Zebra Mussels, macrophytes, and Gobies that were not prevalent in the Bay 15 years ago and to add detritus to the foodweb for completeness. We modeled the fate of 24 chemicals, 4 metals and 11 organic compounds (OCs). We described the findings of the four metals (As, Cd, Cu, Zn) in the companion paper (Gandhi et al., 2011). Here, for the 11 OCs we address three objectives: (1) compare the status of the Bay between 1988 and 2000 in terms of loadings and fate; (2) assess the residence time of contaminants in the Bay; and (3) examine the status of the Bay in 2000 with respect to contaminant guidelines for water, sediments and biota.

Modeling methods

Model framework

Below we summarize the model used in this study. The same model framework was used by Gandhi et al. (2007) to quantify the fate of mercury in the Lahontan Reservoir and Sommerfruend et al. (2010a,b) to quantify the fate of inorganic and organic chemicals in the Venice Lagoon. Full details can be found in these and other references listed below.

Fate and transport model

We used the fate and transport modeling framework of Diamond et al. (1994, 1996), which was originally based on the Quantitative Water Air Sediment Interaction (QWASI; Mackay et al., 1983) model using the fugacity/aquivalence approach of Mackay and Diamond (1989). The Bay was divided into five segments (basins) based on hydrodynamics (Figure A1 in the Appendix in the online supplemental information; Diamond et al., 1994): segment-1 (Upper Bay West), -2 (Upper Bay East), -3 (Hay Bay), -4 (Middle Bay), and -5 (Lower Bay). The water columns of segments 4 and 5 were divided into two layers, the epilimnion and hypolimnion, to account for thermal stratification. Sediment was divided into two vertical layers (surficial and lower sediments) instead of one sediment layer in the previous model of Diamond et al. (1994, 1996). This change was made to increase the fidelity of the model to reality. Contaminants transferred below the lower sediment were assumed to be "permanently" lost through burial. Air was modeled as a compartment with infinite volume and specified contaminant concentrations. Contaminant fate was modeled assuming steady-state, average annual conditions. This assumption implied that contaminant concentrations in water, sediment and biota were constant with respect to time and were supported by specified loadings. This over-simplification was necessitated by insufficient data needed to run a time dependent version of the model that could have accounted for the delayed decline in sediment concentrations in response to reduced loadings to water.

Foodweb model

The foodweb model for the Bay of Quinte was based on that of Campfens and Mackay (1997) as modified by Arnot and Gobas (2004) and Gewurtz et al. (2006). The steady-state model accounted for chemical uptake and loss processes within and between 11 trophic groups that were suggested by Marten Koops (Department of Fisheries and Oceans Canada, personal communication) for the Upper Bay segments (Figure A2). This improvement is in contrast to the six organism classes modeled in the previous version (Diamond et al., 1994, 1996). We assumed that this new trophic structure also applied to the Middle and Lower Bays.

Model parameterization

Fate and transport model

The physical-chemical properties of chemicals are listed in Table A1. Dimensions and properties of each segment and particle transport parameters (e.g. sedimentation and resuspension rates) were taken from Diamond et al. (1994) and are summarized in Table A2.

The sources of OC loadings were categorized into atmospheric input, tributaries, sewage treatment plants (STPs), industrial input, runoff, Lake Ontario, and "other." Atmospheric loadings were modeled through dry deposition of chemical sorbed to particles, wet deposition of chemical in gas- and particle-phases, and chemical absorption from the atmosphere. Meteorological data were taken from Point Petre station of the Integrated Atmospheric Deposition Network (IADN). Atmospheric concentrations of 6 OCs in the gas phase were geometric means of year 2000 measurements taken at Point Petre as part of IADN, TCDD and TCDF were obtained from Environment Canada (Tom Dann, unpublished data), and Gouin et al. (2005) (Table A3).

For those chemicals for which measured concentrations were available, loadings from tributaries, runoff, STPs and industrial emissions were calculated as the product of average volumetric flow rate and contaminant concentrations. Flow rates for tributaries Trent, Moira, Salmon, Napanee and Wilton Creek were geometric means of daily flow rates measured at the monitoring stations closest to the mouth using 2000 as the base year (Minns and Moore, 2004). Contaminant loadings were estimated for 6 STPs entering the Bay (Trenton and CFB Trenton STPs discharged into Segment 1, Napanee, Desoronto, and Belleville STPs discharged into Segment 2, and Picton STP discharged into Segments 4). Storm water loadings were not explicitly considered due to a lack of data. Three industrial sources entered Segments 1 and 4, however of these sources data were only available for TCDD and TCDF from one industrial facility discharging into the Trent River, which was treated as entering Segment 1. Flow rates of STPs and industrial sources were from the Municipal Industrial Strategy for Abatement (MISA) of the Ontario Ministry of the Environment (OMOE). Runoff and hydrologic flows from Lake Ontario and back-flows from segment-to-segment were taken from Diamond et al. (1994), presuming that they had not changed over time. All flow rates for 2000 and 1988 are summarized in Table A4 and show the percent changes in rates from 1988. Since a chemical loading also depends on water flow rates, significantly lower flow rates of Trent, Moira, Salmon and Napanee Rivers in 2000 (Table A4) may have been responsible for overall reduced loadings of several organic chemicals relative to 1988.

Although one of our objectives was to compare loadings and concentrations between 1988 and 2000, few measurements were available from which to calculate loadings. Tables 2 and A5 summarize the measured and mostly assumed concentrations that were used to obtain loading estimates for each source category.

In the absence of measured data from which to obtain loadings for every source category, we used the model to back-calculate *total* loadings. The back-calculation was done by assigning concentrations for the categorized sources of discharge and then comparing modeled results with in-Bay measured concentrations, starting with sediment and water, and if those were not available, then concentrations in biota. If in-bay measurements were lacking, then we used Lake Ontario measurements in sediment or fish (e.g. BDE 47, 17β-estradiol). In the absence of data, we assumed similar concentrations among tributaries, point sources (STPs), and runoff discharging to each segment. For contaminants for which modeled water concentrations were underestimated relative to measurements based on loadings estimated as described above, additional loadings were assigned to the category "other" in order to achieve correspondence between the measured and modeled values.

Table 1 summarizes the measured concentrations within the Bay from which loadings of the 11 OCs were back-calculated. It should be emphasized that these values are highly uncertain and loading source(s) cannot be confidently determined. As mentioned earlier, the foodweb dietary matrix used in the model pertains to the Upper Bay segments only. Therefore, the back-calculation of loadings from fish body burdens was done in the upper segments of the Bay. Another uncertainty that surrounds the estimated loadings was that we assumed that fish, from which loadings were back-calculated, resided within the Bay. Larger fish such as Walleye are known to move between the Bay and Lake Ontario, but it was beyond our scope to account for this. This omission would bias the back-calculated loadings on the low side.

Foodweb model

The fish community in the Bay consists of large piscivorous (Walleye), small piscivorous (White and Yellow Perch), planktivorous (alewife), benthivorous (Pumpkinseed, Freshwater Drum, White Sucker, Brown Bullhead, Channel Catfish, and American Eel), and Gobies (Marten Koops, DFO Canada, personal communication). Thus, the updated foodweb model structure consisted of: (1) detritus, (2) macrophytes, (3) phytoplankton, (4) zooplankton, (5) benthic Invertebrates, (6) bivalves/Zebra Mussels, (7) Gobies, (8) benthivorous fish, (9) planktivorous fish, (10) small piscivorous fish, and (11) large piscivorous fish (Figure A2).

Chemical accumulation mechanisms for fish were applied to filter feeders (bivalves/Zebra Mussels), benthic invertebrates, and zooplankton in the Bay. Dreissenids (Zebra Mussels), which arrived in the eastern basin of Lake Ontario in 1995, were the most abundant species of bivalves in the Bay of Quinte. Oligochaetes and chironomids that comprised 60% of the benthic invertebrates were used to define this trophic group (Marten Koops, DFO Canada, personal communication). Herbivorous zooplankton comprised the zooplankton trophic group. Table A6 summarizes the biomass fractions of each species in these 11 groups.

The Bay of Quinte foodweb structure was converted to an 11 × 11 predator/prey or dietary matrix (Table A7). The characteristics of each trophic level, including lipid fraction, volume, and measured chemical body burdens, were based on the weighted biomass fraction of the species that comprised each trophic level (Table A8). For species for which biomass estimates were unavailable, those species with higher biomass fractions were assumed to be representative of that trophic level. Organism volume and lipid fractions were taken from measured values from the Sport Fish Contaminant Monitoring Program (SFCMP) of OMOE (unpublished data). In the absence of data from SFCMP, values were taken from Morrison (1998). The Walleye growth rate was calculated from measured data (Ontario Ministry of Natural Resources or OMNR, unpublished data). Lipid and non-lipid absorption efficiencies were taken from Morrison et al. (1999).

Results and Discussion

Model evaluation

Fate and transport

The model was first evaluated for its ability to reproduce observed trends using metals concentrations for which most measured data were available (Gandhi et al., 2011). Model performance for OCs was evaluated for ΣPCB and Pentachlorophenol (PCP) by comparing the results from this work

Table 1. Comparison of measured and modeled concentrations of OCs in water, sediment and biota.*

	Water (ng/L)		Sediment (ng/g)		Benthic Invertebrates		Zebra Mussels		Planktivorous Fish		Benthivorous Fish		Large Piscivorous	
Chemical	Mod.	Meas.	Mod.	Meas.	Mod.	Meas.	Mod.	Meas.	Mod.	Meas.	Mod.	Meas.	Mod.	Meas.
PCB - 018	0.001	NA	0.1	NA	0.29	NA	0.01	NA	0.06	NA	0.35	NA	1.65	NA
PCB - 028	0.001	^{a}0.024	0.12	^{c}2.4	0.33	^{c}0.65	0.04	NA	0.08	^{c}0.06	0.43	^{c}0.53	2.28	^{c}0.20
PCB - 052	0.02	^{a}0.05	1.09	^{c}4.3	1.38	^{c}2.73	0.78	NA	0.74	^{c}0.69	3.045	^{c}3.99	9.64	^{c}4.53
PCB - 101	0.003	^{a}0.0058	0.6	^{c}5.5	1.52	^{c}5.15	0.17	NA	0.64	^{c}2.11	2.9	^{c}10.34	22.9	^{c}18.64
PCB - 105	0.0001	^{a}0.0008	0.1	$^{d}0.18 \pm 0.025$	0.27	^{c}1.09	0.02	^{d}2.8	0.11	^{c}0.49	0.53	^{c}2.195	4.215	^{c}3.953
PCB - 118	0.004	^{a}0.0042	0.36	$^{d}0.35 \pm 0.05$	0.87	^{c}5.12	0.07	^{d}7.4	0.34	^{c}2.09	1.73	^{c}10.27	13.69	^{c}18.50
PCB - 138	0.0016	^{a}0.0018	4.7	^{c}6	3.69	^{c}8.58	0.32	NA	1.65	^{c}7.11	7.34	^{c}27.04	55.94	^{c}84.31
PCB - 153	0.001	^{a}0.0014	0.62	^{c}4.6	1.33	^{c}6.24	0.11	NA	0.58	^{c}4.72	2.03	^{c}18.56	19.38	^{c}54.40
PCB - 180	0.02	^{a}0.01	4.42	^{c}2.8	3.6	^{c}4.53	1.05	NA	4.23	^{c}4.83	8.22	^{c}16.81	38.22	^{c}60.83
ΣPCB	0.7	^{b}ND-2.0	130	^{f}120–137	166.5	NA	80.88	NA	229.95	NA	453.88	^{h}365.07	3294	^{h}3080
2,3,7,8-TCDD	0.0000123	^{a}0.00000007	0.0002	$^{d}<0.0008$	0.0152	NA	0.0004	$^{d}<0.0006$	0.0085	NA	0.008	^{h}0.006	0.26	NA
2,3,7,8-TCDF	0.00053	^{a}0.00008	0.0022	$^{d}0.0025 \pm 0.0002$	0.2	NA	0.0029	^{d}0.0067	0.11	NA	0.005	^{h}0.002	3.39	NA
Mirex	0.006	^{b}ND-0.11	2.48	^{b}3.5	1.53	NA	0.54	NA	1.78	NA	5.74	^{h}5.00	25.17	^{h}23.30
Atiazine	75–98	^{e}50–100	0.78	NA	1.25	NA	2.21	NA	1.57	NA	1.51	NA	2.03	NA
B[a]P	0.79	^{b} 0.26	110.6	^{f}145	147.35	NA	83.46	NA	172.5	NA	364.29	NA	2599	NA
Dieldrin	0.06	^{b}0.155–0.34	0.22	^{b}0.11	0.26	NA	0.17	NA	0.15	NA	0.11	NA	0.23	NA
p,p-DDT	0.006	NA	0.57	NA	0.62	NA	0.34	NA	0.83	NA	3.66	^{h}5	12.31	^{h}15
HCB	0.02	^{b}0.003–0.3	2	^{f}1.5–2.5	2.01	NA	1.17	NA	1.97	NA	4.24	^{h}3.43	27.1	NA
17β-estradiol	0.01	NA	0.001	NA	0.01	NA	0.03	NA	0.02	NA	0.003	NA	0.02	NA
BDE-47	0.007	^{i}0.005	2.31	^{g}3.00	5.91	NA	0.73	NA	2.08	NA	13.19	NA	77.05	^{i}95+22

^{a}Morrison et al. (1999); ^{b}Booty et al. (2005); ^{c}Morrison (1998); ^{d}Marvin et al. (2002); ^{e}Struger et al. (2005); ^{f}Thorburn (2004); ^{g}Song et al. (2005); ^{h}unpublished data (SFCMP, OMOE); ^{i}Luross et al. (2002); ^{j}Luckey and Litten (2005). *Most measured data from Lake Ontario except for biota. Modeled data averaged over all segments of the Bay of Quinte.

representative of 2000 and the previous model that was representative of 1988 (Diamond et al., 1994, 1996), where the later are listed in Table A9. Both models predicted water and sediment concentrations within 10% for PCBs and 8% for PCP (Figure A3). The discrepancy between model results was likely due to changes in the foodweb structure, the inclusion of the second layer of sediment in the updated model in addition to the slightly different parameterization of year 2000 contaminant loadings.

Next we compared the estimated concentrations for year 2000 with available measurements (Table 1). Note that most modeled water and sediment concentrations were averaged over the entire Bay, except water concentrations of mirex, B[*a*]P, dieldrin, and PCB congeners for which model results from Segment 5 were compared with those from Lake Ontario given the lack of measured concentrations from the Bay. Modeled concentrations of surface sediment were compared with measured concentrations from surface grab samples or modeled lower sediment concentrations if measured values were taken from deeper sediment samples. Although the modeled concentrations were geographically averaged, we focused the comparison on the Upper Bay since the modeled foodweb structure represents those segments. The modeled concentrations were mostly within less than an order of magnitude of the measured sediment values.

Foodweb

We compared the foodweb model results for organism concentrations in Segments 1 and 2 since the model's dietary matrix was based on these segments. Estimated concentrations of the Bay's foodweb were compared between 1988 (Diamond et al., 1994) and 2000 (present study), except for the PCB congeners for which 2000 estimates were compared with those from Morrison (1998). The comparison was approximate since the foodweb structure significantly changed from 1988 to 2000 and also differed from that of Morrison (1998) due to the invasion of Zebra Mussels and Gobies. For several chemicals such as mirex and DDT, the comparison between measured and modeled body-burden concentrations evaluated the ability of the model to provide back-calculated loadings.

Modeled concentrations were within an order of magnitude of the measured data for contaminants in different trophic levels in the Upper Bay of Quinte (Figure A4). The concentrations of most chemicals decreased by ∼30% for B[*a*]P to 80% for ΣPCB between 1988 to 2000 except for HCB that remained constant. ΣPCB concentrations in fish decreased by ∼half over this time (OMOE, unpublished data). Estimated congener specific PCB concentrations for 2000 were similar to those presented by Morrison (1998) for 1995. We acknowledge that decreases in fish concentrations between 1988 and 2000 could at least partly be attributable to declines in analytical detection limits.

Sources and fate of chemicals

The calibrated model was used to investigate contaminant loadings, fate and persistence. The back-calculated loadings and concentrations are summarized in Table 2. Below we describe the loading and fate of organic chemicals studied.

ΣPCBs

ΣPCBs were modeled because congener specific measurements were only available for some congeners. The obvious short coming of modeling ΣPCBs was that the model treats this group of chemicals as a single compound with "average" values for physical-chemical properties that were intended to approximate the mixture.

Modeled concentrations of ΣPCBs (from PCB-47 to -209) in sediment and biota were within the standard error of the measured values. The estimated total loadings of ΣPCBs to the Bay decreased from ∼79 in 1988 to ∼15 kg year^{-1} in 2000 (Figure 1a). Based on the data used to derive the quantitative loading estimates and the discrepancy between measured and model sediment and fish concentrations, the model suggested an "extra" loading of 2.8 kg year^{-1} of ΣPCBs entering Segment 2. This additional loading could be from the Moira River, which was supported by the pattern of measured ΣPCBs in sediment (Environment Canada, 2001, unpublished data; Frank et al., 1980), and/or inputs from STPs and urban runoff (Diamond et al., 2010). Another likely explanation is that sediment and water were not at steady state but that sediment concentrations reflect past conditions when water concentrations were higher. It is also possible that fish concentrations show enrichment from the benthic foodweb. In addition, there is a possibility of "hot spots" in sediment concentrations from local contamination that are not representative of entire segments.

Based on the loading estimates, tributaries, 'other', and atmospheric deposition were the main sources of ΣPCBs to the Bay, contributing

Table 2. Source concentrations and loadings of OCs to the Bay. Measured concentrations are indicated by the source of data. All other values are back-calculated as described in the text.

Chemical		Tributaries	STPs	Runoff	L. Ontario	Industrial	Others
ΣPCB	Conc. (ng L^{-1})	[a]2.50E+00	N	1.00E-03	[c]4.00E-03	N	
	Loading (kg y^{-1})	1.50E+01		4.74E-05	6.24E-02		[f]2.67
PCB - 018	Conc. (ng L^{-1})	1.00E-03	N	1.00E-03	[c]1.39E-03	N	
	Loading (kg y^{-1})	1.14E-02		4.74E-05	2.17E-02		
PCB - 028	Conc. (ng L^{-1})	1.00E-03	N	1.00E-03	[c]1.00E-03	N	
	Loading (kg y^{-1})	1.13E-02		4.74E-05	1.56E-02		
PCB - 052	Conc. (ng L^{-1})	5.00E-02	N	1.00E-03	[c]1.48E-03	N	
	Loading (kg y^{-1})	2.07E-01		4.74E-05	2.31E-02		
PCB - 101	Conc. (ng L^{-1})	1.00E-02	N	1.00E-03	[c]1.00E-05	N	
	Loading (kg y^{-1})	1.13E-01		4.74E-05	1.56E-04		
PCB - 105	Conc. (ng L^{-1})	1.60E-04	N	1.00E-03	[c]1.60E-04	N	
	Loading (kg y^{-1})	1.83E-03		4.74E-05	2.49E-03		
PCB - 118	Conc. (ng L^{-1})	1.00E-02	N	1.00E-03	[c]3.90E-04	N	
	Loading (kg y^{-1})	1.13E-01		4.74E-05	6.08E-03		
PCB - 138	Conc. (ng L^{-1})	1.00E-01	N	1.00E-03	[c]1.00E-05	N	
	Loading (kg y^{-1})	8.69E-01		4.74E-05	1.56E-04		
PCB - 153	Conc. (ng L^{-1})	1.00E-02	N	1.00E-03	[c]3.90E-04	N	
	Loading (kg y^{-1})	1.13E-01		4.74E-05	6.08E-03		
PCB - 180	Conc. (ng L^{-1})	1.00E-01	N	1.00E-03	[c]2.10E-04	N	
	Loading (kg y^{-1})	4.12E-01		4.74E-05	3.27E-03		
2,3,7,8-TCDD	Conc. (ng L^{-1})	1.00E-07	1.00E-04	N	[c]3.20E-06	[e]0.00153	
	Loading (kg y^{-1})	1.41E-06	2.27E-06		1.56E-06	2.78E-06	[g]2.76E-06
2,3,7,8-TCDF	Conc. (ng L^{-1})	1.00E-07	1.00E-04	N	[c]2.28E-06	[e]0.00133	
	Loading (kg y^{-1})	1.41E-06	2.27E-06		3.56E-06	2.42E-06	[g]3.04E-05
Mirex	Conc. (ng L^{-1})	[b]1.00E-03	N	1.00E-02	1.00E-03	N	
	Loading (kg y^{-1})	1.23E-02		4.74E-03	1.56E-02		
Atrazine	Conc. (ng L^{-1})	5.50E+01	N	1.00E+00	[d]1.20E+02	N	
	Loading (kg y^{-1})	3.25E+02		4.74E-01	1.87E+03		
B[a]P	Conc. (ng L^{-1})	[b]4.30E-01	N	60-120	2.60E-01	N	
	Loading (kg y^{-1})	1.81E+00		2.35E+01	4.05E+00		[h]2.08E+01
Dieldrin	Conc. (ng L^{-1})	4.00E-02	N	N	[c]5.30E-02	N	
	Loading (kg y^{-1})	4.57E-01			8.26E-01		
p,p-DDT	Conc. (ng L^{-1})	[b]1.00E-02	N	1.00E-01	[c]8.10E-04	N	
	Loading (kg y^{-1})	1.14E-01		4.74E-03	1.26E-02		
HCB	Conc. (ng L^{-1})	[b]3.00E-02	N	N	[c]4.31E-03	N	
	Loading (kg y^{-1})	1.04E-01			6.72E-02		[h]1.11
17β-estradiol	Conc. (ng L^{-1})	1.00E-03	1.00E+00	N	1.00E-03	N	
	Loading (kg y^{-1})	4.17E-03	2.27E-02		1.56E-02		
BDE-47	Conc. (ng L^{-1})	[c]5.05E-03	[i]1.05E+01	N	[c]5.05E-03	N	
	Loading (kg y^{-1})	2.08E-02	2.15E-01		7.87E-02		

[a]Trent River (OMOE, unpublished data), other tributaries assigned lower concentration; [b]Boyd and Biberhofer (1999); [c]Luckey and Litten (2005); [d]Struger et al. (2004); [e]OMOE (unpublished data 2000), measured for Norampac; [f]Segment 2 (estimated loadings from "other" sources to segment 2); [g]Segment 1 (estimated loadings from "other" sources to segment 1); [h]Segment 1 & 2; [i]North (2004); [N]negligible.

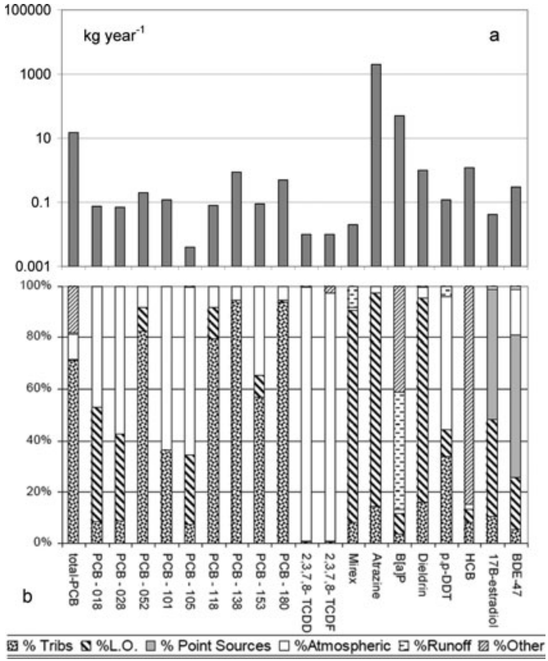

Figure 1. (a) Total loadings (kg year^{-1}) of OCs into the Bay of Quinte, and (b) percentage contributions from various sources estimated for the year 2000.

approximately 70%, 20% and 10%, respectively, to total loadings (Figure 1b). The ΣPCBs discharged from the tributaries to the Upper Bay segments were mainly transported by advective flow to the Lower Bay and then Lake Ontario. About 10–20% of the ΣPCBs loadings were retained by the sediment where they would be ultimately buried and transformed (Figure 2). Volatilization accounted for about 10% of the total loss, followed by $<5\%$ for transformation in water and sediment (Figure 2). Losses due to transformation were highly uncertain in both water and sediment as the transformations rates were poorly known (Jones and de Voogt, 1999).

PCB congeners

Since assessing the status of ΣPCBs was largely a fitting exercise, we assessed the fate of 9 congeners ranging from trichlorobiphenyl (PCB-18) to heptachlorobiphenyl (PCB-180) using the data from Morrison et al. (1999) and Morrison (1998).

Estimated total loadings for each congener ranged from 4 to 870 g year^{-1} for PCB-105 and -180, respectively (Figure 1a). The sum of total loadings for the 9 congeners was 1.85 kg year^{-1} or about 10 times less than total loadings of ΣPCBs. We attribute this discrepancy to the fewer congeners considered in the former, uncertainties in physical-chemical properties that accompany the later estimate, and explanations offered above regarding the "extra" loadings.

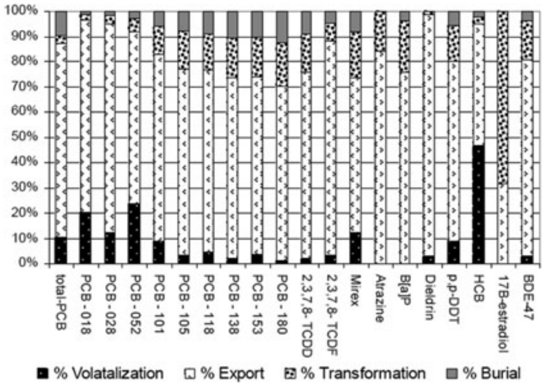

Figure 2. Percentage loss processes of OCs from the Bay of Quinte estimated using year 2000 hydrodynamics and loading data.

The congener-specific loadings suggest that the main source shifted from gas-phase absorption for the less chlorinated congeners (e.g. PCB-18, 52, 101), to tributaries for the highly chlorinated congeners (e.g. PCB-118, 138, 153 and 180), whereas a few congeners (e.g. PCB-28, PCB-105) came from Lake Ontario (Figure 1b). Advective transport (export) accounted for ∼70% of PCB loss from the Bay (Figure 2), with the remainder due to volatilization (lower chlorinated congeners) or burial and transformation (higher chlorinated congeners) (Figure 2). Although transformation rates were poorly known and a slow half-life was specified (55,000 h; Mackay et al., 1992), transformation of more highly chlorinated PCB was attributed to the ∼50 years residence time of PCB in sediment.

2,3,7,8-TCDD and 2,3,7,8-TCDF

Loadings of 2,3,7,8-TCDD (TCDD) and 2,3,7,8-TCDF (TCDF) were back-calculated using measured data in sediment of the Bay, Zebra Mussels taken from segment 5 (Indian point; Marvin et al., 2002), and Channel Catfish (as representative of benthivorous fish) in the Upper Bay (OMOE, unpublished data). Total loadings of both compounds to the Bay were estimated at ∼0.01 g day^{-1} each, mainly through atmospheric deposition (Figure 1) in comparison to 0.56 and 0.79 g day^{-1} for TCDD and TCDF, respectively, in 1988.

The 1988 modeling results suggested that TCDF originated mainly from atmospheric deposition and TCDD from incursions of Lake Ontario water

(Diamond et al., 1994). Despite differences in loading data, the same conclusion was reached with this modeling exercise; >90% of loadings were from atmospheric sources and ∼3% of TCDF from other source(s) possibly STPs. Discharges from Norampac contributed <0.5% of total TCDD and TCDF loadings to the Bay. Approximately ∼73 and 85% of the total loadings of TCDD and TCDF were estimated to be removed by export, respectively (Figure 2). Transformation in, and burial from sediment contributed ∼15% and 9% of total loss for TCDD and 8% and 4% for TCDF, respectively (Figure 2). As with PCBs, the sediment transformation rate was highly uncertain but was set at the slow half-life of 100,000 h (Mackay et al., 1992): transformation losses can be attributed to their long residence time in sediment.

Mirex

Mirex is a persistent, bioaccumulative and toxic pesticide that was banned in 1978 in Canada but remains pervasive in Lake Ontario, in particular (Makarewicz et al., 2003). Loadings to the Bay were back-calculated using measured concentrations in the American Eel, Channel Catfish and Walleye in the Upper Bay (OMOE, unpublished data). Modeled water and sediment concentrations from Segments 5 were within 20% of the measured values from Lake Ontario (Booty et al., 2005). Total loadings of mirex have decreased from 0.9 to 0.02 kg year^{-1} from 1988 to 2000 (Figure A4). Lake Ontario contributed ∼85% and tributaries and runoff were the presumed sources of the remainder of total loadings into the Bay (Figure 1), which is similar to the results of Diamond et al. (1994). More than 50% of total mirex was lost via export and the rest through transformation (18%), volatilization (12%), and burial (8%) (Figure 2). The model results suggested that the Bay was a net sink for mirex.

Atrazine

Since atrazine is more hydrophilic than the older generation of organochlorine pesticides, it is detected more frequently in water than in sediment and biota. Modeling results for atrazine in 1988 were illustrative due to a lack of data. For this study, the loadings were back-calculated using several measured open water concentration from the Upper and Middle Bay and Lake Ontario (Struger et al., 2004). The atmospheric concentration was taken from Schottler and Eisenreich (1997) for Lake Ontario.

Estimated total loadings of atrazine were ∼2000 kg year^{-1} (Figures 1 and A4). Lake Ontario contributed ∼80% of the total loadings, followed by tributaries (Figure 1). This loading pattern was consistent with atrazine use in watersheds of southern Lake Ontario and the Bay of Quinte (Schwab and Beletsky, 1998). Atrazine was mainly lost by export followed by transformation in the water column (Figure 2).

Benzo[a]pyrene

Emissions of polyaromatic hydrocarbons (PAHs), including B[*a*]P, from natural and anthropogenic sources (mostly combustion) continue unabated. Modeled concentrations of B[*a*]P were obtained from back-calculation. In Segments 1 and 2, modeled concentrations were within 30% of measured values after an “extra” loading of ∼20 kg year^{-1} was included (Table 1). Total loadings of B[*a*]P were estimated at ∼50 kg year^{-1} in 2000 (Figure 1) compared to 80 kg year^{-1} in 1988 (Figure A4). Urban runoff contributed ∼46% or 23 kg year^{-1}(Figure 1) with the additional source(s) contributing ∼40% of the total loadings. Possibilities for this “extra” loading include local urban sources such as pavement runoff (Mahler et al., 2005) and STPs, emissions from vehicle traffic and other local combustion sources, and/or unknown sources such as emissions from boating. Results showed that B[*a*]P was lost through export (75%), transformation (20%) and burial (5%) (Figure 2), similarly to that estimated by Diamond et al. (1994).

Dieldrin

Similarly to mirex, dieldrin was used as a pesticide in the past but has not been used in Canada for over 20 years (Thomas, 1995); however, its persistence maintains current environmental concentrations. Since measurements from the Bay of Quinte were not available, loadings were back-calculated from Lake Ontario water (Luckey and Litten, 2005) and sediment concentrations (Booty et al., 2005). Because of high uncertainties in loading estimates, the results for dieldrin are illustrative. Total loadings of dieldrin were estimated at ∼1 kg year^{-1} (Figure 1), 40% less than that from 10 years earlier (1.7 kg year^{-1}; Figure A4). It was lost mainly through export (94%) and volatilization (6%; Figure 2).

DDT

Loadings of DDT to the Bay were back-calculated using the measured concentrations in Brown Bullhead and Walleye in the Upper Bay (OMOE, unpublished data) in addition to the measured air (IADN) and open water concentrations from Lake Ontario (Luckey and Litten, 2005). Estimated total loadings of DDT of ~0.12 kg year^{-1} in 2000 (Figure 1) have decreased by over an order of magnitude from 2 kg year^{-1} in 1988 (Figure A4). DDT was estimated to enter the Bay through atmospheric deposition (50%) followed by tributaries loadings and Lake Ontario (Figure 1) although this distribution was highly uncertain. It was lost from the Bay mostly by export (71%), transformation (14%), volatilization (9%) and burial (5%; Figure 2).

Hexachlorobenzene

HCB is a persistent, bioaccumulative and toxic pesticide that has not been used in Canada for decades; however, small amounts may still be discharged into the environment since HCB is a byproduct of the synthesis of chlorinated solvents and some pesticides (Great Lakes Binational Toxics Strategy Draft, 1999). The loadings and fate of HCB for 1988 were illustrative due to the lack of measured data. In the present study, loadings were back-calculated from sediment concentrations (Thorburn, 2004) and the body burdens of Channel Catfish in the Upper Bay. The estimated loading from tributaries and atmospheric deposition were ~one tenth of the 1.1 kg year^{-1} estimated by the model to enter Segments 1 and 2 in order to reconcile measured and modeled sediment concentrations (Table 2).

The total loadings of HCB into the Bay of Quinte decreased from ~4.5 to ~1.2 kg year^{-1} in 1988 and 2000, respectively (Figure A4). However, this conclusion was based on an "unknown" loading of 1.1 kg year^{-1}, that accounts for ~85% of the total loadings into the Bay. This additional source is unlikely from tributaries given the volatile nature of HCB and is suspect considering the magnitude of the loading and declining uses, production and/or cycling of HCB in the environment (Great Lakes Binational Toxics Strategy Draft, 1999). A likely explanation is that HCB in sediment in Segments 1 and 2 has not yet reached steady state with respect to the water column which can respond rapidly to lower loadings in 2000 relative to 1988. Should this be the case, then the additional source of HCB is fictitious and was only used to "fit" the current measured HCB sediment concentrations which were estimated to have a ~30 year residence time (Figure A5). Due to its high vapor pressure, the main loss pathway for HCB was volatilization from the Bay. Loss from the sediment was due to burial primarily (Figure 2), because of its long sediment residence time.

17β-estradiol

17β-estradiol is a natural hormone that can cause several adverse effects in fish such as feminization and birth defects (Kashiwada et al., 2002). In the Bay of Quinte, Kavanagh et al. (2004) observed intersex gonads in 22–44% of the male White Perch and suggested that estrogenic substances, such as 17β-estradiol, could be responsible for this.

Sources of 17β-estradiol into the Bay were presumed to be STP discharges, and possibly agricultural runoff from fields fertilized with manure or fields on which livestock were maintained. Since there were no measured values of estrogenic compounds from STPs discharging into the Bay, average concentrations from four STPs in Toronto were used (Lee et al., 2004). Concentrations in tributaries and Lake Ontario were taken from Quiros et al. (2005) who reported the average of 17β-estradiol concentrations over a 20 month period in Portuguese rivers. The atmospheric concentration of this compound was assumed to be negligible, which is reasonable given its low volatility and high water solubility.

Loadings of 17β-estradiol into the Bay were estimated to be ~0.04 kg year^{-1} and were, of course, dominated by loadings from STPs (Figure 1). 17β-estradiol was estimated to be lost by transformation (66%) and export (34%) (Figure 2). Due to its high solubility, 80% of the total mass was expected to reside in the water column. The model predicted an average annual water concentration of ~0.01 ng L^{-1} in the Upper Bay segments, which is 100 times below the range at which 17β-estradiol water concentrations can potentially cause reproductive effects in fish (Kavanagh et al., 2004). Although our model did not provide spatially resolved results, it is plausible that 17β-estradiol concentrations at the outfall of the STPs could have been within the range that could cause adverse effects.

BDE-47

BDE-47 is one of the main congeners of the penta formulation of polybrominated diphenyl ethers (PBDEs) that were used as flame retardants mostly in polyurethane foam furniture and other products until controls came into place in late 2004. Due to a lack of data for the Bay of Quinte, the results for this compound were entirely illustrative. We assumed an atmospheric concentration of 4.6 pg m^{-3} which was reported by Strandberg et al. (2001) for Great Lakes air.

Loadings were back-calculated based on sediment and Lake Trout concentrations from Lake Ontario (Luross et al., 2002; Song et al., 2005). The STP effluent concentration was taken from North (2004) who measured BDE-47 in the effluent of a waste water treatment plant in California. Since there were limited measurements of PBDEs in surface waters at the time when data were compiled, the concentration of BDE-47 in Eastern Lake Ontario (Luckey and Litten, 2005) was used for tributary concentrations.

Total loadings of BDE-47 were estimated to be ~0.3 kg $year^{-1}$, mainly originating from STPs (55%) followed by Lake Ontario (20%) and atmospheric deposition (18%). Tributaries contributed about 10% of the BDE-47 total loadings. Losses were due to export followed by transformation in the sediment and burial. Volatilization accounted for 3% of the total loss from the Bay.

Residence times

Chemical residence time is defined as the time necessary for concentrations to decrease by 63% after loadings have ceased. It is calculated as the ratio of chemical mass into total removal rate from a compartment. Chemical loss processes were advective flow, volatilization, transformation, and burial to deeper sediment layers. Figure A5 illustrates residence times of OCs in water and surface sediment which were averaged over all segments of the Bay. Residence times in water ranged from 2 (mirex) to 10 (atrazine) days. However, residence times for OCs in the upper sediment layer (top 3 cm) were estimated to range from <1 (atrazine) to ~50 (ΣPCBs) years. The uncertainties in estimates of OC residence time in sediment were due to large uncertainties in their transformation rates. The short residence time of the water column and slow response of the sediment is consistent with the previous modeling effort and many aquatic systems. The conclusion that can be drawn from this analysis is that chemical concentrations in the water reflect current loadings plus contributions from contaminated sediments. Reductions in water column concentrations are slowed by the long residence time of chemicals in the sediments. However, water column concentrations are anticipated to, and have fallen in response to reduced loadings.

Provincial sediment quality and fish consumption guidelines

Measured and modeled ΣPCBs in the sediment of Segments 1, 2 (which are in agreement) and 5 exceeded by a factor of 2 the Lowest Effects Level (LEL) of 70 ng g^{-1} specified by the OMOE. The model suggested that for sediment concentrations to decrease from the measured and modeled concentrations of 120 and 140 ng g^{-1}, respectively, to the LEL, the concentrations in the Trent River would have to decrease from 2.5 to 1 ng L^{-1}.

Other chemicals such as HCB, mirex, *p,p′*-DDT, and dieldrin met the LELs of 20, 7, 8 and 2 ng g^{-1}, respectively, in the sediment of all segments of the Bay. As mentioned above, the modeled concentrations were averaged over a segment and therefore did not account for sediment “hot spots” that have been found in the Upper Bay.

In nearly all cases, modeled and measured concentrations of ΣPCBs, TCDD, and TCDF in piscivorous fish in the Bay of Quinte exceeded Ontario consumption restrictions for women of childbearing age and children set at 153, 0.00162, and 0.00162 ng g^{-1}, respectively, as well as concentration limits for the general population set at 1220, 0.0129, 0.0129 ng g^{-1}, respectively (Figure A6). Measured and modeled concentrations of mirex approached the consumption guideline of 82 ng g^{-1} (Figure A6). Other chemicals in fish were not of concern (OMOE, 2009).

Conclusions

A mass balance model developed 20 years ago for estimating contaminant fate and transport in the Bay of Quinte and transfer through the Bay’s foodweb (Diamond et al., 1994) was revised in order to compare loadings and concentrations between 1988 and 2000. Estimated loadings, fate, and concentrations in water, sediment and fish were thus analyzed for 11 organic chemicals. Most model results relied on the use of the model to back-calculate loadings from measured concentrations because of the lack of loading data.

Although the modeling results are couched in uncertainty, they suggest that chemical loadings decreased by 1–2 orders of magnitude for TCDD/F to ~40% for B[*a*]P and ~80% for ΣPCB between

1988 and 2000. In addition to lower concentrations contributing to this reduction, lower analytical detection limits and lower tributary discharges in 2000 relative to 1988 could also have been responsible. Loadings of mirex, atrazine and HCB were too uncertain to compare due to lack of data. The estimated loadings for year 2000 ranged from ~0.01 g year^{-1} of TCDD and TCDF each to 2000 kg year^{-1} of atrazine. Atmospheric deposition was estimated as the main source of lower molecular weight PCBs, TCDD, TCDF, and DDT. Loadings of higher molecular weight PCBs were dominated by contributions from tributaries, and mirex, dieldrin and atrazine were from the incursions of Lake Ontario water into the Lower Bay. The source(s) of HCB were uncertain, B[*a*]P were assumed to come from urban sources, and 17β-estradiol and BDE-47 from STP discharges. Loadings from STPs and urban runoff were most uncertain and possibly contributed more than other sources.

Export from the Bay to Lake Ontario was the main loss pathway for OCs due to the dynamic nature of this system with the exceptions of HCB and 17β-estradiol for which losses were dominated by volatilization and transformation, respectively. The residence time of chemicals in the water of the entire Bay was estimated to vary from 2 (ΣPCB) to 10 days (atrazine). In contrast, the residence time in sediment was estimated to be much longer at less <1 year for atrazine to ~50 years for ΣPCB. The concentrations of ΣPCBs, dieldrin, mirex and DDT in fish declined between 1988 and 2000 but concentrations of ΣPCBs, TCDD and TCDF remained above the consumption guidline.

Model results suggest that industrial sources were not major contributors to OCs in the Bay. A first step towards reducing concentrations should be first determining if STPs and urban runoff are important sources, particularly for PCBs, B[*a*]P, 17β-estradiol and BDE-47. It would be challenging to control concentrations of dieldrin, mirex, TCDD/TCDF, and atrazine as they appear to originate from non-point sources including tributaries, the atmosphere and/or Lake Ontario.

Finally, as noted throughout, the data gaps and many uncertainties and assumptions made because of a lack of data constrained our ability to provide information to enable managers to assess whether remedial actions taken have been beneficial. While we can conclude with some confidence that loadings of all compounds (except 17β-estradiol and BDE-47) have decreased in the Bay of Quinte between 1988 and 2000, it is difficult to take the conclusions any farther with one exception – there has definitely been a decrease in monitoring efforts and even more so, a decrease in the institutional capacity to assess the status of the Bay.

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Supplemental material

Supplemental data for this article can be accessed on the publisher's website.

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Appendix

Table A1. Physical chemical properties of organic chemicals modeled in the Bay of Quinte.

Chemical	MWt (g mol^{-1})	MPt (C)	LogKow	Solubility (mol m^{-3})	*Henry's Law Constant (Pa m^3 mol^{-1})	Transformation Half-lifeWater (hr)	Transformation Half-life Sediment (hr)
a PCB - 018	257.5	44	5.55	0.001553398	25.33125	17000	55000
a PCB - 028	257.5	57	5.62	0.001048544	20.265	17000	55000
a PCB - 052	292	87	6.09	0.000164384	20.265	55000	55000
a PCB - 101	326.4	76.5	6.8	4.72E-05	9.11925	55000	55000
a PCB - 105	326.4	105	6.94	1.04E-05	5.8667175	55000	55000
a PCB - 118	326.4	107	7.12	1.19E-05	6.0693675	55000	55000
a PCB - 138	360.9	80	7.44	4.10E-06	2.127825	55000	55000
a PCB - 153	360.9	103	7.75	2.63E-06	2.330475	55000	55000
a PCB - 180	395.3	110	7.92	9.31E-07	1.01325	55000	55000
b ΣPCB	326	0	6.6	0.0000736	12.228	55000	500000
b 2,3,7,8- TCDD	322	305	6.8	5.99E-08	3.34	100000	100000
b 2,3,7,8- TCDF	306	227	6.1	0.00000137	1.46	100000	100000
b Mirex	545.59	485	e 7.18	e 0.000156	e 0.129	4000	100000
b Atrazine	214.68	174	2.4	0.139	0.000288	1000	1000
b B[a]P	252.32	175	6.04	0.0000151	0.0465	10000	30000
b Dieldrin	380.9	176	5.1	0.000446	1.12	100000	100000
b p,p-DDT	354.48	108.5	6.91	1.55E-05	1.29	50000	60000
c 17B-estradiol	272.39	150	3.94	0.0477	0.000000629	96	1200
b HCB	284.78	231.8	5.73	2.18E-05	172.2525	100000	100000
d BDE-47	485.5	78.75	6.11	0.000266	1.6078	15000	45000

a Mackay et al. (1992); b Diamond et al. (1994); c Kuster et al. (2004), Lai et al. (2000);

d Wania and Dugani (2003); e USEPA (EPISUITE - V.3.12)

Table A2. Physical characteristics of segments and particle transport rates in the Bay of Quinte.

Segment	**Upper West**	**Upper East**	**Hay Bay**	**Middle Epi**	**Middle Hypo**	**Lower Epi**	**Lower Hypo**
Dimensions							
Area (10^6 m^2)	37.5	98.9	21.6	27.6	27.6	71.8	71.8
Water Depth (m)	3.3	2.1	2.2	5.2	2.1	8.3	16.1
Volume (10^6 m^3)	122	354	48	144	58	599	1157
Upper Sed. Depth (m)	0.03	0.03	0.03	-	0.03	-	0.03
Lower Sed. Depth (m)	0.2	0.2	0.2	-	0.2	-	0.2
Particles							
Density (kg L^{-1})	1.8	1.8	1.8	1.8	1.8	1.8	1.8
Organic Carbon (g g^{-1})	0.24	0.26	0.3	0.32	0.32	0.32	0.32
Inflow Conc. (mg L^{-1})	10	9	7	6.8	6.8	3.1	3.1
Upper Sediment							
Density (kg L^{-1})	2	2	2	-	2	-	2
Organic Carbon (g g^{-1})	0.13	0.12	0.08	-	0.09	-	0.06
Porosity	0.06	0.05	0.045	-	0.045	-	
Lower Sediment							
Density (kg L^{-1})	2	2	2	-	2	-	2
Organic Carbon (g g^{-1})	0.1	0.1	0.1	-	0.1	-	0.1
Porosity	0.2	0.2	0.2	-	0.2	-	0.2
Particle Balance							
Deposition (g m^{-2} d^{-1})	15	10	4	8	8	5	5

Resuspension (g m^{-2} d^{-1})	13.5	6.7	1	-	3	-	1.8
Burial Used. (g m^{-2} d^{-1})	0.7	0.29	0.28	-	0.24	-	0.19
[a]Mixing_UtoL_Sed (g m^{-2} d^{-1})	0.5	0.5	0.5	-	0.5	-	0.5
[a]Mixing_LtoU_Sed (g m^{-2} d^{-1})	0.3	0.3	0.3	-	0.3	-	0.3
[a]Burial Lsed.(g m^{-2} d^{-1})	0.5	0.2	0.2	-	0.2	-	0.05

Source: Diamond et al. (1994)

[a] assumed values

Table A3. Average seasonal concentrations of OCs in the gas phase of air measured at Point Petre used to calculate atmospheric deposition of these contaminants to the Bay for the year 2000.

a **Chemical (pg m^{-3})**	**Winter**	**Spring**	**Summer**	**Fall**
PCB – 018	7.65	9.49	8.9	6.68
PCB – 028	3.86	4.55	4.94	3.35
PCB – 052	3.22	4.25	5.38	3.41
PCB – 101	1.03	1.42	1.91	4.21
PCB – 105	0.12	0.14	0.21	0.18
PCB – 118	NA	NA	NA	NA
PCB – 138	0.15	0.184	0.28	0.2
PCB – 153	0.4	0.49	2.78	0.56
PCB – 180	0.133	0.08	0.17	0.11
ΣPCB	25.523	42.97	54.88	38.02
2,3,7,8- TCDD	b ND	b ND	b ND	b ND
2,3,7,8- TCDF	b 0.013	b 0.01	b 0.008	b 0.009
Mirex	0.094	0.158	0.229	6.53
Atrazine	NA	NA	NA	NA
B[a]P	1.643	1.643	1.3	1.643
Dieldrin	5.92	7.69	11.95	N/A
p,p-DDT	0.98	2.52	1.59	0.99
17B-estradiol	NA	NA	NA	NA
HCB	33.81	33.86	20.53	24.79
BDE-47	c 4.6	NA	NA	NA

a IADN, Point Petre station, 2000 (Pierrette Blanchard, MSC, unpublished data)

b Tom Dann (Environment Canada, unpublished data)

c Gouin et al. (2005)

NA: not available

ND: non-detectable (0.002-0.007 pg m^{-3})

Table A4. Comparison of water flow rates of various sources used to calculate loadings of organic chemicals to the Bay for years 2000 and 1988.

Sources	**2000** **Flow** (m^3 day^{-1})	**1988** **Flow** (m^3 day^{-1}) [c]	**% Change in 2000**
Trent River	9.87e+06 [a]	1.33E+07	-26.0%
Trenton STP	7.81e+03 [b]	1.07E+04	-26.9%
CFB Trenton	5.18e+03 [b]	5.18E+03	-0.1%
Sonoco	4.97e+03 [b]	2.93E+03	69.7%
Norampac	1.65e+03 [b]	9.43E+02	74.9%
Runoff	1.54e+05 [c]	1.54E+05	0.1%
Moira River	2.11e+06 [a]	2.88E+06	-26.7%
Salmon River	7.63e+05 [a]	9.94E+05	-23.2%
Napanee River	6.62e+05 [a]	8.74E+05	-24.2%
Napanee STP	7.25e+03 [b]	7.25E+03	0.0%
Desoronto STP	1.60e+03 [b]	1.05E+03	52.2%
Belleville STP	3.00e+04 [b]	3.60E+04	-16.7%
Runoff	6.72e+05 [c]	6.72E+05	0.0%
Wilton Creek	8.10e+04 [a]	1.47E+05	-44.9%
Runoff	3.91e+05 [c]	3.91E+05	-0.1%
Picton STP	4.74e+03 [b]	3.31E+04	-85.7%
Essroc Cement/Picton Heights	6.68e+03 [b]	8.33E+04	-92.0%
Runoff	5.02e+04 [c]	5.02E+04	0.1%
Lake Ontario Epi.	4.80e+06 [c]	2.40E+06	100.0%
Lake Ontario Hypo.	1.10e+08 [c]	4.03E+07	172.8%
Runoff	3.12e+04 [c]	3.12E+04	0.0%

a Minns and Moore (2004)

b MISA (Andreas Radman, OMOE, unpublished data)

c Diamond et al. (1994). All 1988 water flows are taken from Diamond et al. (1994).

Table A5. Measured concentrations of organic chemicals in various sources contributing to annual loading estimates to the Bay for the model simulation of year 2000.

Chemical	**Air (pg m^{-3})**	**Trent River (ng L^{-1})**	**STPs & Industries (ng L^{-1})**	**Runoff (ng L^{-1})**	**Lake Ontario (ng L^{-1})**
PCB – 018	[a]6.68				[J]0.00139
PCB – 028	[a]3.86				[J]0.00001
PCB – 052	[a]3.41				[J]0.00148
PCB – 101	[a]4.21				[J]0.00001
PCB – 105	[a]0.18				[J]0.00016
PCB – 118	[a]0.133				[J]0.00039
PCB – 138	[a]0.2				[J]0.00001
PCB – 153	[a]0.56				[J]0.00039
PCB – 180	[a]0.11				[J]0.00021
ΣPCB	[a]54.88	[d]2.5			[J]0.004
2,3,7,8- TCDD	[b]ND		[g]0.00153		[J]<0.0000032
2,3,7,8- TCDF	[b]0.01		[g]0.00133		[J]0.00000228
Mirex	[a]0.062	[f]<0.01			[J]0.00018
Atrazine	[c]10				[k]200
B[a]P	[a]1.643	[f]0.43		[f]17-531	
Dieldrin	[a]5.92				[J]0.053
p,p-DDT	[a]0.99	[f]0.02			[J]0.00081
17B-estradiol			[h]0.1		
HCB	[a]24.79	[f]0.03			[J]0.00431
BDE-47	[d]4.6				[J]0.00505

[a] IADN, 2000 (Pierrette Blanchard, MSC, unpublished data)

[b] Environment Canada, 2000 (Tom Dann, unpublished data)

[c] Schottler and Eisenreich (1997)

[d] Gouin et al. (2005)

[e] OMOE 2000 (Duncan Boyd, unpublished data)

[f] Boyd and Biberhofer (1999)

[g] OMOE 2000 (MISA, unpublished data), measured for Norampac

[h] Lee et al. (2004)

[i] Liu et al. (unpublished data)

[j] Luckey and Litten (2004)

[k] Struger et al. (2004)

Table A6. Relative proportions of biomass (g. m^{-3} water) of each functional species group in the Bay of Quinte foodweb.

Functional Group	Species	Biomass (g/m^3)
Large Piscivorous	Walleye	0.777
	Largemouth Bass	0.035
	Northern Pike	
	Bowfin	
	Longnose Gar	
Small Piscivorous	Smallmouth Bass	0.018
	White Perch	2.19
	Yellow Perch	2.16
Planktivorous	Alewife	0.67
	Gizzard Shad	0.46
	Emerald Shiner	0.09
	Spottail Shiner	
	Brook Silverside	
Benthivorous	Pumpkinseed	0.7798
	Bluegill	
	Freshwater Drum	0.48
	Common Carp	0.46
	White Sucker	3.73
	Brown Bullhead	
	Channel Catfish	
	American Eel	
	Johnny Darter	
	Logperch	
	Trout-perch	0.033
Gobies	Round Goby	0.00081
Bivalves	Native bivalves	0.27
	Dreissenids	359.5
Benthic Inverts	Insect larvae	1.74
	Other benthos	
	Oligochaetes	7.58
	Chironomids	
	Gastropods	0.91
	Amphipods	2.69
	Isopods	
Zooplankton	Herbivorous zooplankton	3.58
	Copepods	0.93
	Cercopagis	0.004
	Rotifers	0.032
	Predatory cladocerans	0.018
Algae	Phytoplankton	10.85
	Epiphyton	64.41
	Periphyton	2.28
Macrophytes	Macrophytes	64.41
Detritus	DOC	21.19
	Pelagic detritus	27.8
	Sedimented detritus	8.34

Source: Marten Koops, DFO, unpublished data

Table A7. Dietary composition (% by volume) of each functional species group for the foodweb of the Bay of Quinte (estimates are based on segments 1 and 2).

Prey \ Predator	Large Piscivorous	Small Piscivorous	Planktivorous	Benthivorous	Gobies	Benthic Invertebrates	Bivalves	Zooplankton	Phytoplankton	Macrophytes	Detritus
Large Piscivorous	0.00051	0.00047	0.00027								
Small Piscivorous	0.74822	0.006	0.00055								
Planktivorous	0.21952	0.15386									
Benthivorous	0.02461	0.02456									
Gobies	0.00043	0.00004									
Bivalves/ZM		0.04951		0.23692	0.8	0.00242					
Benthic Inverts	0.0017	0.62263	0.01373	0.72965	0.15	0.034					
Zooplankton	0.00502	0.14293	0.68381	0.02101	0.05	0.01118		0.13116			
Phytoplankton			0.26393			0.67996	0.64989	0.789			
Macrophytes				0.00822		0.10578					
Detritus			0.0377	0.00419		0.16665	0.35011	0.07984			
Sum	1	1	1	1	1	1	1	1	0	0	0

Source: Marten Koops, DFO, unpublished data

Table A8. Parameter values used in the foodweb model of Bay of Quinte.

	[a] **Fish size**	**Lipid Fraction**	[c] **Non-Lipid Fraction**	[d] **Lipid Abs. Efficiency**	[d] **Non-Lipid Abs. Efficiency**	[e] **Water Abs. Efficiency**
L. Piscivorous	3000	[b] 0.08	0.2	0.83	0.57	0.8
S.Piscivorous	330	[b] 0.06	0.2	0.83	0.57	0.8
Planktivorous	70	[a] 0.02	0.2	0.6	0.5	0.8
Benthivorous	200	[b] 0.05	0.2	0.83	0.57	0.8
Gobies	15	0.035	0.2	0.83	0.57	0.8
Zebra Mussels	0.11	[a] 0.04	0.2	0.6	0.5	0.8
Benthic Inverts	0.008	[a] 0.04	0.2	0.6	0.5	0.8
Zooplankton	0.000017	[a] 0.03	0.2	0.6	0.5	0.8
Phytoplankton	4.10E-15	[a] 0.015	0.2	0.6	0.5	0.8
Macrophytes	0.00001	0.00001	0.2	0.6	0.5	0.8
Detritus	1	0.02565	0.2	0.6	0.5	0.8

a Morrison (1998)

b Emily Awad (SFCMP, personal communication)

c Arnot and Gobas (2004)

d Morrison et al. (1999)

e Olsen and Ringo (1998)

Table A9. Data from year 1988 used to calculate loadings of ΣPCB and PCP for model evaluation.

Segments	Source	Flow Rate ($m^3\ h^{-1}$)	PCB ($ng\ L^{-1}$)	PCP ($ng\ L^{-1}$)
Upper West (1)	Trent River	5.56E+05	1.01E+01	1.00E-01
	Trenton STP	4.45E+02	1.00E-03	4.10E+02
	CFB Trenton	2.16E+02	1.00E-03	1.10E+02
	Dom Preserving	3.93E+01	1.00E-03	8.40E+02
	Dom Packaging	1.22E+02	1.00E-03	6.37E+05
	Runoff	6.41E+03	1.00E-03	1.00E+02
Upper East (2)	Moira River	1.20E+05	1.15E+01	1.00E-10
	Salmon River	4.14E+04	1.15E+01	1.00E-10
	Napanee River	3.64E+04	1.10E+01	1.00E-10
	Belleville STP	1.50E+03	1.00E-03	1.71E-01
	Deseronto STP	4.38E+01	1.00E-03	9.00E-02
	Napanee STP	3.02E+02	1.00E-03	7.00E-02
	Bakelite)	3.46E+02	1.00E-03	5.00E-02
	Runoff	2.80E+04	3.54E+01	1.00E-10
Hay Bay (3)	Wilton Creek	6.12E+03	1.00E-03	1.00E-04
	Runoff	1.63E+04	1.00E-03	1.00E-04
Middle Bay (4)	Picton STP	1.38E+03	1.00E-03	2.00E-02
	Picton Heights	3.47E+03	1.00E-03	2.00E-02
	Runoff	2.09E+03	1.00E-03	1.00E-04
Lower Bay (5)	Lake Ontario Epi.	1.00E+05	1.00E+00	1.00E-01
	Lake Ontario Hyp.	1.68E+06	1.00E+00	1.00E-01
	Runoff	1.30E+03	1.00E+03	1.00E-04

Air Conc. (pg m$^{-3)}$	-	-	1.00E+03	1.00E+02

Source: Diamond et al. (1994)

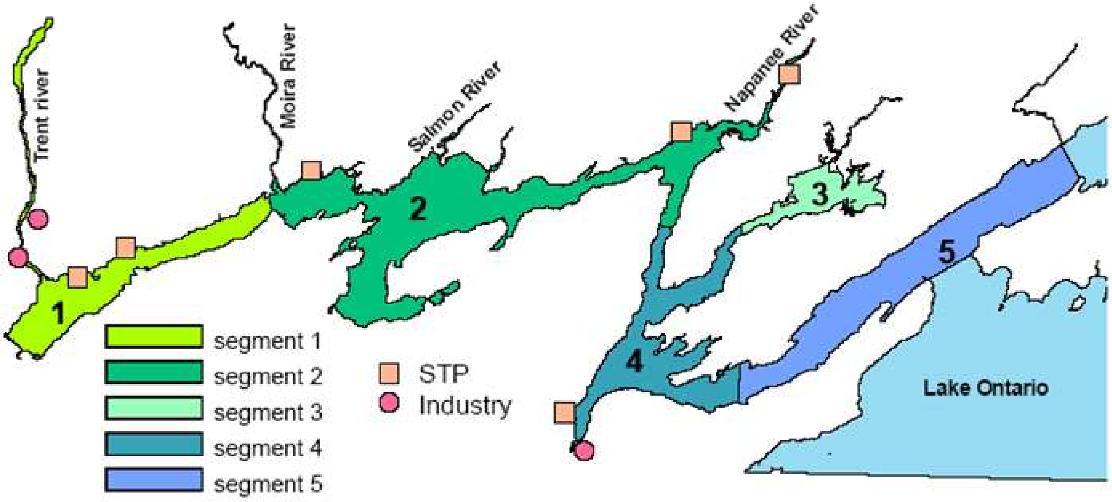

Figure A1. Study area and model boundaries for the Bay of Quinte contaminant model.

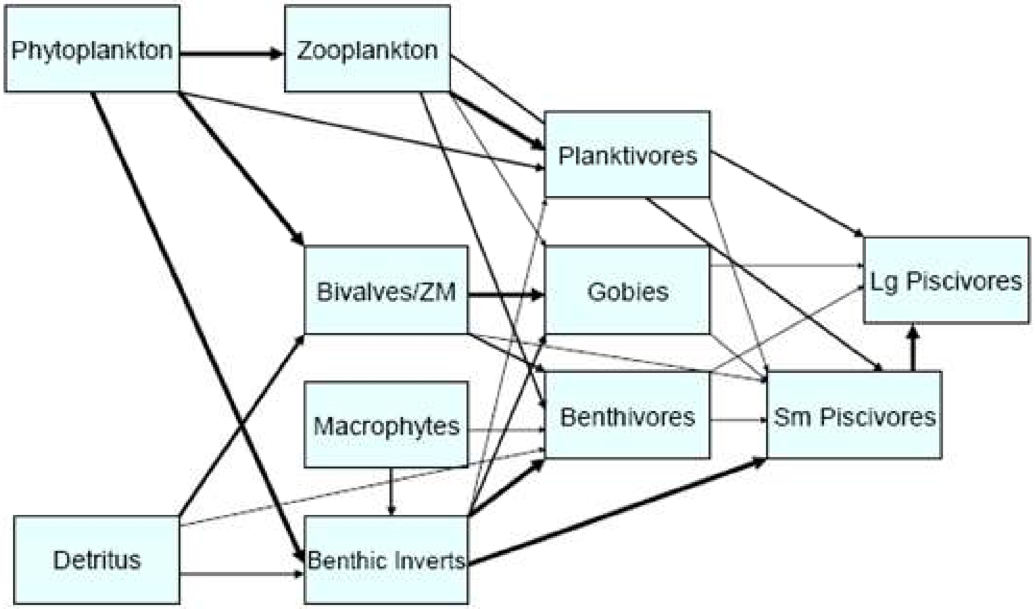

Figure A2. Trophic structure used to depict the contaminant dynamics in the Bay of Quinte foodweb model.

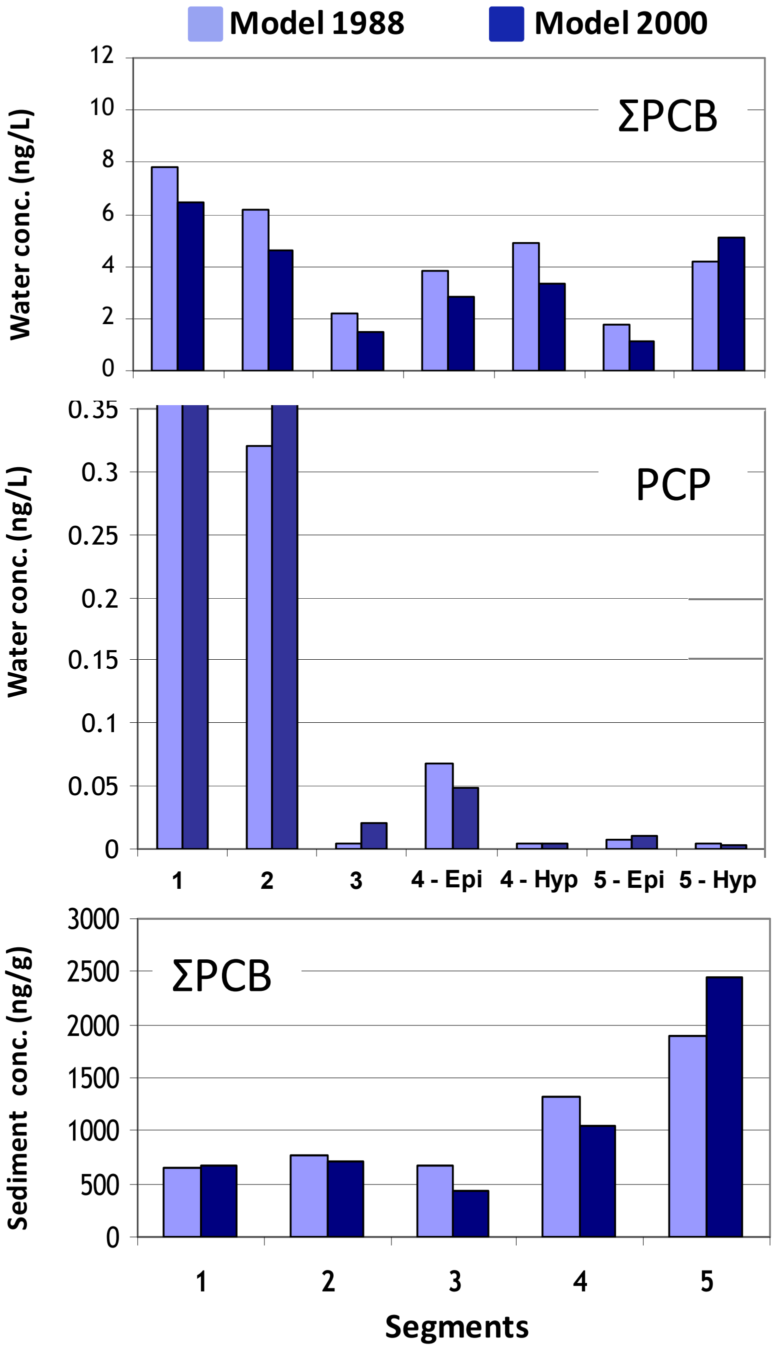

Figure A3. Comparisons of modeled chemical concentrations in the water (ng L^{-1}) and sediments (ng g^{-1}) of Bay of Quinte between Diamond et al. (1994) and this study to evaluate model performance.

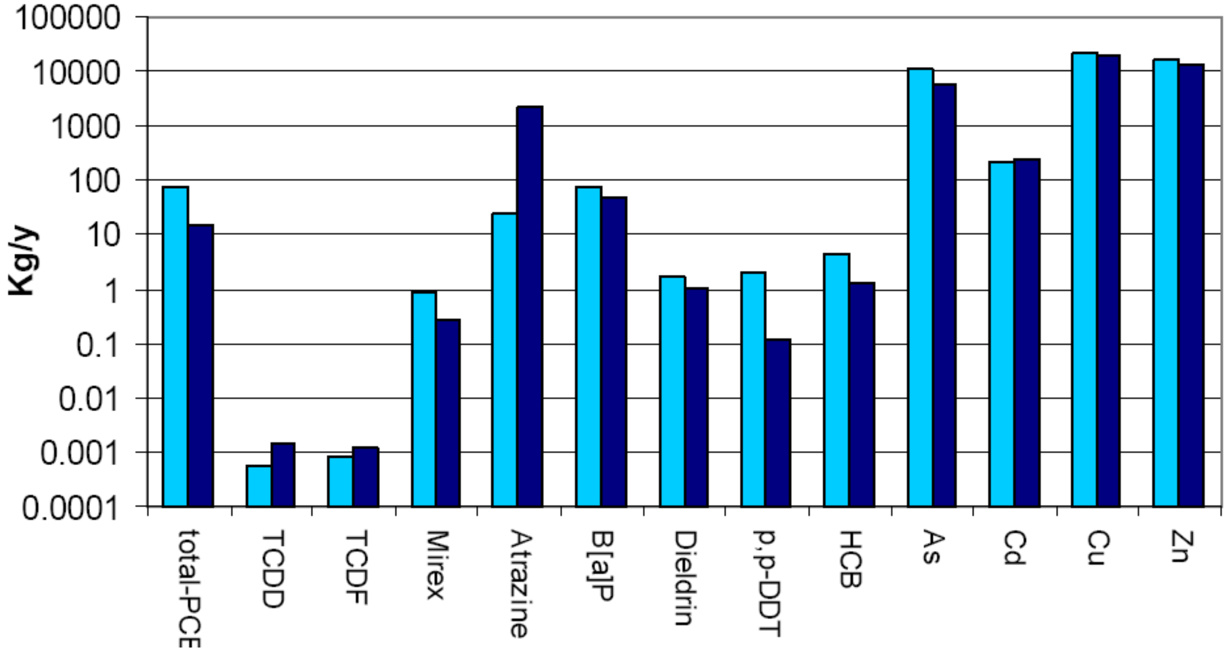

Figure A4. Comparison of annual loadings (kg year^{-1}) of organic chemicals and metals between 1988 (light blue bars) and 2000 (dark blue bars).

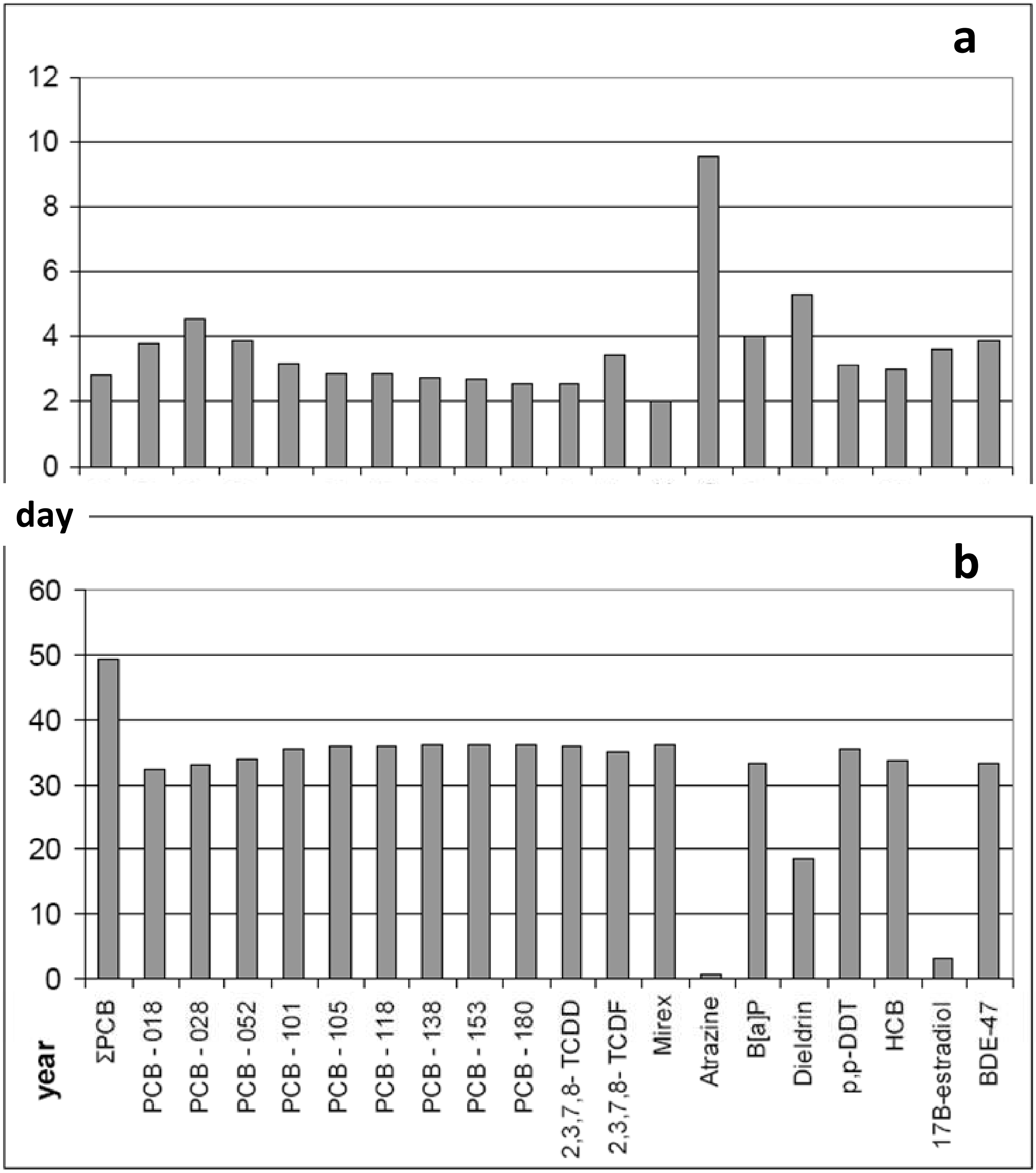

Figure A5. Residence times of OCs in (a) water column (days) and (b) sediments (years) of the Bay of Quinte.

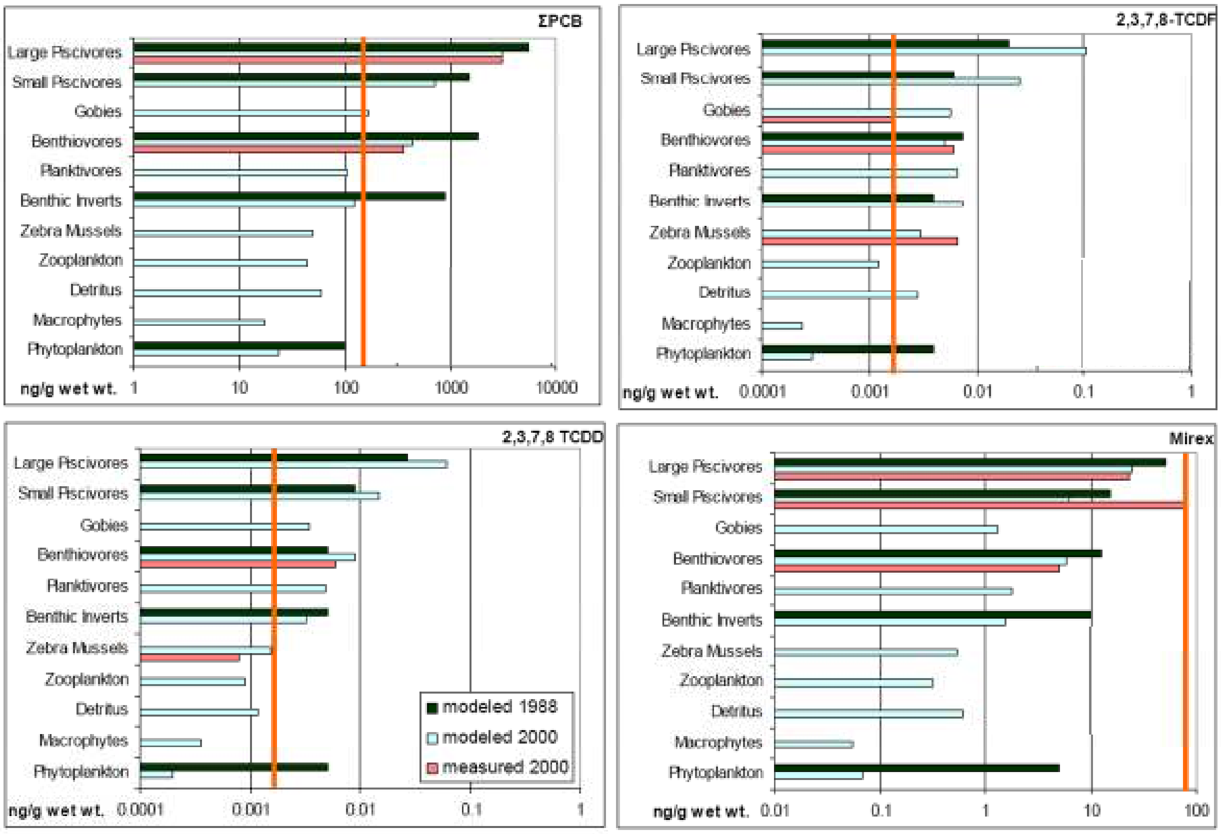

Figure A6. Comparison of modeled and measured fish concentrations of organic chemicals with the provincial fish consumption guidelines. Note that only chemicals of concerns for human consumption are shown here.