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Release of polychlorinated biphenyl congeners in a contaminated harbor and canal

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RELEASE OF POLYCHLORINATED BIPHENYL CONGENERS IN A CONTAMINATED HARBOR AND CANAL

by

Andres Jose Martinez Araneda

An Abstract

Of a thesis submitted in partial fulfillment
of the requirements for the Doctor of
Philosophy degree in Civil and Environmental Engineering
in the Graduate College of
The University of Iowa

July 2010

Thesis Supervisor: Professor Keri C. Hornbuckle

ABSTRACT

The overall hypothesis of this thesis addresses the release of polychlorinated biphenyls (PCBs) in the sediments of a highly contaminated harbor. I collected, analyzed and quantified PCB congeners in more than 130 samples of air, water and sediment. Then I constructed a chemical fate model as function of chemical concentrations, physical-chemical properties, local meteorological and hydraulic conditions. Indiana Harbor and Ship Canal in East Chicago (IHSC), Indiana, was selected for its expected high levels of PCBs in the sediment and because of future plans for dredging. I found that PCB concentrations in air, water and sediment in this area were much higher than background levels in the Great Lakes region. PCB sediment concentrations were above the threshold limit to designate IHSC as a Superfund site (≥ 50 ppm), although it is not. The PCB signature in surficial sediment strongly resembles the original Aroclor 1248 but deeper layers show evidence of mixtures of Aroclors and weathering processes. The fate model showed that IHSC contaminated sediments are a continuous source of PCBs to the water and overlying air, and also produce a PCB input to Lake Michigan, even under quiescent conditions. The PCB signature in sediment, water, and air support my determination that the contaminated sediment is a major source of PCBs into the water and air above it. Simulations considering different surficial sediment concentrations post-dredging demonstrated that PCB concentrations in the sediment should be considered in the dredging operation to minimize the release of PCBs into the environment. Finally, I examined the role of the dissolved sediment porewater concentration in the prediction of sediment-water soluble fluxes, using a passive sampler technique (SPME PDMS-fiber) and calculated values from a one-parameter linear free energy relationship (op-LFER). I determined that the latter overestimates the freely dissolved porewater concentration but are nevertheless the most appropriate values for predicting PCBs soluble release from contaminated sediments.

Abstract Approved: ____________________________________

Thesis Supervisor

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Title and Department

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Date

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Graduate College
The University of Iowa
Iowa City, Iowa

CERTIFICATE OF APPROVAL

PH.D. THESIS

This is to certify that the Ph.D. thesis of

Andres Jose Martinez Araneda

has been approved by the Examining Committee
for the thesis requirement for the Doctor of Philosophy
degree in Civil and Environmental Engineering at the July 2010 graduation.

Thesis Committee: ___________________________________
Keri C. Hornbuckle, Thesis Supervisor

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Thomas Peters

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Larry W. Robertson

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Jerald L. Schnoor

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Peter S. Thorne

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Kai Wang

To my parents for their support
And to Amaia, Paz and Paola for making every day a new experience

Making the simple complicated is commonplace; making the complicated simple, awesomely simple, that's creativity.

Charles Mingus, jazz musician

ACKNOWLEDGMENTS

Due to all the people that helped me in a direct or indirect way through this degree, it is not easy to properly acknowledge all of them, but I will try to do my best.

I would like to start by acknowledging Keri Hornbuckle. Since I met Keri in August 2006 she has been an outstanding advisor. There are many qualities that I can mention about her, but I would just like to say that she was always available to discuss any issue, even though it was very small. She always made time to talk about it. I think everything worked quite well during these 4 years.

When I started my degree I did not have much knowledge and practical expertise in the lab. Karin Norström was an excellent analytical chemistry instructor. Karin gave me the necessary *push* to start working in the lab. I really appreciate it. Dingfei or as I sometimes call him *Dr.Hu*, was also a very helpful person in the lab. We also had many interesting conversations, and not only regarding our scientific work. Kai Wang was also very helpful, especially in relation to the Monte Carlo simulation and writing the scripts in R software. I do not know how many hours of work he saved me. I believe too many hours to be counted. I would also like to thank my colleagues Carolyn, Rachel and Paul. The *girls* helped me in the lab as well as giving me feedback in my writings and presentations. Paul was the computer, especially Excel, support.

I would also like to thank the undergraduate students Tom Ledolter, Christoffer von Schwerin, Alex Poss and Zach Rodenburg for helping me in the lab with all the *dirty* work, or in other words, wet chemistry. I cannot leave out Collin Just. Thank you for all the help in the lab, especially maintaining the instruments lab in perfect conditions, so I could run my *dirty* samples.

It is also a good opportunity to thank the Department of Civil and Environmental Engineering at the University of Iowa, from Judy and Angie to all the professors and graduate students. It has been a pleasure to be studying and working here for 4 years.

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I am also very thankful to the Great Lakes National Program Office of the U.S. EPA for the donation of the R/V *Mudpuppy* and crew (chapters II, III, IV and V), and David Wethington (U.S. Army Corps of Engineers, Chicago Office) for assistance in sampling sediment from IHSC (chapters II and III). I also thank Dr. Kristina Sundqvist (Umeå University in Sweden) for her helpful discussion regarding the core sediment analysis (Chapter IV) and Professor Danny Reible (University of Texas-Austin) for the PDMS-fibers and related discussion of their use (Chapter V).

I am especially grateful to my parents for their support and incentive to go to graduate school. I am absolutely convinced that I would not have undertook this challenge if it was not for them. Finally, I have to thank my family, my daughters Amaia and Paz, and my wife Paola, especially Paola, for her patience, support and understanding. Thank you!

ABSTRACT

The overall hypothesis of this thesis addresses the release of polychlorinated biphenyls (PCBs) in the sediments of a highly contaminated harbor. I collected, analyzed and quantified PCB congeners in more than 130 samples of air, water and sediment. Then I constructed a chemical fate model as function of chemical concentrations, physical-chemical properties, local meteorological and hydraulic conditions. Indiana Harbor and Ship Canal in East Chicago (IHSC), Indiana, was selected for its expected high levels of PCBs in the sediment and because of future plans for dredging. I found that PCB concentrations in air, water and sediment in this area were much higher than background levels in the Great Lakes region. PCB sediment concentrations were above the threshold limit to designate IHSC as a Superfund site (≥ 50 ppm), although it is not. The PCB signature in surficial sediment strongly resembles the original Aroclor 1248 but deeper layers show evidence of mixtures of Aroclors and weathering processes. The fate model showed that IHSC contaminated sediments are a continuous source of PCBs to the water and overlying air, and also produce a PCB input to Lake Michigan, even under quiescent conditions. The PCB signature in sediment, water, and air support my determination that the contaminated sediment is a major source of PCBs into the water and air above it. Simulations considering different surficial sediment concentrations post-dredging demonstrated that PCB concentrations in the sediment should be considered in the dredging operation to minimize the release of PCBs into the environment. Finally, I examined the role of the dissolved sediment porewater concentration in the prediction of sediment-water soluble fluxes, using a passive sampler technique (SPME PDMS-fiber) and calculated values from a one-parameter linear free energy relationship (op-LFER). I determined that the latter overestimates the freely dissolved porewater concentration but are nevertheless the most appropriate values for predicting PCBs soluble release from contaminated sediments.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER I. INTRODUCTION

1.1 Polychlorinated Biphenyls as Pollutants

Polychlorinated biphenyls (PCBs) are stable chlorinated aromatic compounds that were commercially produced as complex mixtures for a variety of applications, including dielectric fluids for capacitors and transformers. Approximately 2 million tons of PCBs were produced worldwide (1). Two hundred and nine different discrete chemical compounds, called congeners, have been identified, which differ in the number as well as in the position of chlorine atoms located in the biphenyl (2) (Figure 1-1).

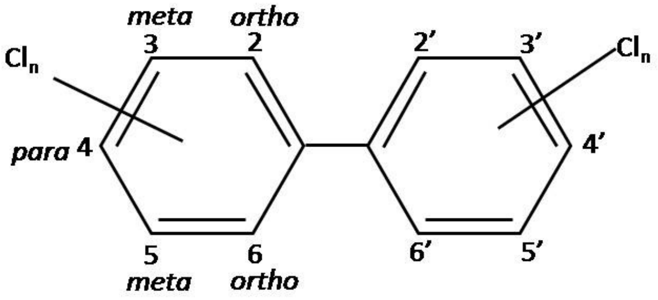


Figure 1-1 Polychlorinated biphenyl structure

These differences in the amount and location of the chlorines also result in different physical and chemical properties, such as Henry's Law constant (3), octanol-water partition coefficient (4) (Figure 1-2) and vapor pressure (5). Due to the presence of chlorine atoms in the biphenyl molecule, PCBs do not readily degrade in the environment (persist) and because they are lipophilic, they tend to bioconcentrate, biomagnify in the food chain, and bioaccumulate in organisms, including humans.

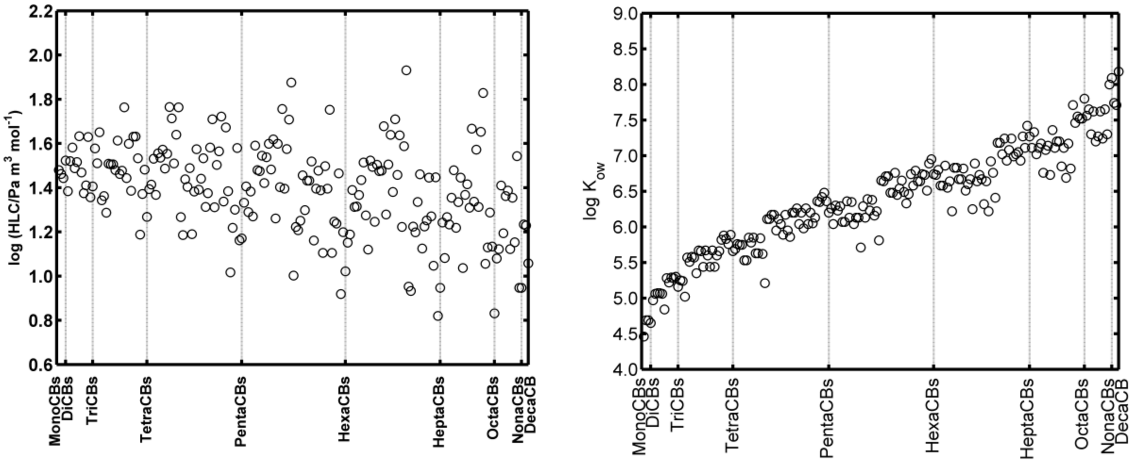


Figure 1-2 Henry’s Law constants (3) (left) and octanol-water partition coefficient (4) (right) at 298.15 K for 209 PCB congeners. Congeners are ordered by “IUPAC” nomenclature (2). Two examples of the different chemical properties of PCB congeners

PCBs are listed in the Stockholm Convention as Persistent Organic Pollutants (POPs) (6). This international treaty establishes the measures to reduce or eliminate the production and use of these chemicals around the globe. PCBs are probable animal carcinogens and endocrine disruptors, and new evidence links PCB exposure to neurodevelopment disorders and autism (7-12).

Despite the fact that PCBs were banned in open, and semi-closed sources and production in North America in the mid 1970’s, it is still possible to detect these pollutants in many environmental matrices, including human tissues (13). Scientists now understand much more about PCB behavior than was clear when PCBs were first implicated as environmental contaminants forty years ago (14).

1.2 Study Area: Indiana Harbor and Ship Canal and Dredging Project

1.2.1 Indiana Harbor and Ship Canal

Penetrating the city center of East Chicago is the Indiana Harbor and Ship Canal (IHSC), located on the southern shore of Lake Michigan (Figure 1-3). The construction of IHSC was authorized in 1913 to serve industries and provide a connection between Lake Michigan and the Grand Calumet River. The connection is no longer maintained for navigational purposes. The IHSC system is approximately 7 km long, with two branch canals (Lake George Branch and Grand Calumet River Branch). Currently, the main industries located in this area are Mittal Steel USA Inc, LTV Steel Company Inc, Safety Kleen Oil Recovery Co and BP Products North America Inc. The IHSC is an active canal system that continues to support large vessels.

Due to years of heavy industrial operation, the area has been contaminated with heavy metals, polycyclic aromatic hydrocarbons (PAHs) and PCBs. As a result, the International Joint Commission designated the IHSC as an Area of Concern, which ideally results in the development of remedial action plans to restore and protect ecosystem health so that the water is drinkable and fish are safe to eat (15).

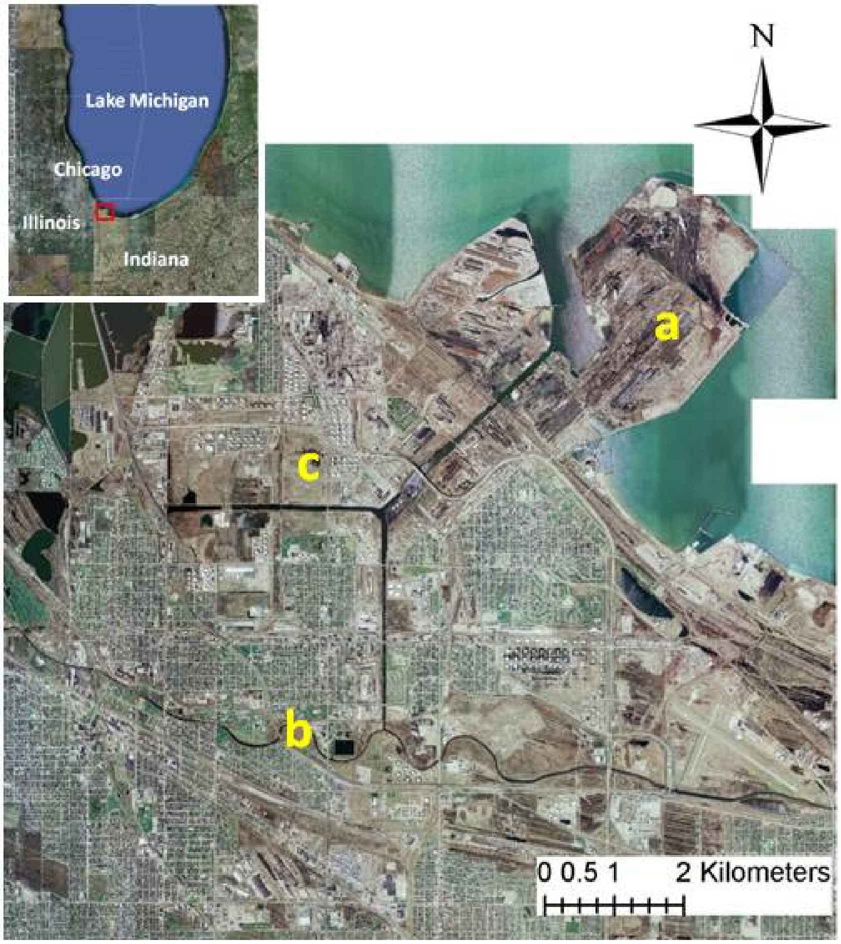
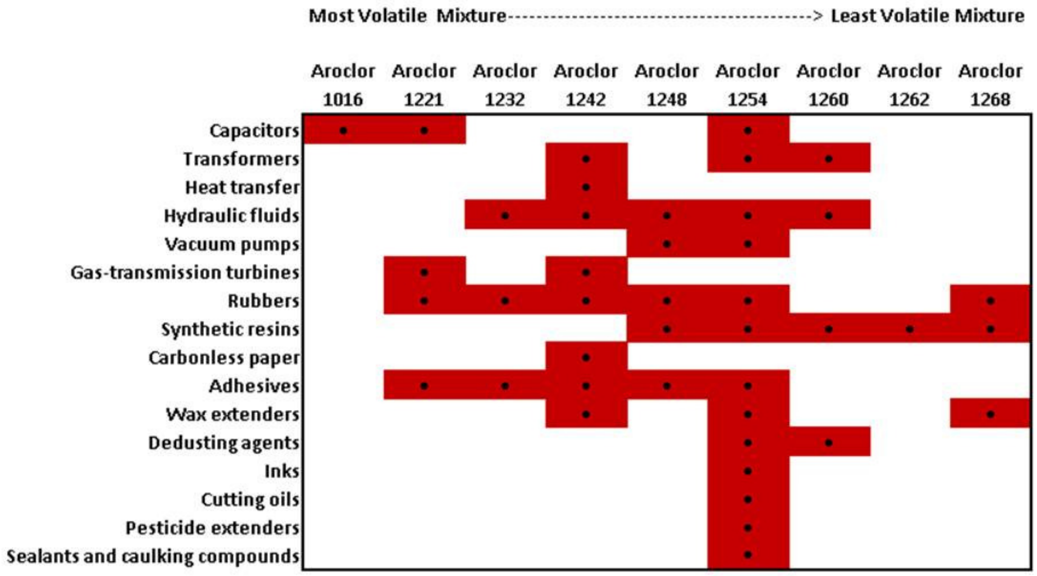


Figure 1-3 Aerial photograph of Indiana Harbor and Ship Canal. The city surrounding IHSC is East Chicago. The identified locations are: a) Mittal Steel USA Inc, b) East Branch Grand Calumet River and c) Confined Disposal Facility (CDF) for the future disposal of the sediment from IHSC. The refinery tanks located northwest of the canal are part of BP Products North America Inc. facility

PCBs are expected to be present in the IHSC because of the intense industrial activities that have occurred there. Aroclor mixtures and their common industrial uses are shown in Figure 1-4.



Most Volatile Mixture---------------------------------------> Least Volatile Mixture

	Aroclor 1016	Aroclor 1221	Aroclor 1232	Aroclor 1242	Aroclor 1248	Aroclor 1254	Aroclor 1260	Aroclor 1262	Aroclor 1268
Capacitors	●	●				●			
Transformers				●		●	●		
Heat transfer				●					
Hydraulic fluids			●	●	●	●	●		
Vacuum pumps					●	●			
Gas-transmission turbines		●		●					
Rubbers		●	●	●	●	●			●
Synthetic resins					●	●	●	●	●
Carbonless paper				●					
Adhesives		●	●	●	●	●			
Wax extenders				●		●			●
Dedusting agents						●	●		
Inks						●			
Cutting oils						●			
Pesticide extenders						●			
Sealants and caulking compounds						●			

Figure 1-4 Commercial Aroclor mixtures produced by Monsanto Company and their common industrial uses (7)

However, there are few published data of PCB concentrations in air, water and sediment in IHSC. The United State Army Corps of Engineers (USACE) has monitored airborne PCB concentrations in the region since 2001 (16). They also report that PCBs were found in IHSC sediment since 1977 but they have not published a full report (Pittman, personal communication). Table 1-1 summarizes part of the air and sediment core data from IHSC for different time periods.

Table 1-1 Air gas phase and bulk sediment core concentrations from IHSC

Location [a]	Year	Air – gas phase (pg m^{-3})	Sediment Concentration (ng g^{-1})	Notes	Reference
Lake George Branch	2001-2004	190 - 310		Mean summers	(16)
Lake George Branch	1979		7,900	depth -13.3' to -16.3'	[b]
			1,000	depth -16.3' to -19.3'	[b]
			20	depth -19.3' to -23.3'	[b]
Calumet River Branch	1979		68,000	depth -22.3' to -25.3'	[b]
	1983		35,000	depth -23.9' to -25.4'	[b]
	1993		46,000	depth -32' to -36'	[b]
	1993		100,000	depth -28' to -32'	[b]
Indiana Harbor Canal	1979		89,000	depth -23.7' to -26.7'	[b]
	1983		70,000	depth -21.9' to -23.9'	[b]
Harbor Entrance	1979		8,100	depth -31.7' to -34.7'	[b]
	1984		46,000	depth -33.3' to -35.3'	[b]

[a] locations are shown in Figure 2-1.

[b] Personal communication.

1.2.2 Dredging Project

The USACE, Chicago District, will commence an important dredging project in IHSC, East Chicago, Indiana. Due to lack of an adequate disposal site for the sediments, the last time this water system was dredged was in 1972. Although it is not clear when it will start, an appropriate sediment disposal site (confined disposal facility, CDF) has been built near IHSC (Figure 1-3). It is estimated that 1.2x10^{6} m^{3} (1.6x10^{6} yd^{3}) of sediment will be dredged from this system, and it will require 8 to 10 years to be completed. The removed sediment will be loaded onto barges that will be then moved to the CDF (17). The main purpose of the project is to maintain congressionally authorized navigation depths for large barges to pass through the canals. The project will require the removal of PCB-contaminated sediments although contamination is not the main design criterion for this project. Even though dredging is one of the most common remediation technologies for large contaminated sediment sites, there is still uncertainty in the final outcomes with respect to reducing environmental and human health impacts (15). Additionally, people in East Chicago have long been concerned about PCBs in the sediment from the IHSC (18).

1.3 Objectives and Hypotheses

The overall hypothesis of this study is the following:

The sediment of the navigational regions of Indiana Harbor and Ship Canal is an important source of PCBs to the overlying air and to Lake Michigan waters.

To address this overall hypothesis, we have divided this research into four objectives with their respective hypotheses. Each objective has been carefully chosen in a sequential order, thus there is no gap between them and it is easier to answer the overall hypothesis. The objectives and their respective hypotheses are the following:

a) Objective 1: Investigate the spatial extent and concentration magnitude of PCB congeners in surficial sediment from Indiana Harbor and Ship Canal.
   i. Hypothesis 1.1: The IHSC surficial sediment is heavily contaminated with PCBs.
   ii. Hypothesis 1.2: The current congener distribution of PCBs in the surficial sediment continues to resemble the original commercial mixtures distributed by Monsanto Company in the middle part of the last century.

b) Objective 2: Determine and evaluate the fate of PCB congeners in IHSC.
   i. Hypothesis 2.1: PCBs are continuously released from the sediments to the water above it.

  ii. Hypothesis 2.2: Once PCBs are released from the sediments, they are exported from the canal into Lake Michigan and also emitted to the air over the canal.

c) Objective 3: Estimate the PCB emissions after sediment dredging has occurred in IHSC.
  i. Hypothesis 3.1: PCB concentrations in deeper sediment are above the threshold for establishing IHSC a Superfund site.
  ii. Hypothesis 3.2: After the dredging project is finished, sediments with higher levels of PCBs may be exposed and induce higher emissions from the sediment to the water and water to the overlying air, as well as an increase in the tributary loading to Lake Michigan.

d) Objective 4: Understand the role of sediment porewater in the prediction of PCB emissions from contaminated sediments in IHSC.
  i. Hypothesis 4: Sediment porewater PCB concentrations are similar when measured using passive sampler technique to those predicted by employing a one-parameter linear free energy relationship (op-LFER).

1.4 Thesis Overview

The thesis is outlined with respect to the above objectives and respective hypotheses. Chapters II address objective 1 and hypotheses 1.1 and 1.2 with respect to PCBs in surficial sediment in IHSC. Chapter III undertakes objective 2 and hypotheses 2.1 and 2.2 regarding the fate of PCBs in IHSC. Chapter IV uses the PCB fate model developed in Chapter III to address objective 3 and hypothesis 3.1 and 3.2. Chapter V is an investigation of the role of sediment porewater concentration in the estimation of soluble PCBs release from the contaminated sediment in IHSC (objective 4, hypotheses 4.1 and 4.2).

Chapter II presents the results of PCB surficial sediment concentrations from IHSC, obtained from the first campaign in IHSC in August 2006. The PCB analytical method in sediment is described, where tandem mass spectrometry in multiple reaction monitoring mode was utilized. The total PCB concentrations found are comparable to other PCB concentrations at contaminated tributaries in the United States, most of them (although not IHSC) established by law as Superfund sites. The PCB congener signal strongly resembles the original technical mixture Aroclor 1248 that has experienced a small amount of weathering. We believe this is the first publication that reports levels of PCBs in sediments in IHSC.

Chapter III contains the PCB release model developed for sediment-water and air-water exchanges in IHSC. We estimated the release of 4 kg of ΣPCBs from the sediment to the water and 7 kg of ΣPCBs were volatilized from the water to the overlying air annually. The congener profiles in sediment, water, and air support our determination that the contaminated sediment is a major source of PCBs into the water and air above it. We found that IHSC is currently a significant source of PCBs to the air and to Lake Michigan, even under quiescent conditions

Chapter IV examines the potential effect of dredging in IHSC system regarding PCBs release from the surficial sediment to the water and from the water to the overlying air, as well as the tributary loading to Lake Michigan. Two cores samples from the second campaign in IHSC, May 2009, are analyzed and the PCB concentrations are used in the release model developed in Chapter III. We found that even though the cores are located quite near to each other, there are important differences in terms of total PCB concentration and congener distributions (profiles). Results show that the total PCB concentration in the sediment is a major key in the prediction of the release of PCBs.

Chapter V investigates the role of sediment porewater measurements to determine the soluble sediment-water PCB fluxes. We compared our predicted values using a one-parameter linear free energy relationship (op-LFER) with freely dissolved porewater concentrations obtained from a passive sampler technique (SPME PDMS-fiber). Although the op-LFER overestimates the freely dissolved porewater concentration, the scientific community's current understanding of the nature of PCBs in sediment porewater indicates that these values are the more appropriately applied to the empirical equations developed for predicting PCBs soluble release from contaminated sediments.

Appendix A contains supplementary information referenced in Chapter II, such as tables and figures. Additionally, there is extra information, such as raw data per sample, PCB chromatograms and photographs from the field campaign. Appendix B contains supplementary information referenced in Chapter III, such as quality assurance and control, sediment, dissolved-phase and air gas-phase concentrations of individual congeners used in the flux model, equations used to develop the release of PCB model, and additional information, such as the release of PCB model in R program. Appendix C presents supplementary information referenced in Chapter IV, such as sample information, supporting table and photographs from the core sampling. Appendix D encloses supplementary information referenced in Chapter V, mainly raw data resulted from the passive sampler experiments.

Due to the fact that chapters II through V are intended for publication in a scientific journal, they have more than one author and were all written in first person plural or third person. Together with me, the coauthors of Chapter II are Dr. Karin Norström, Dr. Kai Wang and my advisor Dr. Keri Hornbuckle. Karin helped me in the development and analysis of PCBs in sediment, Kai was very useful in the statistical analysis, and Keri reviewed the manuscript. In the case of Chapter III the coauthors are Kai and Keri. Kai helped me write the codes for the fate model in R software, and Keri reviewed the manuscript. For chapters IV and V Keri reviewed both chapters.

CHAPTER II: INVESTIGATION OF THE SPATIAL EXTENT AND CONCENTRATION MAGNITUDE OF PCB CONGENERS IN SURFICIAL SEDIMENT FROM IHSC[1]

2.1 Abstract

We report the results of the first intensive survey of polychlorinated biphenyls (PCBs) in the surficial sediment of the Indiana Harbor and Ship Canal (IHSC) in East Chicago, Indiana, a part of the Calumet River tributary of Lake Michigan that will be dredged to maintain depth for ship traffic. The tributary has previously been reported to be a large source of PCBs to Lake Michigan. PCB congeners were measured using tandem mass spectrometry in multiple reaction monitoring mode, a method that provides a high level selectivity and sensitivity for PCBs in complex environmental samples. The PCB concentrations (sum of 163 congeners or coeluting peaks) range from 53 to 35000 ng g^{-1} dry weight (d.w.) and are comparable to other PCB concentrations at contaminated tributaries in the United States, most of them (although not IHSC) established by law as Superfund sites. The PCB congener signal strongly resembles the original technical mixture Aroclor 1248 that has experienced a small amount of weathering — less than 2.5% by mass for the statistically different congeners — consistent with desorption, volatilization, and microbial dechlorination. The origin of the PCBs in IHSC is not known but Aroclor 1248 was used in hydraulic fluids, vacuum pumps, plasticizers and adhesives. Possible uses of this mixture in East Chicago included the equipment and auxiliary services for the adjacent steel mill and gas refinery and/or lubrication for the drawbridges spanning the canal.

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[1] Martinez, A.; Norström, K.; Wang, K.; Hornbuckle, K. C. Polychlorinated biphenyls in the surficial sediment of Indiana Harbor and Ship Canal, Lake Michigan. *Environ. Int.* **(2009),** *in press.*

2.2 Introduction

East Chicago is a heavily industrialized urban community on the southern shore of Lake Michigan. Penetrating the city center is the Indiana Harbor and Ship Canal (IHSC). The construction of IHSC was authorized in 1913 to serve industries and provide a connection between Lake Michigan and the Grand Calumet River. The connection is no longer maintained for navigational purposes. The IHSC system is approximately 7 km long, with two branch canals (Lake George Branch and Grand Calumet River Branch). Currently, the main industries located in this area are Mittal Steel USA Inc, LTV Steel Company Inc, Safety Kleen Oil Recovery Co and BP Products North America Inc. The IHSC is an active canal system that continues to support large vessels. To remain viable for industrial shipping, the U.S. Army Corps of Engineers, Chicago District, is planning to begin a long-term dredging project in 2009 to restore adequate navigational depth. The sediment will be disposed in a Confined Disposal Facility (CDF), which is under construction, and will be located north of Lake George Branch, less than 100 m from the canal (19)

Due to years of heavy industrial operation, the area has been contaminated with heavy metals, polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs). As a result, the International Joint Commission designated the IHSC as an Area of Concern (20). The IHSC and Grand Calumet River has been shown to include regions that are toxic to invertebrates (21-24). Sediment collected from IHSC presents the highest toxicity in comparison to Buffalo and Saginaw rivers (22, 24), and are among the most contaminated and toxic Great Lakes sediments that have been evaluated (23).

There is little published data of spatial extent and concentration magnitude of PCBs in the sediment in IHSC. The Army Corps reports that PCBs were found in IHSC sediment since 1977 but has not published a full report (Pittman, personal communication). There is no data about methods of quantification of individual PCB congeners or quality control. Custer and coworkers report high levels of PCBs in tissue of lesser scaup (*Aythya affinis*), a diving duck dwelling in IHSC (25). Although not commonly used for food, the authors noted that the PCB concentration in 88% of the birds exceeded the PCB human consumption guidelines for edible poultry in USA (N3.0 μg g^{-1} lipid wt.) (26).

The U.S. Army Corps of Engineers has monitored airborne PCBs in the region since 2001 (16). They have reported concentrations of PCB congeners that are comparable to concentrations measured in Chicago (a region of elevated airborne PCBs) and much higher than reported for remote and rural locations around Lake Michigan (27).

Due to the intense industrial activity in the area surrounding the IHSC during the time that PCBs were heavily used, we hypothesized that the IHSC surficial sediment would be heavily contaminated. We further hypothesized that the current congener distribution of PCBs in the surficial sediment continues to resemble the original commercial mixtures distributed by Monsanto Company in the middle part of the last century. Therefore, the central purpose of this study was to investigate the spatial extent and concentration magnitude of PCB congeners in surficial sediment from Indiana Harbor and Ship Canal, which presumably will be the first sediment layer to resuspend into the water column when dredging operations begin.

2.3 Methods

2.3.1 Sampling Method

During August 2006, 60 surficial sediments were sampled in IHSC, East Chicago, Indiana (Figure 2-1 and Table A-1 in Appendix A) from aboard the U.S. Environmental Agency's R/V *Mudpuppy*. A standard Ponar dredge sampler (clamshell-bucket) was used to collect the top 10 cm layer of surficial sediment. The sediment sample from each site was homogenized on the ship deck and divided into 3 precleaned amber jars, around 200 g each. Jars were completely filled and capped, avoiding any headspace. The samples were brought to The University of Iowa and kept refrigerated at 4 °C until extraction and analysis.

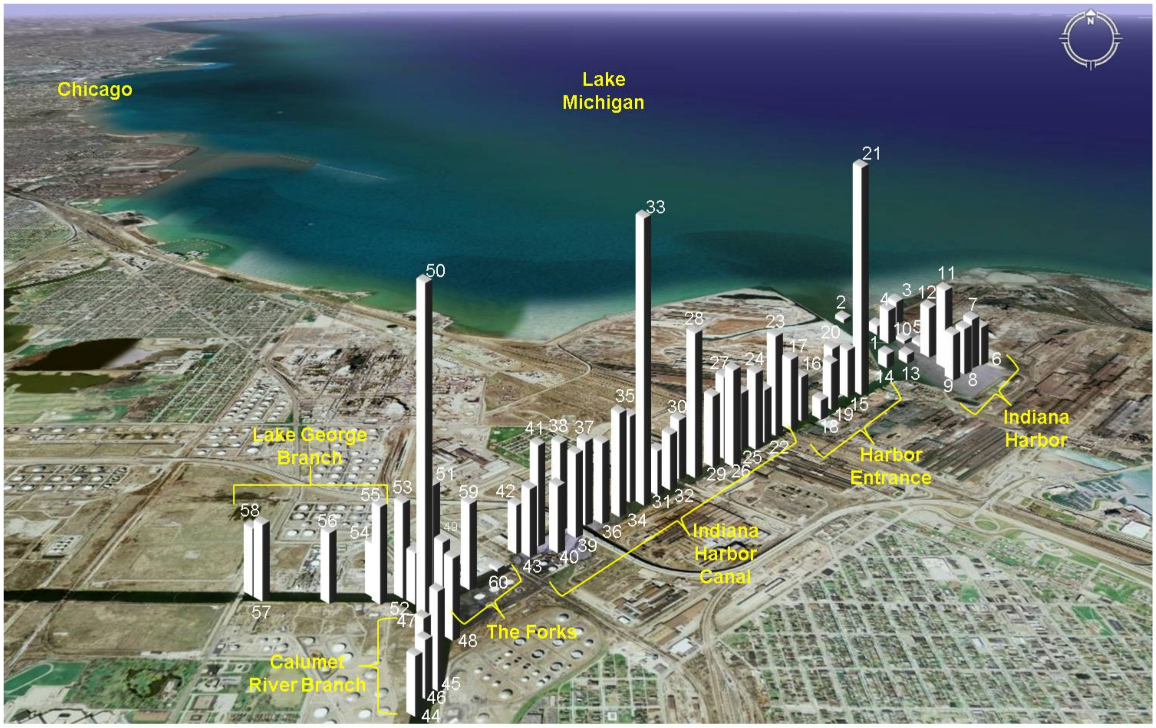

Figure 2-1 Spatial location and measured ΣPCB concentration (ng g^{-1} d. w.) in surficial sediment of IHSC. The height of the bars represents the total PCB concentration and the number over or next to each bar is the sample ID (see also Table A-1 in Appendix A). The canals regions are U.S. Army Corps of Engineers designations

2.3.2 Analytical Method

The analytical method employed for sample extraction is a modification of U.S. EPA Method 3545 (28-31). Briefly, samples were weighed (~3 g) and mixed with a known amount of combusted diatomaceous earth and spiked with 500 ng surrogate standard, PCB14 (3,5-dichlorobiphenyl), PCB65 (2,3,5,6-tetrachlorobiphenyl) and PCB166 (2,3,4,4′,5,6-hexachlorobiphenyl) (Cambridge Isotope Laboratories, Inc.). The sediments were extracted utilizing a pressurized fluid extraction (Accelerated Solvent Extractor, Dionex ASE-300), of equal parts acetone and hexane. The sediment water content was determined gravimetrically for each sample from a separate aliquot by drying for 12 h at 104 °C.

Polar interferences and other compounds were removed by extraction with KOH and then with sulfuric acid. The final hexane extract was passed through a Pasteur pipette filled with 0.1 g of combusted silica gel and 1 g of acidified silica gel (2:1 silica gel:acid by weight) (31) and eluted with hexane. PCB204 (2,2′,3,4,4′,5,6,6′-octachlorobiphenyl) was added as internal standard (100 ng; Cambridge Isotope Laboratories, Inc.). PCB quantification was carried out employing a modification of EPA Method 1668a (32). Tandem Mass Spectrometry GC/MS/MS (Quattro Micro™ GC, Micromass MS Technologies) in multiple reaction monitoring (MRM) mode was utilized to quantify all 209 congeners in 163 individual or coeluting congener peaks (Table A-2 in Appendix A), of which PCB14, PCB65 and PCB166 are surrogate standards and PCB204 is internal standard. The gas chromatogram (GC) was equipped with a Supelco SBP-Octyl capillary column (30 m×0.25 mm ID, 0.25 µm film thickness) with helium as carrier gas at a constant flow rate of 0.8 ml min^{-1}. The GC operates at the following conditions: injector temperature 270 °C, interface temperature 290 °C, initial temperature 75 °C, initial time 2 min. The GC temperature program is 75 to 150 °C at 15 °C min^{-1}, 150 to 290 °C at 2.5 °C min^{-1}, and final time 1 min. Figure A-1 in Appendix A includes a calibration chromatogram, as well as a sample chromatogram. Linearity of the instrument response was confirmed and PCB congener mass calculation was performed applying relative response factor (RRF) obtained from the calibration curve for each congener. Total organic carbon (TOC) was analyzed by Minnesota Valley Testing Laboratories. Inc (SW-846 Method SW 9060).

2.4 Results and Discussion

2.4.1 Quality Assurance and Control

Quality assurance and control (QA/QC) was rigorously assessed using surrogate PCB standards, blanks, replicates and standard reference material. Percentage recovery of surrogate standard PCB14 and PCB166 yielded a mean of 93% and 85%, and a median of 83% and 85%, respectively. Their standard deviations were 36% and 16%, and within a range of 49%–191% for PCB 14, and 58%–130% for PCB 166. Surrogate standard PCB65 yield high values due to coelution issues. PCB congener masses were corrected using the percentage recovery of congeners PCB14 (congeners 1 to 39) and PCB166 (congeners 40 to 209). Congener masses were not corrected for lab blanks, which were negligible. Table 2-1depicts the results from 5 samples that were each extracted and analyzed multiple times. Sample 16 yielded an unusually high relative standard deviation (66%) that may indicate poor mixing in the sample jar. Standard Reference Material 1944, New York, New Jersey Waterway sediment (SRM 1944, National Institutes of Standards and Testing) was quantified. The analysis of SRM 1944 resulted in identification of all congeners, with an acceptable quantification results with respect to the certified values (Figure 2-2). The average percent difference between the measured and certified values (27 congeners) was 15 ± 15%. The congener masses were corrected as explained above.

Table 2-1 Replicate results for 5 sediment samples, including number of replicates, mean, standard deviation and range in (ng g^{-1} d.w.), and relative standard deviation in percentage

Sample ID	Number of replicates	Mean (ng g^{-1} dw)	Stdev (ng g^{-1} dw)	Range (ng g^{-1} d.w.) Min	Max	RSD %
2	3	180	6	170	180	3
16	4	4300	2900	2800	8600	66
18	4	1800	220	1500	2100	12
21	4	24000	5600	19000	32000	23
42	3	4900	1200	4000	6300	25

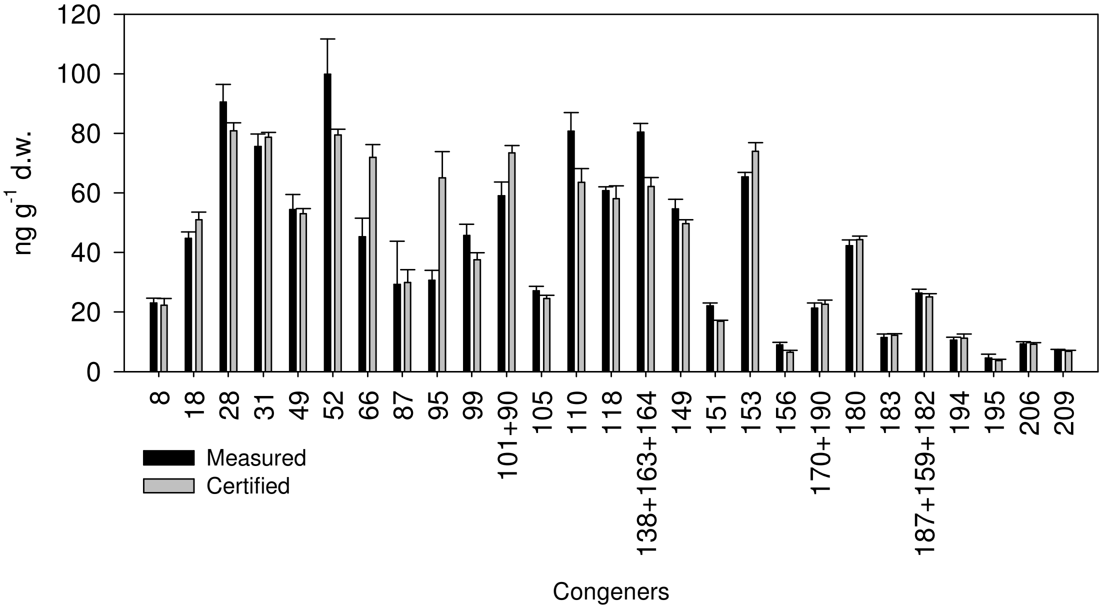

Figure 2-2 Standard Reference Material® 1944 quantification results. The error bars represent one standard deviation above the arithmetic mean. The black bars represent the measured value obtained in the lab using our analytical method. The gray bars are the values certified by the National Institute of Standard and Technology

2.5 Total PCB Concentration Analysis

The concentration of ΣPCBs (sum of all congeners, ng g^{-1} d.w.) in the 60 samples ranges from 53 ng g^{-1} d.w. to 35000 ng g^{-1} d.w. with an arithmetic mean 7400 ng g^{-1} d. w. and a coefficient of variation of 90%. The geometric mean of the ΣPCB concentrations is 4800 ng g^{-1} d.w., with a geometric standard deviation of 3.5 ng g^{-1} d.w. The total PCB concentration follows a log normal distribution (Figure 2-3). Total organic carbon content (TOC) in the sediments ranged from 0.43% to 7%, with an arithmetic mean of 4.6%, standard deviation of 1.5% and coefficient of variation of 32%. Neither linear nor logarithmic transformation correlations were strong between ΣPCB concentrations and % TOC (R^2=0.23 and 0.49, respectively), indicating that equilibrium of PCBs with particulate organic carbon does not control or predict ΣPCB concentration in the sediment of IHSC.

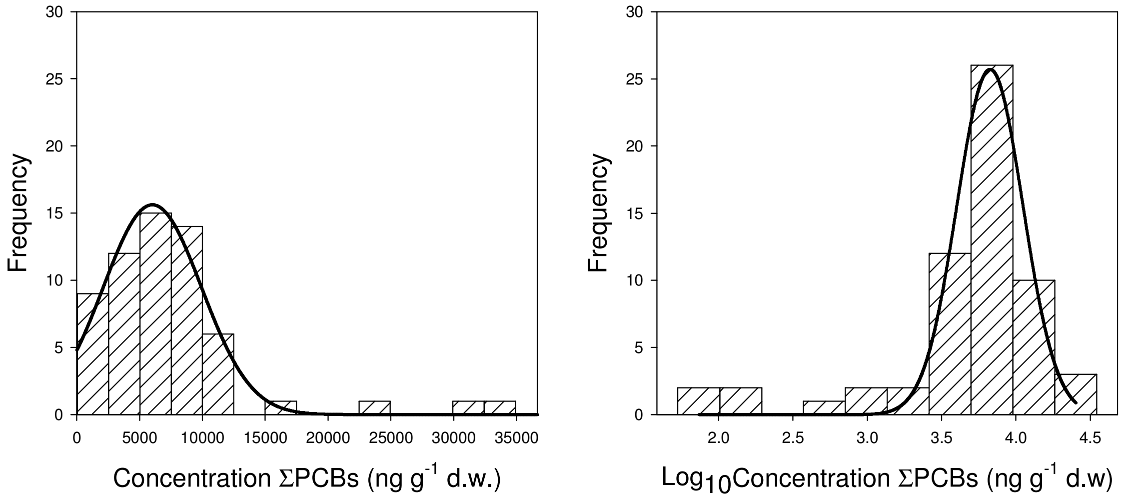

Figure 2-3 Histograms of surficial sediment. Left plot in ng g^{-1} d.w. and right plot transformed to common logarithms. The curve in the left plot shows the lognormal distribution, while the curve in the right plot shows the fitted normal distribution

These results differ from an EPA study of Lake Michigan sediments (33) where logarithmic transformation showed a strong relationship between both variables. IHSC samples normalized to % TOC range from 2800 to 680000 (ng PCB g^{-1} TOC), with an arithmetic mean of 160000 (ng PCB g^{-1} TOC) and a coefficient of variation of 80%. The ΣPCB concentration in IHSC surficial sediment is lowest in the harbor near Lake Michigan (Table 2-2). The difference in concentrations between the Indiana Harbor samples and the rest of the IHSC is statistically significant (95% confidence level using log-transformed data). The concentration of surficial sediment of southern Lake Michigan is approximately 30 ng g^{-1} d.w. (33), lower than in any location sampled in the IHSC. The much greater concentrations in the IHSC relative to Lake Michigan suggest that the sediment from IHSC could be a source of PCBs to the lake. Indeed, the Lake Michigan Mass Balance Study reports a total net load of 29.86 kg $year^{-1}$ PCBs from Calumet River, passing through IHSC, to Lake Michigan (34). Desorption and/or sediment transport from the IHSC may be the origin of those PCBs (35, 36).

Table 2-2 Sample number, mean and range of total concentration of PCBs (ng g^{-1} d.w.) for the sections of Indiana Harbor and Ship Canal, East Chicago, Indiana

Location	**Number Samples**	**Mean (ng g^{-1} dw)**	**Range (ng g^{-1} dw)**	
			Min	**Max**
Indiana Harbor	14	2800	53	8000
Harbor Entrance	7	7300	1800	24000
Indiana Harbor Canal	23	8700	140	30100
Calumet River Branch	5	7200	5200	10300
Lake George Branch	5	7500	5400	10000
The Forks	6	13000	5200	35000

The maximum ΣPCBs in surficial sediment found in IHSC falls within the range of other well-known contaminated sites in USA (Figure 2-4). The concentrations are much higher than the Milwaukee Harbor (37) and Sheboygan River Inner Harbor (38), similar to Hudson River (39), but lower than the Fox River and lower Green Bay (40, 41), Little Lake Butte des Morts Reach (42), Manistique River (43), Waukegan Harbor (34) and New Bedford Harbor (44). Most of these sites have been designated as Superfund Sites, which require that remediation actions be implemented. IHSC is not a Superfund Site and is not being dredged for environmental remediation.

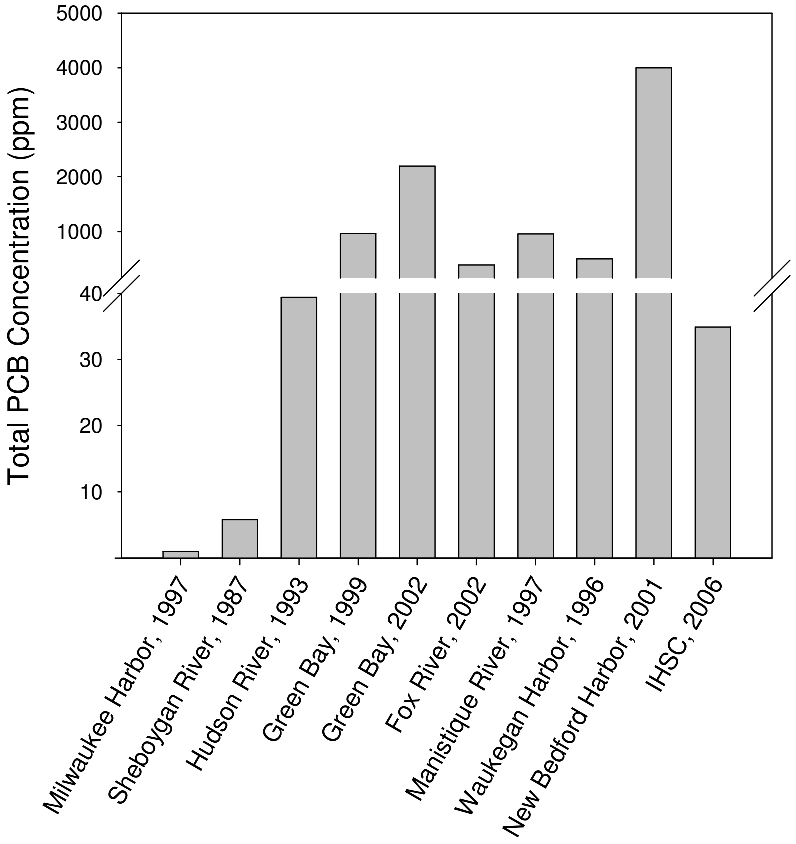

Figure 2-4 Comparison of total concentration of PCB in surficial sediment with nine different sites across the United States, including IHSC (this study)

2.5.1 Congener Profile Distribution Analysis

The PCB homolog and congener distributions in the IHSC are nearly uniform from site to site and resemble Aroclor 1248 (Figure 2-5) (the arithmetic mean and standard deviation for each congener are presented in Table A-2, Appendix A). We compared the congener distribution of Aroclor 1016 lot A2, 1242 mean of 3 lots, 1248 lot A3.5, 1248 lot G3.5, 1254 lot A4, 1254 lot G4 and 1260 mean of 3 lots, reported by Frame et al. (45), with the average congeners profile distribution of our samples.

Both Aroclor 1248 lots yielded the best linear correlation ($R^2 \geq 0.91$). Aroclor 1248 (Accustandard Lot B4020171) was then analyzed by our analytical method and the resulting R^2 with Aroclor 1248 was 0.94. Despite the strong relationship found, 53% of the congeners are statistically different (99% confidence level) from this commercial mixture. The following are the 10 most different, in order of difference: PCB48, PCB15, PCB158, PCB187, PCBs98+102, PCBs26+29, PCB25, PCB177, PCBs135+151 and PCBs129+138+160+163. However, the differences between the Aroclor and IHSC congeners are less than 2.5% by mass (Figure 2-5).

It appears that the IHSC was originally contaminated with Aroclor 1248, and that the small differences that now exist are the result of chemical, physical and biological transformations (weathering) in the sediments. The last time the IHSC was dredged was in 1972 —thirty-four years before our expedition; thus the surficial sediments may have been at the water–sediment surface for many years. Over time the lower chlorinated congeners (e.g. PCB 48) may have been lost to volatilization, desorption and/or aerobic microbial degradation (46), and the high chlorinated ones due to anaerobic microbial dechlorination (47). The relative enrichment of the lower-chlorinated and ortho-substituted congeners (PCBs 25 and 26+29) is probably a result of anaerobic microbial dechlorination (47).

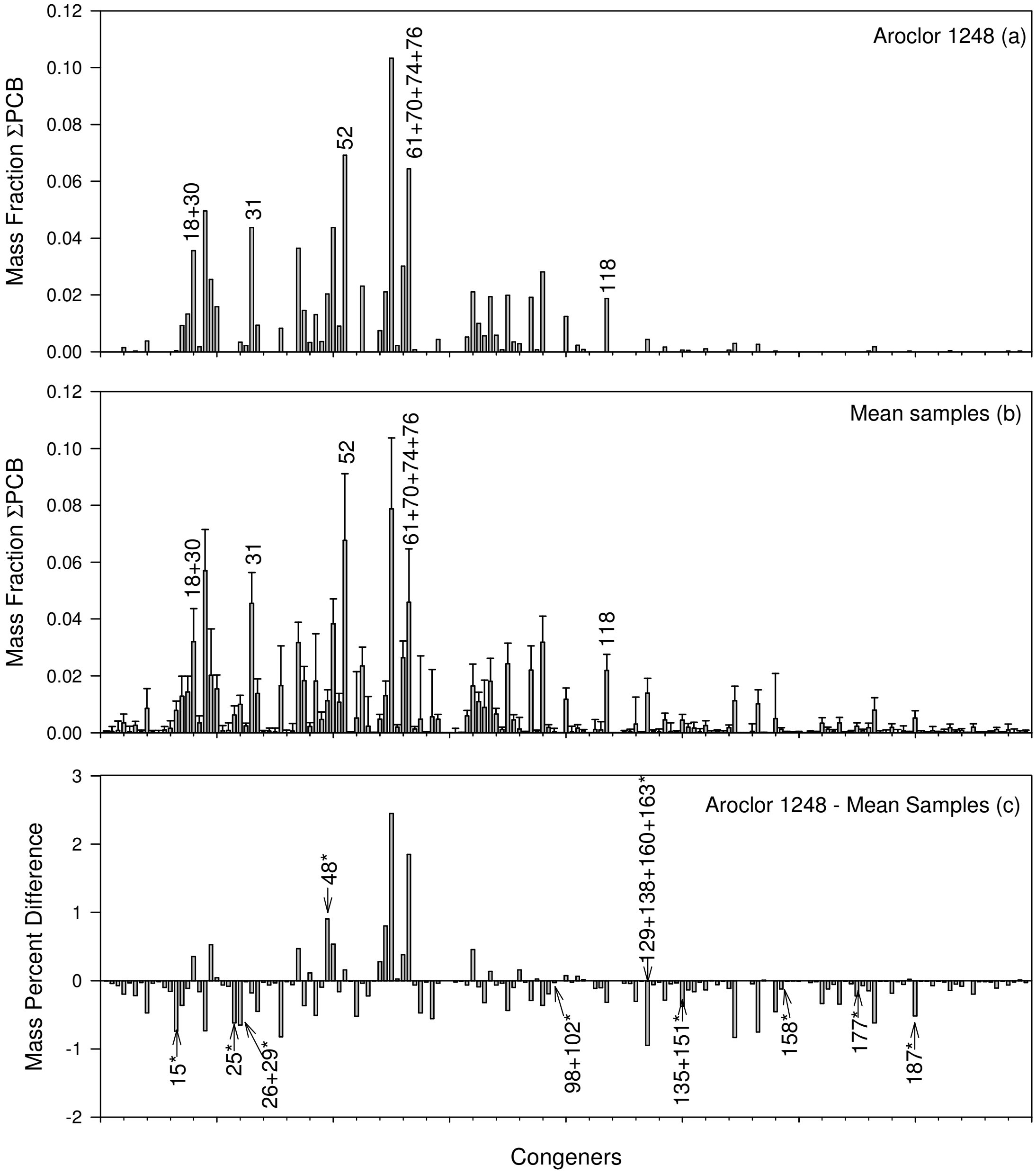

Figure 2-5 Congener distributions in mass percentage for Aroclor 1248 (Lot B4020171) (a), mean congener distribution of the 60 sediment sites (b) and Aroclor 1248 minus mean samples (c). In the case of (b), each sample was normalized to its total concentration, and the error bars represents one standard deviation about mean. Congeners are ordered by "IUPAC" nomenclature (2)listed in full in Table A-2 in Appendix A, including the values depicted in (b). The asterisk (*) indicates a difference at the 99% confidence level as described in the text

2.6 Conclusions

Employing tandem mass spectrometry we have conclusively determined that IHSC surficial sediments are contaminated with PCBs. The PCB levels found here are comparable to other PCBs contaminated sites in USA, most of them (although not IHSC) established by law as Superfund Sites. The analytical method used also allowed us to determine the PCB congener profile distribution in the sediment. The origin of the PCBs is not known but strongly resembles the original technical mixture Aroclor 1248. This mixture was used in hydraulic fluids, vacuum pumps, plasticizers and adhesives (48). Possible uses of this mixture in East Chicago included the equipment and auxiliary services for the adjacent steel mill and gas refinery and/or lubrication for the drawbridges spanning the canal. Finally, the PCBs in the sediments have undergone a small amount of weathering compared to the original 1248. The current congener profiles provide evidence of desorption, volatilization, and microbial dechlorination.

CHAPTER III: FATE OF PCB CONGENERS IN AN INDUSTRIAL HARBOR OF LAKE MICHIGAN[2]

3.1 Abstract

We have quantified the release of polychlorinated biphenyls (PCBs) from Indiana Harbor and Ship Canal (IHSC) to Lake Michigan and the atmosphere. Navigational dredging is planned for this system, and there is concern that dredging will result in releases of PCBs. We have analyzed greater than 158 PCBs in surficial sediment, water, suspended particles, and air. We predicted the release of PCBs from sediments to water and from water to air. To quantify the level of confidence in our calculations, we used a Monte Carlo simulation for each congener flux. We determined that 4 ± 0.05 kg of ΣPCBs were released from the sediment to the water and 7 ± 0.1 kg of ΣPCBs were volatilized from the water to the air annually. We measured input from the upstream regions of the canal system of 45.0 kg yr^{-1} and export to Lake Michigan of 43.9 kg yr^{-1}. The ΣPCBs mass balance accounts for nearly all the PCB inputs and losses to the navigational regions. The congener profiles in sediment, water, and air support our determination that the contaminated sediment is a major source of PCBs into the water and air above it. We have shown that the system is currently a significant source of PCBs to the air and to Lake Michigan, even under quiescent conditions.

3.2 Introduction

Indiana Harbor and Ship Canal (IHSC) is one of the most heavily polluted water systems in the United States. It is contaminated with polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons, chlorinated solvents, volatile organic compounds, heavy metals, and is home to a former lead smelter (20). The IHSC discharges water to

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[2] Martinez, A.; Wang, K.; Hornbuckle, K. C. Fate of PCB Congeners in an Industrial Harbor of Lake Michigan. *Environ. Sci. Technol.* **2010,** *44*, (8), 2803-2808.

Lake Michigan and may be one of the largest sources of many of these chemicals to the freshwater lake, one of the largest in the world. This is certainly the case for PCBs (34, 49, 50). This is a major environmental threat because of PCBs' known toxicity (7, 12, 51) and very strong bioaccumulation potential in the aquatic food web (52, 53). As a result of PCB contamination of fish, consumption advisories are still necessary in Lake Michigan (54).

The sediments of IHSC are to be dredged for navigational purposes within the next few years (55), allowing deep-hulled barge traffic to serve local industries, which include a major steel mill (Mittal Steel Indiana Harbor) and a major gas refinery (BP America Inc. in Whiting, Indiana). It has not been determined when dredging will commence, although a confined disposal facility (CDF) has been constructed close to the site in East Chicago, Indiana. Despite these plans for dredging, the impact of removing the contaminated sediments is unclear (15). In fact, even in the absence of dredging, the current fate of PCBs in the sediments is unknown.

We have previously shown that PCBs in the surficial sediment of IHSC resemble the commercial mixture Aroclor 1248 and are comparable in magnitude to those identified as Superfund sites by the Comprehensive Environmental Response, Compensation, and Liability Act. The concentrations range from 53 to 35000 ng PCB g^{-1} dry weight (d.w.) of sediment (56).

The goal of the study was to investigate the fate and quantify the release of PCBs from the sediments to the water, as well as from the waters to the air above it, and to quantitatively evaluate the uncertainty over a week and on an annual basis. We hypothesized that PCBs are continuously released from the sediments to the water. Furthermore, we hypothesized once they are released from the sediments, PCBs are exported from the canal into Lake Michigan and also emitted to the air over the canal. To test our hypotheses, we measured PCB congeners in the air, water, and surficial sediment in the canal and modeled the potential release. We predicted the release and emission of

PCB congeners as a function of their physical-chemical properties, the local meteorology and the levels of PCBs in each of the environmental compartments. We used a Monte Carlo simulation approach to assess our confidence in the model results.

3.3 Methods

We conducted an intensive sampling expedition to collect samples of surficial sediment, water (dissolved-phase and suspended particles), and air (gas-phase) in the IHSC. The study was designed for an internally consistent and matched sample set of 158 PCB congeners quantified in those four environmental compartments. This dataset is the basis for the determination of the potential movement of PCB congeners between sediment, water, and air.

3.3.1 Sampling Method

During the second week of August 2006, samples were collected in IHSC (Figure 3-1) from aboard the U.S. Environmental Protection Agency's *R/V Mudpuppy*. Details of sampling methods are provided in Appendix B. Meteorological data such as wind speed, atmospheric pressure, water and air temperatures were obtained from the National Oceanic and Atmospheric Administration (NOAA), Calumet Harbor, IL, Station. Daily average volumetric flows from IHSC were obtained from U.S. Geological Survey (USGS). Figure 3-2 depicts the wind speed, air and water temperatures and water flows for 2006.

Figure 3-1 Indiana Harbor and Ship Canal, East Chicago, Indiana. The blue circles (○) and red diamonds (◊) represent the sites where sediment and water samples, respectively, were collected

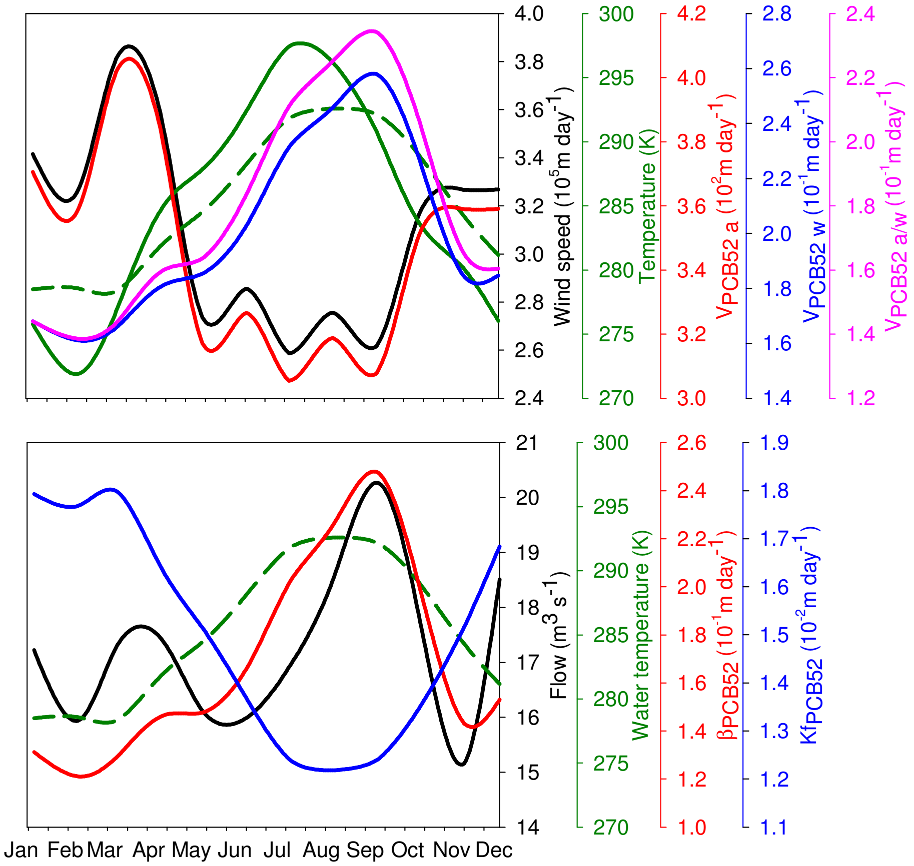


Figure 3-2 Seasonal variation of meteorological and hydraulic conditions, and transfer coefficients for PCB52. Top plot depicts air-water coefficients and bottom one, sediment-water coefficients. Note the difference in scale on the right for each parameter. The green lines on the top plot describe the air and water temperatures (dash line), respectively. Transfer coefficients are strongly dependent on the congener. See text for abbreviations

3.3.2 Analytical Methods and Quality Assurance and Control

The extraction method of PCBs in bulk sediment and airborne PCBs sorbed to XAD-2 resin required pressured fluid extraction with acetone and hexane and has been described in detail elsewhere (57). Extraction of water-borne PCBs collected on glass fiber filters and XAD-2 resin required Soxhlet apparatus, also refluxed with acetone and hexane (58). PCB quantification was carried out employing a modification of USEPA method 1668a (32). Tandem Mass Spectrometry GC/MS/MS (Quattro Micro^{TM} GC, Micromass MS Technologies) in multiple reaction monitoring mode was utilized to quantify all 209 congeners in 158 individual or coeluting congener peaks (see congener order in Table B-1), of which PCB14 (3,5-dichlorobiphenyl), PCB65 (2,3,5,6-tetrachlorabiphenyl) and PCB166 (2,3,4,4′,5,6-hexachlorobiphenyl) are surrogate standards and PCB204 (2,2′,3,4,4′,5,6,6′-octachlorobiphenyl) is internal standard (see Appendix B for additional details and QA/QC).

3.3.3 Mathematical Approach

The mathematical structure of the mass transfer phenomena used in this study is well established and has been used and described in numerous papers and textbooks (59-63). Our study applied this structure using the most accurate, recently reported, and/or well characterized parameters. In all cases, we used data specific to each PCB congener and the local environment. The sediment-water and air-water interfacial boundary layer coefficients were determined from reported experimental and modeling studies. Figure B-1 depicts the equations utilized in this model.

3.3.4 Sediment-water Exchange

A theoretical resistance-in-series model between two phases was utilized to model the sediment-water exchange (62). Fluxes were computed for each congener or coeluting congeners, and equilibrium between sediment and porewater concentrations were assumed (eq 3-1)

$$F_{PCBi\,s/w} = k_{f\,PCBi} \times \left(C_{PCBi\,pw} - C_{PCBi\,w}\right) \tag{3-1}$$

where $F_{PCBi\ s/w}$ is the flux between sediment and water for the ith PCB (ng m^{-2} day^{-1}), $k_{f\ PCBi}$ is the solubilization mass transfer coefficient for the ith PCB (m day^{-1}), $C_{PCBi\ pw}$ is the concentration in the porewater for the ith PCB (ng m^{-3}), and $C_{PCBi\ w}$ is the concentration in the water column for the i^{th} PCB (ng m^{-3}). A positive flux value indicates a flux from the sediment into the water. This model assumes the process of PCBs solubilization from the surficial sediment bed to the water column, and resuspension is not included. Even though solubilization of hydrophobic compounds is a slower process in comparison to resuspension, recent studies have shown that the resuspension phenomenon balanced by deposition and is a less significant process than solubilization in terms of net release of contaminants into the water column (36, 64). The solubilization mass transfer coefficient ($k_{f\ PCBi}$) was developed by Thibodeaux (62) and tested in different studies (36, 60, 64). It lumps both bioturbation and chemical sorption/desorption processes (eq 3-2).

$$k_{f\,PCBi} = \frac{1}{\frac{1}{\beta_{PCBi}} + \frac{z}{D_b \times K_{PCBi\,oc} \times f_{oc} \times \rho}} \qquad (3\text{-}2)$$

where β_{PCBi} is the benthic boundary layer coefficient for the i^{th} PCB (m day^{-1}), z is the bioturbated depth (m), D_b is the biodiffusion coefficient (m^2 day^{-1}), $K_{PCBi\ oc}$ is the organic carbon base partition coefficient corrected by water temperature for the i^{th} PCB (L kg^{-1} oc), foc is the total organic carbon fraction (kg oc kg^{-1}) and ρ is the bulk dry density of the bed (kg L^{-1}).

3.3.5 Parameter Estimation: Sediment-water

The parameters used in the sediment-water exchange model were chosen based on their applicability to IHSC. Details are provided in the Appendix B and briefly summarized here. We used the congener-specific octanol-water equilibrium coefficient, $K_{PCBi\ ow}$ (4) with water temperature correction (5, 65). A one-parameter linear free energy relationship (op-LFER) (66) was employed to calculate $K_{PCBi\ oc}$. The β_{PCBi} were computed using a relationship between the water-to-bed friction velocity and the Schmidt number.

The water-to-bed friction velocity was calculated from the mean flow velocity, a coefficient of roughness, mean hydraulic radius, the water depth and the gravitational acceleration constant (62). The bioturbation component of the solubilization mass transfer coefficient was computed using values from literature (60, 64). The biodiffusion coefficient was selected from a seasonal range and the lowest value was considered for the calculation because we did not observe any evidence of macro-fauna during our sampling of the surficial sediments.

3.3.6 Air-water Exchange

We calculated the direction and magnitude of air-water exchange of each PCB congener using the gradient-flux law, i.e. a mass transfer velocity multiplied by a concentration gradient (eq 3-3) (61)

$$F_{PCBi\,a/w} = V_{PCBi\,a/w} \times \left(C_{PCBi\,w} - C^{eq}_{PCBi\,w}\right) \tag{3-3}$$

where $F_{PCBi\,a/w}$ is the flux between air and water for the ith PCB (ng m^{-2} day^{-1}), $V_{PCBi\,a/w}$ is the air-water exchange velocity for the ith PCB (m day^{-1}), $C_{PCBi\,w}$ is the concentration in the water column for the ith PCB (ng m^{-3}), and $C^{eq}_{PCBi\,w}$ is the concentration in water in equilibrium with the gas-phase for the ith PCB (ng m^{-3}). A positive flux value indicates a flux from the water into the atmosphere. The air-water exchange velocity was separated into velocities for the compounds in air and water using diffusivity ratios between a known chemical and the congeners. Once both terms are computed, the air/water exchange velocity is calculated from eq 3-4

$$\frac{1}{V_{PCBi\,a/w}} = \left(\frac{1}{V_{PCBi\,w}}\right) + \left(\frac{1}{V_{PCBi\,a} \times K_{PCBi\,a/w}}\right) \tag{3-4}$$

where $V_{PCBi\,w}$ is the water exchange velocity for the ith PCB (m day^{-1}), $V_{PCBi\,a}$ is the air exchange velocity of the ith PCB (m day^{-1}), and $K_{PCBi\,a/w}$ is the equilibrium air-water partition constant (nondimensional Henry's Law constant) for the ith PCB corrected by air and water temperatures. The aqueous concentration in equilibrium with the atmospheric concentration for each congener (C_{PCBiw}^{eq}) was obtained from the division of the gas-phase concentration and $K_{PCBi\,a/w}$. This is a well accepted approach for determining volatilization flux potentials (63, 67, 68).

3.3.7 Parameter Estimation: Air-water

The choice of Henry's Law constant in Pa m^3 mol^{-1} (HLC_{PCBi}) affects the direction and magnitude of the PCB flux and many studies have reported different values for congener HLC_{PCBi} (3, 5, 69, 70) , although the differences are most pronounced for the highest molecular weight PCBs. The selection of HLC_{PCBi} has been source of considerable discussion in the literature (71, 72). For this study, the internal consistency of the measurements and availability of the measurement's uncertainty is the most important factor. We chose the values from Dunnivant et al. (R = 0.95, standard error = 0.66 or 1.9% of the mean value) (3). Temperature correction for $K_{PCBi\,a/w}$ was carried out using van't Hoff equation (65), where the $\Delta U_{PCBi\,a/w}$ was from Li et al. (5) (eq 3-5).

$$K_{PCBi\;a/w(T_2)} = K_{PCBi\;a/w(T_1)} \times \mathrm{e}^{\left(-\frac{\Delta U_{PCBi\;a/w}}{R}\left(\frac{1}{T_2}-\frac{1}{T_1}\right)\right)} \qquad (3\text{-}5)$$

where $K_{PCBi\;a/w(T_2)}K_{PCBia/w(T_2)}$and $K_{PCBi\;a/w(T_1)}$are the dimensionless Henry's Law constant at temperatures T_2 and T_1 (K) for the ith PCB, $\Delta U_{PCBi\,a/w}$ is the internal energy for the transfer of water to air transfer for the ith PCB (J mol^{-1}) and R is the gas constant (J mol^{-1} K^{-1}) (more details in Appendix B).

3.3.8 Annual Emissions

Because sediment, water and air concentrations were measured only in August, we estimated concentrations over the rest of the year as follows. We assumed that the bulk sediment PCB concentration was constant during the entire year. However, porewater concentration of PCBs varied during the year due to temperature difference in the water which modifies the octanol-water equilibrium coefficient. Total water concentrations (dissolved-phase + suspended particulates) were assumed to be the same as measured from June to September but 2.5 times higher during the rest of the year. We made this assumption due to two pieces of information. First, Offenberg and Baker (73) measured total water concentrations in the southern Lake Michigan region (Chicago, IL and Gary, IN) and found that total concentration of total PCBs were 2.5 higher in January than in July. Second, USEPA measured total water concentrations (dissolved-phase + suspended particulates) in IHSC from August 1994 to September 1995 and found a similar trend of 1.3 to 2.7 times higher levels during winter and spring months than the rest of the year (49, 50). The ratio between dissolved-phase and suspended particulates was assumed to be constant for the whole year, but a 20% error in the dissolved-phase concentration was included in the Monte Carlo simulation.

Air concentrations increase as a function of air temperature: we assumed that gas-phase PCBs in IHSC varied as a function equivalent to what we have observed in the City of Chicago of the same 158 congeners in 184 air samples collected in Chicago, IL (74). The resulting extrapolation predicted ΣPCBs in summer are about three times larger than in winter. All physical-chemical parameters as well as mass transfer coefficients were corrected for meteorological and hydraulic conditions obtained from NOAA and USGS, respectively. Emissions were calculated in a monthly basis and then added for the entire year. Emissions were calculated as flux multiplied by the total water surface area of IHSC (1300000 m^2).

3.3.9 Monte Carlo Simulation

We evaluated the precision of the calculated fluxes and emissions by considering the frequency distribution for each model parameter instead of single average values. These frequency distributions were determined from the original reports of the parameter's confidence intervals or standard deviations. Some estimate of uncertainty was available for all the parameters. Wind speed, HLC_{PCBi} and $K_{PCBi\ ow}$ were described as lognormal distributions and the rest of the parameters as normal distributions (more details in Appendix B). The Monte Carlo simulation then randomly probes the distributions to generate a set of input parameter values from which fluxes were computed. This was repeated 10000 times and provided a frequency distribution of PCB congener fluxes. From the frequency distribution, we determined the arithmetic mean, the standard error, and the 95% confidence intervals. This Monte Carlo simulation procedure was applied to each congener flux and emission for the air/water and sediment/water exchanges. It was a powerful method to assess the variability of the flux results as a function of the variability in the independent variables.

3.4 Results and discussion

3.4.1 Air, Water and Sediment Total Concentrations

The concentrations of ΣPCBs in gas-phase, dissolved-phase and suspended particulates, and sediments are presented in Figure B-2. The ΣPCBs average gas-phase concentration during the sampling period was 4500 ± 1800 pg m^{-3} (n=16). Dissolved ΣPCB water phase concentrations averaged 33 ± 16 ng L^{-1}(n=10). The particulate water phase samples averaged 20.0 ± 8.5 ng L^{-1}(n=7). The dissolved-phase represents 61% of ΣPCB in water (all samples). Similar dissolved/particulate PCB distributions have been reported by many studies in different locations (73, 75). Surficial sediment ΣPCB concentrations have been previously reported (57) and ranged from 53 to 35000 ng g^{-1} d.w. (n=60) with an arithmetic mean of 7400 ± 6700 ng g^{-1} d.w. The three sites with concentrations above the 95th percentile were not considered in the model simulation, resulting in an arithmetic mean of 5900 ± 1200 ng g^{-1} d.w. Total organic carbon fraction (*foc*) in the sediments ranged from 0.43% to 7%, with an arithmetic mean of 4.6 ± 1.5% kg oc kg^{-1} sediment. The concentration of each PCB congener in the sediment, dissolved-phase and the gas-phase used to compute the week fluxes are presented in Table B-1.

It is difficult to compare PCB levels in heterogeneous systems between different studies, but Table B-2 provides some perspective to the level of contamination in IHSC. It is especially difficult to compare airborne PCBs concentrations because the variation and seasonal time periods collection, site location, wind direction, analytical methods and quantity of congeners analyzed can significantly impact the results. For example, airborne PCB measurements by USACE (76) and Hsu et al. (77) indicate concentrations were 1/10 to 1/100 times (lower) than our results (Table B-2). Our samplers were located directly over the water while the other samplers were located on land. The air directly over the IHSC water is enriched in PCBs, as has been reported for air over other contaminated waters (63, 67).

The congener distributions in the IHSC (Figure B-3) are quite similar and their similarity is consistent with the strong potential for chemical fluxes from sediment to water to air. As expected, the gas-phase and dissolved water profiles are slightly skewed to less chlorinated congeners while the sediment and suspended particulate profiles are skewed toward the more chlorinated congeners. Nevertheless, the profiles in the sediment and gas phases are remarkably similar as indicated by linear ($R^2 = 0.69$ and $s = 0.0061$) and non-linear correlations ($\cos \theta = 0.81$(78, 79)). Indeed, the difference between each congener fraction (congener mass to total congeners mass ratio) in the gas-phase and sediment is less than 5%. The same analyses of the sediment-water and air-water profiles (compared as averages or pairs) are even stronger. Overall, these findings are consistent with our model that predicts the sediments are one of the major sources of waterborne and atmospheric PCBs.

3.4.2 Flux: Sediment-water

The ΣPCBs net sorption/desorption flux yielded 9700 ± 130 ng m^{-2} day^{-1}, and ranged from -7 ± 2.3 to 800 ± 210 ng m^{-2} day^{-1}, for PCB192 and PCBs61+70+74+76, respectively. Figure 3-3 depicts the average flux of each congener, including the 97.5th percentile. Gross desorption from the sediment to the water yielded a flux of 10300 ± 140 ng m^{-2} day^{-1} and gross sorption from water to sediment yielded a flux of -610 ± 7 ng m^{-2} day^{-1}.

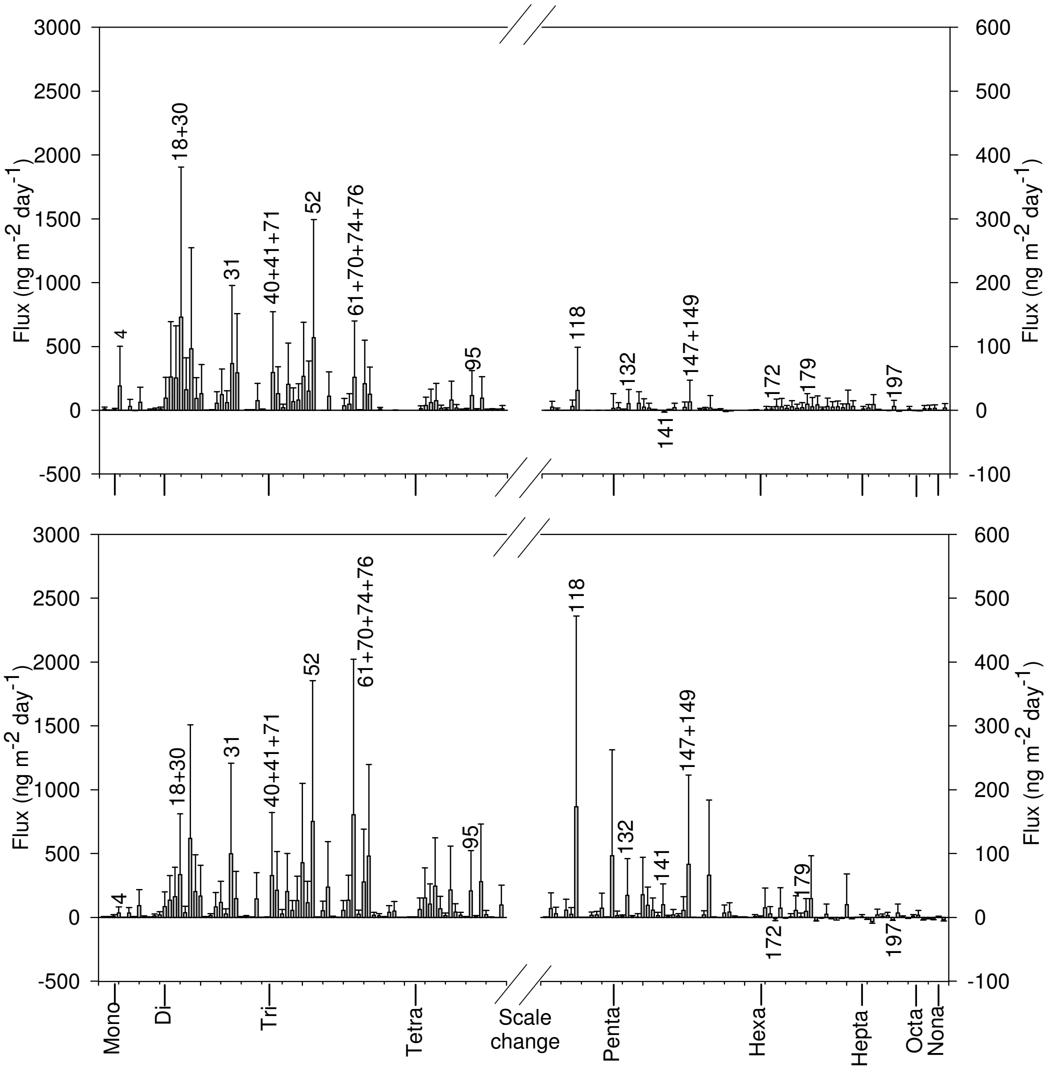


Figure 3-3 Top plot is the net air-water flux and bottom plot the net sediment-water flux for PCB congeners in IHSC. Bars represent the arithmetic average, and the error bars represent the 97.5th percentile. Note the different scales for the vertical axes

To illustrate how the independent parameters affect each congener fate, Figure 3-4 shows the probability distribution of PCB52 and PCB205 for the simulated fluxes during the sampling period, including the 95% CI. All the fluxes calculated for PCB52 are positive, thus the net flux of PCB52 is from sediment to water. PCB205, on the other hand, exhibited negative flux values and is predicted to sorb or desorb into the sediment. Our study results indicate that 70% of congeners or coeluting congeners are desorbing and 5% are sorbing. The net direction of flux cannot be identified within a 95% CI for the other 25% of congeners.

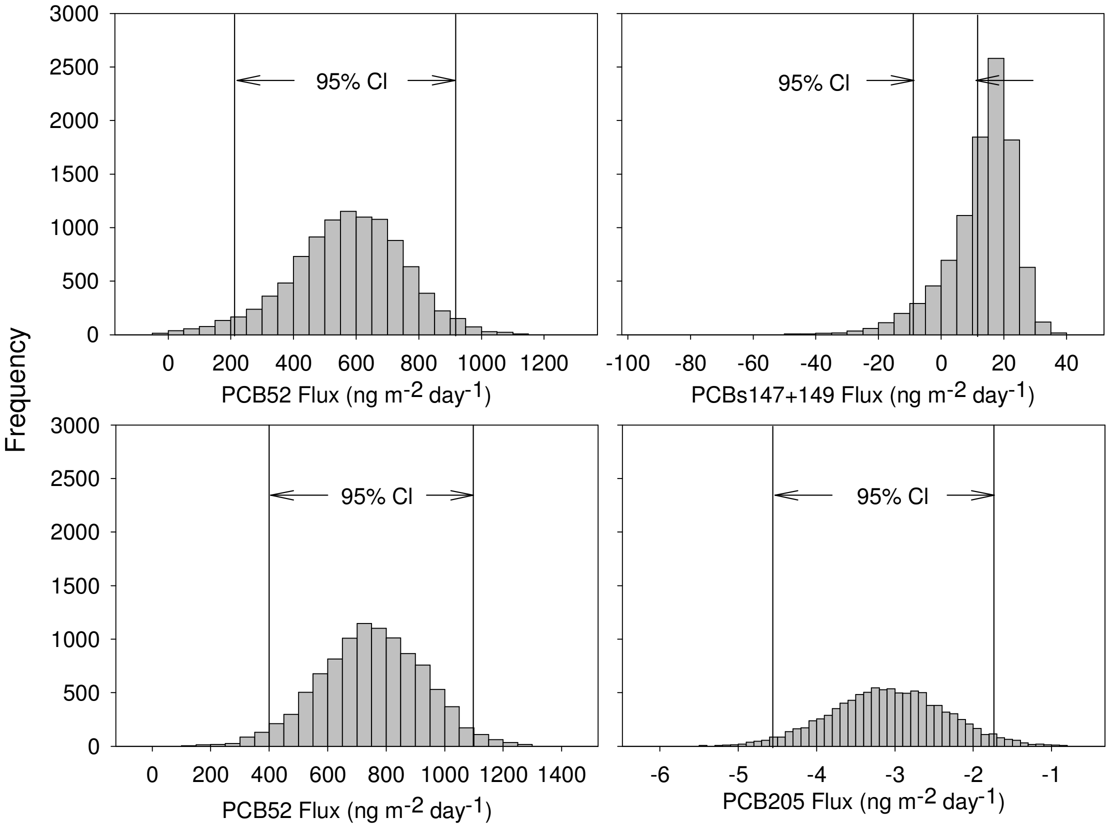


Figure 3-4 Histograms of simulated PCB fluxes during the sampling period for three congeners. Top left plot depicts PCB52 and top right plot PCBs147+149 (coeluting congeners) for the air-water interface. Bottom left plot depicts PCB52 and bottom right depicts PCB205 for the sediment-water interface

3.4.3 Flux: Air-water

The ΣPCB net volatilization/gas absorption flux yielded 6800 ± 100 ng m^{-2} day^{-1}, and ranged from -1.4 ± 1.6 to 730 ± 230 ng m^{-2} day^{-1} for PCB141 and PCBs18+30, respectively. Figure 3-3 depicts the average flux of each congener, including the 97.5th percentile. The total net average flux is at least 3 times higher than total fluxes for Lake Michigan or the Delaware River (59, 63, 67, 68), where they employed a similar flux model. Gross gas absorption yielded a total flux of -220 ± 2.4 ng m^{-2} day^{-1} and gross volatilization resulted in 7100 ± 110 ng m^{-2} day^{-1}.

Figure 3-4 shows the probability distribution of PCB52 and the coeluting PCBs147+149 for the simulated fluxes during the sampling period. Because all the fluxes within the 95% CI are positive, PCB52 will volatilize from water to air. However, PCBs147+149 do not behave as PCB52 and we cannot state with the same level of confidence that PCBs147+149 will volatilize. Our study results indicate that 64% of congeners or coeluting congeners are volatilizing from the water and no congeners are absorbing into the water. The net direction of flux cannot be identified within a 95% CI for the other 36% of congeners.

3.4.5 Annual Release of PCBs from IHSC

The 2006 gross emissions in kg per year are presented as part of the steady state mass budget (Figure 3-5). The mass balance includes annual gross desorption, sorption, volatilization and gas absorption emissions, input from upstream flow, and direct discharge to Lake Michigan. To calculate the annual emissions, we used monthly mean values for parameters that had known seasonal variability. For example, Figure 3-2 shows the seasonal variation for air ($V_{PCB52\ a}$), water ($V_{PCB52\ w}$), air-water exchange ($V_{PCB52\ a/w}$) velocities, benthonic boundary layer (β_{PCB52}) and the solubilization mass transfer coefficient ($k_{f\ PCB52}$) for PCB52. For gas-phase, dissolved-phase and sediment porewater

PCB concentrations, water flow, and temperature, we used monthly averages and calculated monthly emissions.

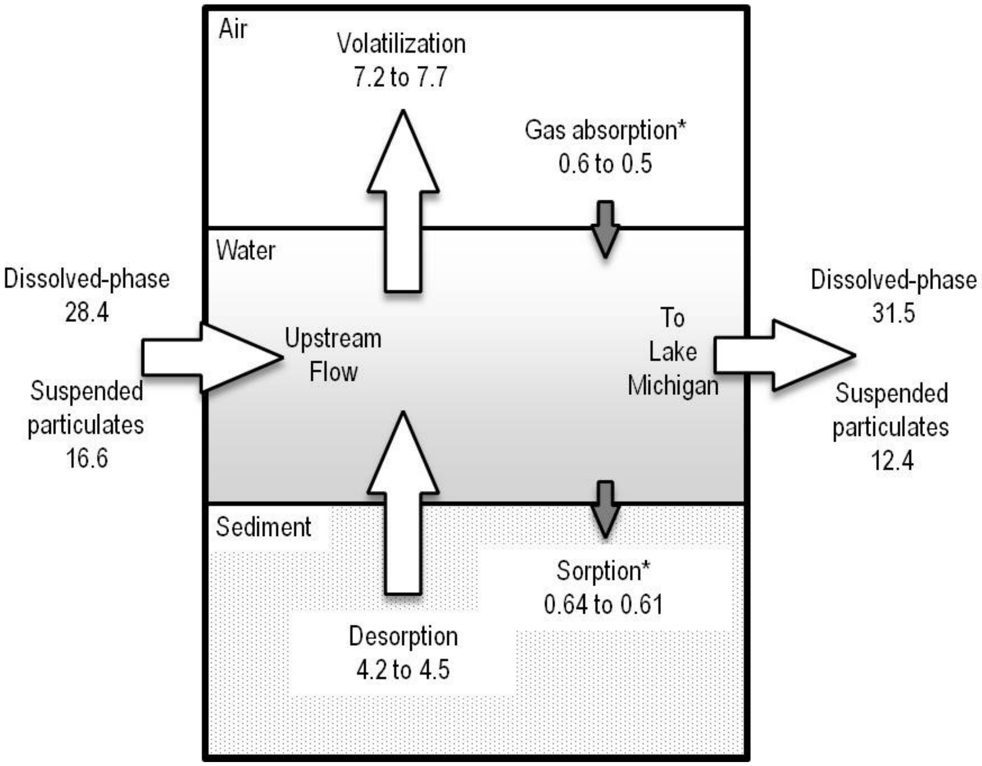


Figure 3-5 Steady state mass budget for total PCBs in IHSC for 2006 in kilograms per year. Ranges shown for sediment, water, and air fluxes are the 2.5th and 97.5th percentiles. Asterisk (*) means negative values

The emissions and uncertainties were determined using the same congener-specific and Monte Carlo methods described above. Net desorption of ΣPCBs from IHSC sediment was determined to 4 ± 0.05 kg yr^{-1} and net volatilization of ΣPCBs from IHSC water was determined to be 7 ± 0.1 kg yr^{-1}. The input from upstream flow was calculated using water samples collected in the middle of the canal (45.0 kg yr^{-1}). The direct discharge to Lake Michigan was calculated using water samples collected near the lake side of the harbor. Both mass flows assumed the same monthly USGS water flow rates and considered PCBs sorbed to suspended particles as well as in the dissolved-phase. The downstream PCB flow to Lake Michigan equals a net load of 43.9 kg PCB yr^{-1}. This finding is somewhat higher than the 29.86 kg PCB yr^{-1} determined in the mid-1990s by the USEPA (34). Although each term of the mass balance is determined independently, the inputs and losses nearly balance. We conclude that the approach we used to extrapolate from August measurements to the rest of the year is reasonable and representative of the major processes controlling PCB fate in IHSC.

3.4.6 Implications

The approach we used to determine that the sediments are one of the major sources of PCBs to the overlying water could be used to determine emissions of PCBs if the dredging at IHSC exposes sediments that are more contaminated than the surficial sediments we sampled. If the underlying sediment is three times more concentrated than the surficial sediment, and all other things remain equal, then the gross annual desorption fluxes and volatilization fluxes increase by a factor of three.

The IHSC sediments are an indirect source of PCBs to the atmosphere. Our value, 7 ± 0.1 kg yr^{-1}, is lower than estimated from the municipal sludge drying beds from Stickney and Calumet (~90 kg yr^{-1}) and insignificant to the 70 kg day^{-1} of ΣPCBs emission estimated for Chicago (77, 80). However, if we consider just the immediate community of East Chicago, the emissions may account for a significant fraction of the gas-phase PCBs in the local community. Despite the lack of information available and the many assumptions made to develop this model, we believe the approach undertook and the information resulted from this investigation could be used in other similar places to assess the fate of not just PCBs, but other persistent organic pollutants around the world. Moreover, POPs are dispersed worldwide from their original emission sites to vulnerable regions the world. The findings of this study may also be used to more accurately determine the impact of local decisions on global emissions of POPs.

CHAPTER IV: CURRENT AND POTENTIAL RELEASE OF PCB CONGENERS IN SURFICIAL AND DEEP SEDIMENTS OF INDIANA HARBOR AND SHIP CANAL

4.1 Abstract

Indiana Harbor and Ship Canal (IHSC) will be dredged in the near future. It is unclear if the dredging could decrease or increase the levels of polychlorinated biphenyls (PCBs) in this system. Through the collection of two core samples in IHSC we have attempted to investigate and predict the amount of PCBs that will be released from the sediment to the water and from the water to the overlaying air, as well as the tributary load to Lake Michigan, post dredging operations. Vertical distributions of ΣPCBs ranged from 500 to 89000 and 1800 to 30000 ng g^{-1} d.w. for cores 1 and 2, respectively. Core 1 showed its highest accumulation rate for the year 1966 (19000 μg m^{-2} yr^{-1}). Core 2 could not be dated because of evidence of sediment disturbance, perhaps due to dredging. The PCB signatures at the surface of both cores have a strong Aroclor 1248 signal, but deeper layers show evidence of mixtures of Aroclors and weathering processes that are different for each core. We examined three scenarios to predict the effect of sediment dredging on potential release of PCBs from newly exposed deep sediments. The magnitude of potential release depends strongly on the surficial PCB concentration left post dredging. For example, Scenario I (1 m of sediment removed, with a sediment profile represented by Core 1) yielded an increase in relation to the base line of 1500%, 510% and 170%, emissions from the sediment to the water, water to the overlying air, and the tributary load to Lake Michigan, respectively. Conversely, scenario II (surficial sediment concentration = 3700 ng g^{-1} d.w.) yielded a reduction in relation to the base line of 45%, 25% and 10%, emissions from the sediment to the water, water to the overlying air, and the tributary load to Lake Michigan, respectively. No appreciable effects were found in the total emissions due to organic carbon fraction, water depth and congener profiles

from the samples. Although the purpose of dredging is to provide navigational depth, PCB concentrations in the sediment should be considered so that release of PCBs to the environment is minimized.

4.2 Introduction

The United State Army Corps of Engineers (USACE), Chicago District, will commence an important dredging project in Indiana Harbor and Ship Canal (IHSC), East Chicago, Indiana. Due to lack of an adequate disposal site for the sediments, the last time this water system was dredged was in 1972. Although it is not clear when it will start, an appropriate sediment disposal site (confined disposal facility, CDF) has been built near IHSC (Figure 4-1). It is estimated that $1.2\text{x}10^6$ m^3 ($1.6\text{x}10^6$ yd^3) of sediment will be dredged from this system, and it will require 8 to 10 years to be completed. The removed sediment will be loaded onto barges that will be then moved to the CDF (17). The main purpose of the project is to maintain congressionally authorized navigation depths for large barges to pass through the canals. The project will require the removal of PCB-contaminated sediments although contamination is not the main design criterion for this project. Even though dredging is one of the most common remediation technologies for large contaminated sediment sites, there is still uncertainty in the final outcomes with respect to reducing environmental and human health impacts (15).

In previous studies we have reported the level of polychlorinated biphenyls (PCBs) contamination in IHSC. The amount of PCBs found in the surficial sediment ranged from 53 to 35000 ng g^{-1} dry weight (d.w.) and the PCB signature resembled the commercial mixture Aroclor 1248 (56). We have also determined the potential flux of these pollutants under quiescent conditions from the sediment to the water, which contributes to the tributary load to Lake Michigan, and from the water to the overlying air. Our estimates indicate that IHSC is a source of airborne PCBs, and that the contaminated sediment in IHSC is a major source of PCBs into the IHSC system and into Lake Michigan (81).

Figure 4-1 Indiana Harbor and Ship Canal, East Chicago, Indiana. Red circles show the core sample locations (Core 1: latitude 41° 38.7425 N and longitude 87° 28.3277 W, Core 2: latitude 41° 39.9058 N and longitude 87° 26.2944 W). The blue and yellow polygons represent the dredging area and the confined disposal facility (CDF), respectively (17)

Fate and transport models for different environmental compartments have been developed and employed for almost 25 years. Valsaraj et al. (82) demonstrated theoretically and with field data that the transport rate from sediment is relevant in establishing the concentration of a series of persistent organic pollutants (POPs) along its pathway from sediment to air. Connolly et al. (83) developed a fate, transport and bioaccumulation PCB model for the Upper Hudson River, where elimination of the upstream source is predicted to reduce the PCB levels in the system. Similarly, a steady-state mass balance model was used to determine the polychlorinated dibenzo-p- dioxins and –furans distribution and fluxes in the Venice Lagoon, Italy (84). These models predicted the concentrations, environmental accumulation and intermedia fluxes in the different compartments, although in some cases the model outcomes underestimated the concentrations in all the compartments (85).

However, none of these or other published articles that the authors have knowledge of have predicted the effect in terms of release of POPs from post dredging in a contaminated sediment site. Therefore, the aims of this study were i) to investigate and understand the PCB signature (total concentration and congener profiles) of two highly contaminated core samples from IHSC, including the comparison of the entire core samples, as well as the different sections with commercial Aroclor mixtures and ii) evaluate new emissions to the water and air above generated after the dredging project is carried out. We hypothesized that if deeper sediment presents higher levels of PCBs, higher emissions from the sediment to the water and water to the overlying air will be generated, as well as an increase in the tributary loading to Lake Michigan.

4.3 Methods

4.3.1 Sampling Method

Two IHSC core samples were collected May 8th 2009 from aboard the U.S. Environmental Protection Agency's *R/V Mudpuppy* (Figure 4-1). A submersible vibro-coring system was employed, with a PVC tube (length 457 cm, internal diameter 9.5 cm). Core 1 was segmented every 0.15 m (6 in), resulting in 29 slices and Core 2 every 0.305 m (1 ft), resulting in 15 slices. After segments were sliced, the segments were homogenized on the ship deck and divided into 3 precleaned amber jars, around 200 g each. The samples were brought to The University of Iowa and kept refrigerated at 4 °C until extraction and analysis.

4.3.2 Analytical method

Samples extraction and sulfuric acid cleanup were carried out as explained in detail elsewhere (56). Briefly, wet sediment (~3 g) was homogenized with combusted diatomaceous earth (7 – 15 g d. w.). Surrogate standard consisted of 500 ng of PCB14 (3,5-dichlorobiphenyl), d-PCB65 (2,3,5,6-tetrachlorabiphenyl-d5) and PCB166 (2,3,4,4',5,6-hexachlorobiphenyl) were added. Pressurized fluid extraction (Accelerated Solvent Extractor, Dionex ASE-300) was employed to extract the samples, using an acetone:hexane solution (1:1). After the extracted solution was concentrated, sulfuric acid (~2 mL) was added to the solution and mixed. This step was repeated twice. The top layer was collected and concentrated again to 5 mL. Three reservoir columns and a sulfur reducing step were used for the final cleanup method (86-89). Reservoir columns were packed as follow (from bottom to top); combusted glass wool, combusted silica gel (1 g), KOH-silica (30% v/v) (3 g), combusted silica gel (2 g) and H_2SO_4-silica gel (2:1 w/w) (6 g). The columns were eluted with 20 mL of fresh hexane which was discarded. The sample extract was added to the column and eluted with hexane (70 mL), followed by two additional elutions of hexane (70 mL). The final eluate was concentrated to 10 mL.

Activated granulate copper was used to remove sulfur in solution. The activation of the copper was carried out with concentrated HCl (12N), and rinsed with deionized water, methanol, methylene chloride and hexane. Activated copper (~3 g) was added to the concentrated solution. When necessary, the sediment extract was eluted through a fresh cleanup column one or two additional times. The solution was concentrated to 0.5 mL and set into GC vials and internal standard was added (100 ng PCB204 (2,2',3,4,4',5,6,6'-octachlorobiphenyl)). PCB quantification was carried out employing a modification of U.S. EPA method 1668B (90). Tandem mass spectrometry GC/MS/MS (Quattro Micro GC, Micromass MS Technologies) in multiple reaction monitoring mode was utilized to quantify all 209 congeners in 161 individual or coeluting congener peaks. Total organic carbon (TOC) was analyzed by Minnesota Valley Testing Laboratories. Inc (SW-846 Method SW 9060).

4.3.3 Quality Assurance and Control

Average percentage recovery of PCB14, d-PCB65 and PCB166 were 64 ± 21%, 71 ± 19% and 62 ± 10% respectively. Percentage recoveries of surrogate standards were used to correct mass congeners as follow: PCB14 from PCB1 to PCB39, d-PCB65 from PCB40 to PCB127 and PCB166 from PCB128 to PCB209. Laboratory blanks contained < 5% of total mass of PCBs detected in the samples, except for sample 396-411 cm Core1 (= 8.7%). Limit of quantification (LOQ) for each congener was obtained as 6 times the standard deviation from 3 laboratory blanks. Congener masses were calculated using two substitution methods for values below the LOQ, i.e. substitution with zero and with original values. Results showed no variation between both methods, thus, the first method is reported here.

4.3.4 Fate Model Approach

The theoretical and mathematical construction of the fate model are described in Martinez et al. (81). Briefly, fluxes for sediment-water and air-water exchanges were calculated as described below (eqs 4-1 and 4-2)

$$F_{PCBi\,s/w} = k_{f\,PCBi} \times \left(C_{PCBi\,pw} - C_{PCBi\,w}\right) \tag{4-1}$$

$$F_{PCBi\,a/w} = V_{PCBi\,a/w} \times \left(C_{PCBi\,w} - C^{eq}_{PCBi\,w}\right) \tag{4-2}$$

where $F_{PCBi\ s/w}$ and $F_{PCBi\ a/w}$ are the fluxes between sediment-water and air-water for the ith PCB (ng m^{-2} day^{-1}), $k_{f\ PCBi}$ is the solubilization mass transfer coefficient for the ith PCB (m day^{-1}), $V_{PCBi\ a/w}$ is the air-water exchange velocity for ith PCB (m day^{-1}), $C_{PCBi\ pw}$ is the concentration in the porewater for the ith PCB (ng m^{-3}), $C_{PCBi\ w}$ is the concentration in the water column (dissolved phase) for the ith PCB (ng m^{-3}), and $C^{eq}_{PCBi\ w}$ is the concentration in the water in equilibrium with the gas phase for ith PCB (ng m^{-3}). A (+) flux value from eqs 1 and 2 indicate desorption and volatilization, respectively. Emissions were calculated as flux multiplied by the total water surface area of IHSC (1300000 m^2), and computed in a monthly basis and then added for the entire year (2006). In addition, we included a Monte Carlo simulation to evaluate the precision of the calculated emissions (81).

4.3.5 Parameter Estimation

Selection, estimation and temperature correction of the different parameters are explained in detail in ref. (81). Concentration of PCBs in the sediment ($C_{PCBi\ s}$, ng g^{-1} d.w.) and organic carbon fraction (*foc*, kg oc kg^{-1}) were obtained from the core data (Table C-3, Appendix C). Although both dissolved and particulate-associated PCBs were measured in the water column in 2006, the dissolved phase concentrations under the proposed scenarios were predicted as a function of load of PCBs from upstream and from newly exposed deep sediment. Under the proposed scenarios, we expect that the flux of PCBs to the dissolved phase from the sediment will change. We assume that the PCBs associated with suspended particles do not change under any of the proposed scenarios. The concentrations of dissolved PCBs in the water column under the proposed scenarios were estimated as follows. Water dissolved concentration was divided into concentrations due to advection ($C_{PCBi\ w,\ ad}$) and due to the sediment-water exchange ($C_{PCBi\ w,s}$), $C_{PCBi\ w} = C_{PCBi\ w,ad} + C_{PCBi\ w,s}$. The $C_{PCBi\ w,s}$ was estimated using a mass balance one-box model approach to the water column in IHSC, assuming that the advection input and output are the same, the air PCB concentration is negligible, and there is no PCB degradation (eq 4-3)

$$d(C_{PCBi\,w,s} \times V)\big/_{dt} = F_{PCBi\,s/w=0} \times A - V_{PCBi\,a/w} \times \left(C_{PCBi\,w,s}\right) \times A \qquad (4\text{-}3)$$

where V and A are the total volume (m^3) and total area (m^2) of IHSC, respectively, employed in the simulation and $F_{PCBi\ s/w=0}$ is the gross desorption flux ($C_{PCBi\ w}$ =0) for the i^{th} PCB (ng m^{-2} day^{-1}). The analytical solution of eq 4-3 is shown in eq 4-4

$$C_{PCBi\,w,s} = \frac{F_{PCBi\,s/w=0}}{V_{PCBi\,a/w}} \times \left(1 - e^{-\frac{t}{h} \times V_{PCBi\,a/w}}\right) \qquad (4\text{-}4)$$

where h is the water depth (m) and t time (day). Water concentration due to advection was estimated from the difference between the total concentration in the water and the concentration due to sediment-water exchange, employing data prior to dredging (81). $C_{PCBi\ w,ad}$ was maintained constant (no new upstream sources) for all the rest of the simulations. The new concentrations due to sediment-water exchange were calculated as explained above (eq 4-4) and total concentrations were computed as = $C_{PCBi\ w,ad}$ + $C_{PCBi\ w,s}$. Hence, the total concentration varies merely because of the sediment water exchange process. A similar approach has been described by Valsaraj et al. (82). Due to the seasonal variation obtained in (81), calculations were made monthly and summed to the year.

PCB load (kg yr^{-1}) to Lake Michigan was calculated through a steady state mass balance to IHSC, where suspended particulates where assumed constants and equal to what was found in (81), and gas absorption was considered negligible.

4.3.6 Congener Profile Analysis

We estimated the flux of PCBs as a function of the individual congener concentrations in the sediment and water compartments. However, we were also interested in evidence of industrial use of specific PCB mixtures (Aroclors), especially as they may be preserved in dated sediment. A multivariate curve resolution – alternating least squares (MCR-ALS) was utilized to determine the relative contribution of four commercial Aroclors (1016, 1221, 1242, 1254 and 1248) in each sample, i.e. cores layers (91). Similar statistical methods, such as polytopic vector analysis (PVA) (78, 79) and modified polytopic vector analysis (M-PVA) (92) have being used to determine possible sources of PCBs and dioxins from field samples. Due to the fact that our source patterns are well-defined (Aroclors) and that determining weathering processes in the sediment is not one of our main goals of this study, the chosen method is valid (92). Moreover, the outcomes are easily interpreted. MCR-ALS software was obtained free from http://www.mcrals.info/ and performed using Matlab (R2009a).

Cosine theta metric (cos θ) was employed to determine similarities between congener profiles. The cosine theta metric (cos θ) allows us to examine similarities between congener profiles. This metric uses the cosine of the angle between two multivariable vectors (the profiles) where a value of 0.0 describes two completely different vectors and 1.0 describes two identical vectors (78, 79, 93).

4.4 Results and Discussion

4.4.1 Vertical ΣPCBs Concentration

The vertical distributions of ΣPCBs in both cores are depicted in Figure 4-2. Core 1 ranged from 500 to 89000 ng g^{-1} d.w. (n=29). The lowest concentration is found in the 0.396-0.411 m section and the highest at 0.107-0.122 m section. Core 1 distribution presents 5 distinct sections, from top to bottom: constant (0-0.76 m), fast increase (0.76 - 0.122 m), constant (0.122 - 0.213 m), fast decrease (0.122-0.244 m), and constant (0.244

- 0.457 m) concentrations. Total organic carbon fraction (*foc*, kg oc kg^{-1} sediment) ranged from 3.1 to 8.2%, with an average of 6.7 ± 1.5%.

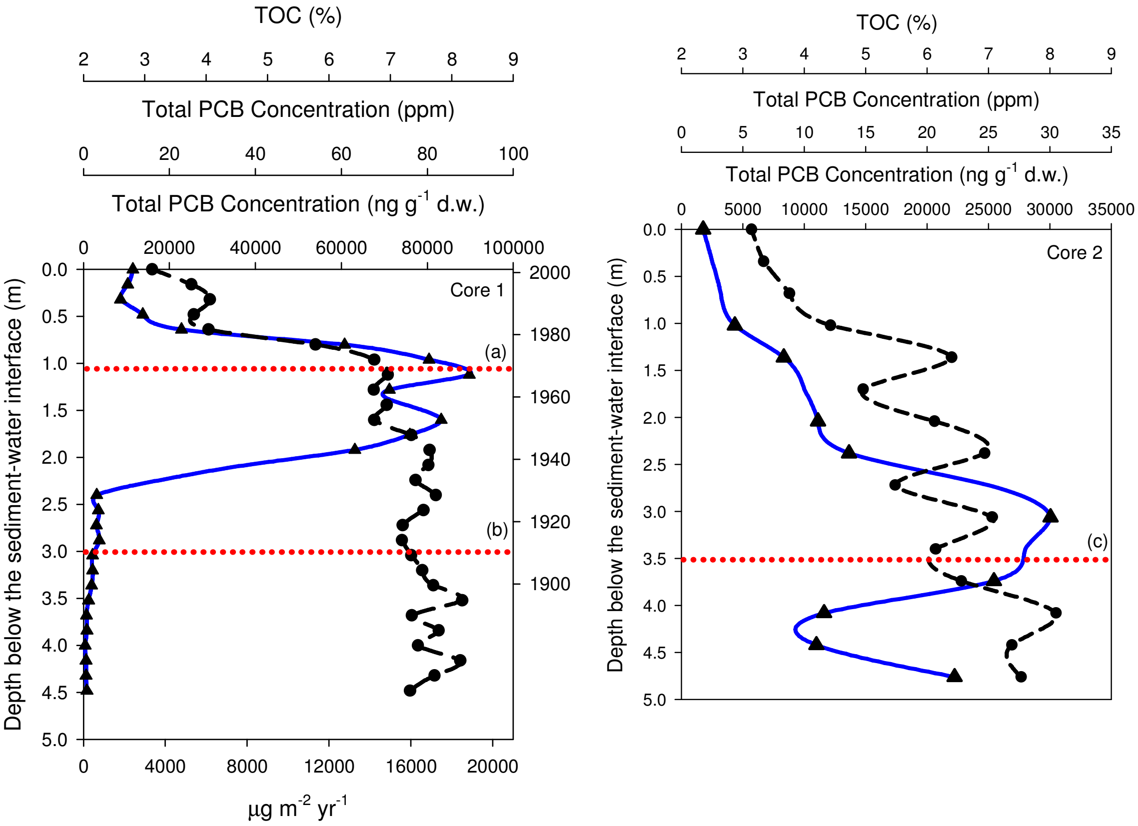


Figure 4-2 Vertical profiles of total PCB concentrations in Core 1 (left) and Core 2 (right). The solid blue line represents the PCB concentration and the black dash line is the percentage total organic carbon. Red dotted lines represent the 3 PCB release scenarios, (a) = Scenario I, (b) = Scenario II and (c) = Scenario III

From the sediment surface to section 0.198 - 0.213 m there is a strong linear relationship between ΣPCBs concentration and *foc* ($R^2 = 0.88$, $p < 0.0001$), but then, for the rest of the core there is no relationship between these two parameters ($R^2 = 0.15$, $p < 0.17$). This suggests that other types of carbon materials are involved in the sorption (absorption + adsorption) of PCBs into the sediment, such as black carbon (94, 95). Core 2 ranged from 1800 to 30000 ng g^{-1} d.w. (n=15). The lowest concentration is found in the first 0.30 m (top layer) and the highest at 0.244 - 0.274 m section. This core distribution presents 3 sections, from the top to the bottom: steady increase (0 - 0.274 m), constant (0.274 - 0.335 m), and a fast decrease-increase-decrease (0.335 - 0.457 m) concentrations. *foc* ranged from 3.1 to 8.1%, with an average of 5.8 ± 1.5%. A weak relationship was found between ΣPCBs concentration and *foc* ($R^2 = 0.38$, $p < 0.07$), similar behavior to what was found in the deepest sections of Core 1 (0.213 to 0.457 m).

The difference in PCB concentrations and congener distributions between the cores could be mainly due to the cores' location in IHSC (Figure 4-1). Core 1 was collected far from Lake Michigan and the main canal where there is less vessel traffic, less water flow interaction with Lake Michigan, and is generally a quiescent area. Core 2 was collected from the harbor, which is opposite to Core 1 in relation to its hydrodynamic conditions (turbulent). Although we do not know the spatial history of dredging in the IHSC, it is possible that the area where Core 2 was collected was dredged the last time IHSC was dredged (1972), and while Core 1 has never been dredged (96).

Core 1 was dated using an average mass sedimentation rate for IHSC from Petrovski (96) of 2.1 g cm^{-2} yr^{-1}. This rate is 100 fold higher than rates reported for Lake Michigan and 10 fold for Green Bay (97), but because of the quiescent conditions of IHSC and the industrial activities in the area, the value used is reasonable. The variability in PCB accumulation is consistent with data reported elsewhere (97, 98), except for the years around 1960 which exhibits an unexpected drop in PCB accumulation, and in the most recent year when PCB accumulation appears to increase. The highest accumulation rate (19000 μg m^{-2} yr^{-1}) was found in the 107-122 cm section, corresponding to the year 1966, which matches the historical records of the sales/production volumes of PCBs in the United States (peaks in 1966-1969) (98). Due to the disturbed characteristic of the vertical profile of Core 2, it was not possible to date this core.

4.4.2 Congener Profile Distributions

Figure 4-3 depicts the depth versus homolog group fractions of both cores. Both cores are enriched in tri- and tetrachlorobiphenyls (> 60% in mass), where generally tetra- is predominant in Core 1 and tri- is in Core 2. Tri- and tetra- in Core 1 show a decrease, with a constant penta- and an increase from hexa- to deca- with depth. Core 2 also shows a similar trend of Core 1 for tri-, but tetra- maintains constant, and an increase in the penta- to hexa-, but not much for the octa- to deca-, as it appears in Core 1. It appears that in Core 1 there is a slight decrease in mono- and di- and an increase in penta- to octa- fractions from bottom to top, which could suggests that aerobic microbial degradation is occurring in the top layer (46). This is not the case for Core 2. It appears that the trend is contrary to Core 1, which could suggest that Core 2 top layer might be affected by anaerobic microbial degradation (99).

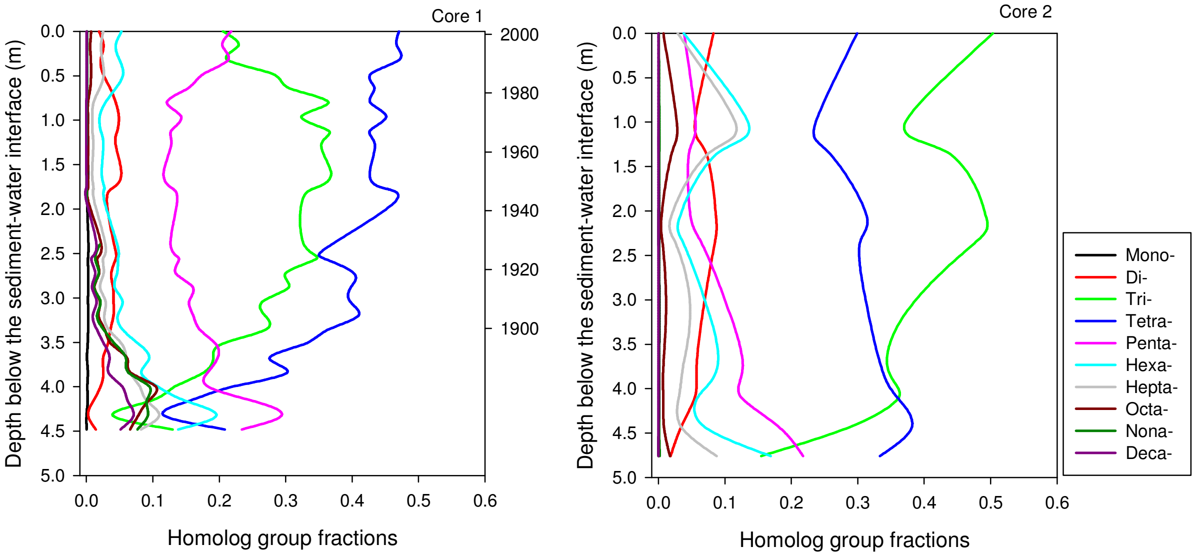


Figure 4-3 Depth versus homolog group fractions in Core1 (left) and Core 2 (right)

The results from the MCR-ALS are presented in Figure 4-4 for both cores. Certainly, the top layer of both cores, even until 0.10 m deep in Core 2, Aroclor 1248 is the predominant mixture in the sediment (> 40% in mass). This finding is consisted with our previous work in IHSC (56). The vertical distribution of Core 1 shows that during the last 20 years, mainly Aroclor 1248 has been accumulated in this area and little weathering of PCBs is evident. As at a depth of 0.50 m, there is evidence of Aroclor 1016 and well as a PCB mixture that is dissimilar to a commercial Aroclor (non-Aroclor PCBs). Around 0.250 cm, Aroclor 1254 appears and there are four mixtures contributing to the congener profile of that section. At this depth, the non-Aroclor PCBs start to be the predominant mixture (> 50%) and 1016, 1248 and 1254 are generally in the same proportion. As sections of Core 2 go deeper, 1016 starts to be the main mixture (> 40%) and 1248 almost becomes negligible. Aroclor 1254 is found in most of the sections, although it does not follow any pattern in relation to depth.

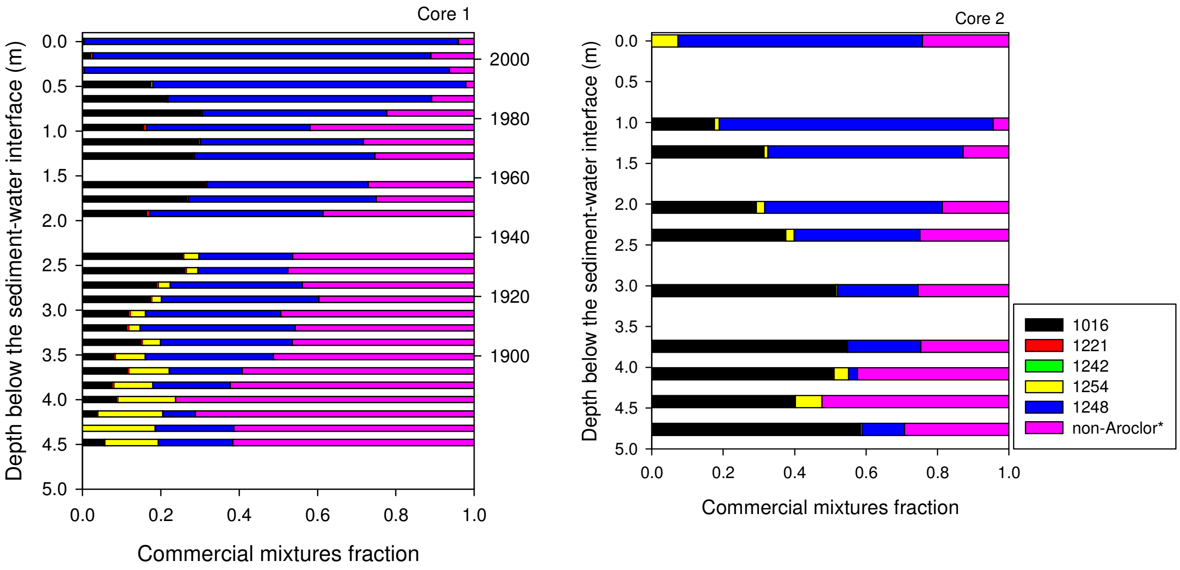


Figure 4-4 Vertical commercial fraction of Aroclor in Core 1 (left) and Core 2 (right) obtained from the MCR-ALS analysis. Each color represents the commercial Aroclor fraction. Aroclors were measured in our laboratory, using the method explained in the text. Non-Aroclor* (pink) refers to none of the Aroclors presented

Cos θ also yielded similar results. Samples with a major proportion of one of the Aroclors (Figure 4-4) returned a correlation value near 1.0, between the sample and the Aroclor chosen. Samples without a contribution from any of the commercial mixtures yielded a value near 0.0. For example, the top layer of Core 1 and Aroclor 1248 yielded a value of 0.97 ($p < 0.0001$), but the top layer of Core 2 and Aroclor 1221 yielded a value of 0.41 ($p < 0.0001$).

The difference in vertical patters in both cores could suggest that various sources of PCBs were impacting IHSC or a significant difference in core disturbance could have lead to different processes in both cores (e.g. mobilization, desorption, chemical oxidation, and dechlorination), causing major differences in both vertical profiles. The congener distributions of the three scenarios, the base line (average IHSC surficial sediment (56)), and Aroclors 1248, 1016 and 1245, are provided in Figure 4-5.

4.4.3 Annual Release of PCBs post Dredging

Three scenarios were selected to estimate the release of PCBs after dredging was completed (see Figure 4-2). Although we have shown that the cores are completely different with respect to total concentration, vertical distribution, and congener profiles, here we assumed that the core chosen for the simulation is representative for the entire IHSC. Also, due to the lack of information available (i.e. precise depth of dredging or sediment removal), these 3 scenarios describe extreme situations. Under Scenario I, dredging leaves the highest PCB concentration in the surficial sediment (Core 1: 0.107 – 0.122 m section, 89000 ng g^{-1} d.w., *foc* = 7.0 ± 0.1%, *h* = 6.2 ± 0.1 m). Under Scenario I, around 1 m of sediment is removed. Under Scenario II, 3 m of sediment with the PCB profile of Core 1 is removed, leaving a relatively low concentration of PCBs in the surficial sediment (3700 ng g^{-1} d.w., *foc* = 7.2 ± 0.1%, *h* = 8.0 ± 0.1 m). Under Scenario III, a 3.5 m sediment layer of Core 2 is removed, leaving a surficial sediment PCB concentration of 25400 ng g^{-1} d.w. (*foc* = 6.6 ± 0.1%, *h* = 7.7 ± 0.1 m). Scenario III is based on the report of the Federal Navigation Project, which establish the authorized depth in the harbor (8.5 m, 28 ft) (96). The estimated current average water depth is 5 m.

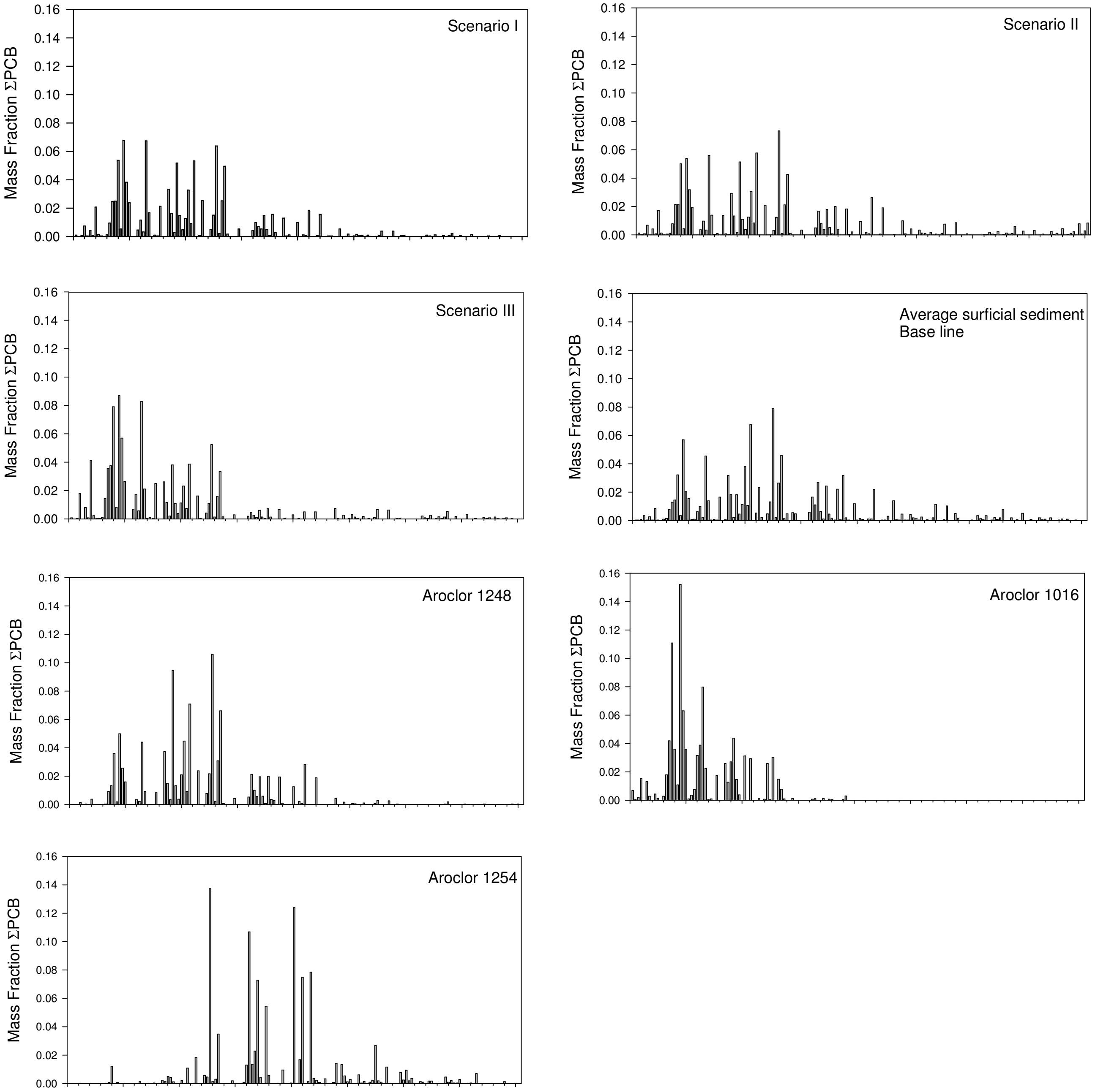


Figure 4-5 Congener profile distribution in surface sediment for scenarios I, II, III, base line (average surficial sediment IHSC (56)), and Aroclors 1248, 1016 and 1254 (analyzed by our analytical method). Each congener was normalized to the total concentration of PCBs in the sample

The flux of PCBs from the surficial sediments contributes to the concentration of PCBs dissolved in the overlying water. Under the current (pre-dredging) conditions, flux of PCBs from the surficial sediment contributes 44 ± 17% of the total water column concentration, although the contribution is a strong function of season. The sediment flux contribution to PCBs in the overlying water ranges from 31% in the coldest month to 68% in the warmest months. The seasonal trend is caused by the wintertime increase in upstream PCB flow (81) and the summertime increase in the solubilization mass transfer coefficients (36, 64, 83). This finding agrees with the increase in dissolved water concentration found in the tributary loading to Lake Michigan, in comparison with the upstream load (81).

Scenarios I, II and III yielded an annual average of the dissolved PCB water concentration due to the sediment flux of 89 ± 6%, 30 ± 17% and 73 ± 6% of $\Sigma C_{PCBi\,w}$, respectively. The difference in the proportions is mainly due to the sediment flux produced in each scenario (82).

Final results from the mass balance simulations post dredging are presented in Table 4-1, as well as prior dredging (5900 ng g^{-1} d.w., $foc = 4.6 \pm 0.15\%$, $h = 5.0 \pm 0.1$ m). As the concentration in the sediment increases, so does the sediment flux, the emissions from the sediment to the water, from water to the overlying air, and the tributary loading to Lake Michigan. Indeed, when Scenario I is compared to the current condition, there is an increase of 1500% in emission from the sediment to the water, a 510% from the water to the air, and a 170% in tributary loading to Lake Michigan. Conversely, if Scenario II is compared with the current condition, there will be a reduction in the current emissions from the sediment to the water, water to the air, and the tributary loading to Lake Michigan of 45, 25 and 10%, respectively. These emission reductions are attenuated due to the effect of the upstream load.

Table 4-1 Prior and post dredging results from the simulations. Ranges shown for desorption, sorption and volatilization are the 2.5th and 97.5th percentiles. Only the dissolved phase is presented in the loading to Lake Michigan

Condition	**Core**	**ΣPCB sediment concentration (ng g^{-1} d.w.)**	**Desorption (kg yr^{-1})**	**Sorption (kg yr^{-1})**	**Volatilization (kg yr^{-1})**	**Tributary loading to Lake Michigan (kg yr^{-1})**
Scenario I	1	89000.0	63.0- 66.2	4.5 – 4.8	37.0 – 39.1	54.0
Scenario II	1	3700.0	2.3 – 2.4	0.63 - 0.71	5.5 – 5.8	28.6
Scenario III	2	25400.0	17.9 – 19.0	1.55 – 1.63	14.4 – 15.3	34.5
Base line		5900.0	4.2 - 4.5	0.61 – 0.64	7.2 – 7.7	31.5

The ratio of sediment emission to sediment concentration is very similar between all the scenarios and the base line, even if the sediment concentration is normalized to the organic carbon content. The same is valid for the emission from the water to total dissolved water concentration. No appreciable effects were found in the total emissions due to *foc*, *h* and congener profiles from the samples.

4.4.4 Implications

Results from this investigation have exposed the following issues. First, two sediment cores cannot describe the actual extent of PCB sediment contamination in IHSC (area of 1300000 m^2). Qualitatively and quantitatively both cores present important differences, such as vertical ΣPCBs concentration and congener profiles distributions, which influence the fate of PCBs in this system. Second, Core 1 presents PCB concentration higher than 50 ppm (28% of Core 1 layers > 50 ppm), which is considered a hazardous waste (100) and therefore, IHSC could be designed as a Superfund site by the Comprehensive Environmental Response, Compensation, and Liability Act. Third and as we have predicted previously (81), the PCB concentration in the surficial sediment is a key parameter in estimating the release of PCBs from the sediment to water and from the water to the overlying air. Therefore, PCB concentrations in the sediment should be included in the dredging strategy, so that release of PCBs to the environment is reduced.

4.4.5 Limitation of the Predicted Release of PCBs

One of the major limitations of the model's outcomes (see Table 4-1) is that all the simulations were performed assuming that the sediment is homogeneous in terms of individual PCB concentrations and organic carbon content throughout all IHSC. We have already shown that both cores are different in PCB concentration, congener profile distributions and organic carbon content. It is difficult to determine whether our calculations are underestimating or overestimating the release of PCBs in this system, without having more core samples collected. However, we attempted to tackle this problem selecting two extreme scenarios in relation to PCB concentrations (scenarios I and II), so it was possible to obtain an emission range.

The other important limitation is the lack of information about the exact dredging depth. As showed before, total PCB concentration is directly related to sediment depth, so if the dredging depth is unknown, the PCB concentration is also unknown.

Another limitation is the water temperature obtained from the National Oceanic and Atmospheric Administration (NOAA), Calumet Harbor, IL Station, used to temperature correct the dimensionless Henry's law constants and the octanol-water partition coefficient (see Figure B-1). Because Calumet Harbor, IL Station is located in the Calumet River, which is bigger than IHSC, it is possible that the temperature utilized is cooler than the temperature in IHSC.

CHAPTER V: THE ROLE OF POREWATER MEASUREMENTS IN THE PREDICTION OF PCB EMISSIONS FROM THE SEDIMENTS OF A CONTAMINATED INDUSTRIAL HARBOR OF LAKE MICHIGAN

5.1 Abstract

Sediments contaminated with persistent, bioaccumulating and toxic compounds (PBTs) are an important source of these chemicals to the environment. PBTs release from sediments is caused by both episodic resuspension and continuous soluble release from the bed sediment. The latter is a predictable function of the sediment porewater concentration, although this is a measurement that is difficult for PBTs because of their relatively low water solubilities. PBT concentration in sediment porewater is required for the determination of the concentration gradient that drives the release of PBTs from the sediments. Here, we present measurements of polychlorinated biphenyls (PCBs) freely dissolved porewater concentrations from Indiana Harbor sediment using a novel passive sampler technique (SPME PDMS-fiber). The concentrations are compared to calculated values from a one-parameter linear free energy relationship (op-LFER) and bulk sediment PCB concentrations. Isotherm experiments showed that less than 20 days were enough to achieve equilibrium between the PDMS-fiber and the sediment porewater concentration. Measured sediment porewater concentration in the sediments were 110 ± 7.30 ng L^{-1}, which represents 8% of the concentration calculated using op-LFER (1390 ng L^{-1}). However, comparison between both congener profile distributions showed remarkable similarities ($\cos \theta = 0.91$), and the difference between each congener fraction (congener mass to total congeners mass ratio) in the measured and calculated porewater concentrations is less than 5%. The op-LFER overestimates the freely dissolved porewater concentration, but the measured freely dissolved porewater concentration is not necessarily the correct parameter required for the prediction of the sediment-water

soluble flux. Currently, the values obtained from the op-LFER are more appropriately applied to the empirical equations developed for predicting PBTs soluble release from contaminated sediments. Therefore, it is necessary to identify the *effective* porewater concentration to be used in the sediment-water soluble flux estimations, and how to accurately measure it.

5.2 Introduction

Contaminated sediment is one of the most important sources of persistent, bioaccumulating and toxic compounds (PBTs) into the environment (101). Emissions of PBTs are a function of the relative chemical activity in the sediment relative to the overlying water (61). Polychlorinated biphenyls (PCBs) are one of the most well studied PBTs in sediments and certainly a group of chemicals that has prompted many sediment remediation activities in natural systems. The Hudson River has become one of the best examples of sediments as a source of PCBs into the environment. Connolly et al. (83) estimated that 36% of the PCB emission into the Upper Hudson River was due to sediment-water exchange. Sediments from Indiana Harbor and Ship Canal (IHSC) have been also reported as source of PCBs into the system (15%) (81). The release of PBTs from sediment is a function of geochemical, biological and hydrodynamic conditions of the site as well as the physical chemical properties of the contaminant of interest (102, 103). In general, the sediment-water soluble PBTs flux or non-particulate flux can be estimated as mass transfer coefficient times the gradient concentration between the sediment porewater and the overlying water concentrations (eq 5-1), particularly under steady flows or quiescent conditions.

$$F_{i\,s/w} = MTC_i \times \left(C_{i\,pw} - C_{i\,w}\right) \tag{5-1}$$

where $F_{i\ s/w}$ is the sediment-water flux for the i^{th} compound (ng m^{-2} d^{-1}), MTC_i is the mass transfer coefficient for the i^{th} compound (m d^{-1}), $C_{i\ pw}$ and $C_{i\ w}$ (ng m^{-3}) are the dissolved sediment porewater and overlying water concentrations for the i^{th} compound. The general approach used to determine MTC_i has been rearranging eq 5-1, leaving MTC as function of the flux and the gradient concentrations. For PCBs in particular, MTC_is have been estimated using field measurements (36, 64) as well as laboratory experiments (101, 104-106). Most of the estimated values are within the range, with some deviation ~0.02 to 0.5 m d^{-1}. Thibodeaux et al. (103) developed a mathematical model to estimate MTC_i, and coupled the bedside bioturbation process and the transport through the benthic boundary layer to the overlying water. In this case, truly dissolved PCBs plus PCBs associated with dissolved organic carbon (DOC) fractions must be considered in the gradient concentration. DOC is a strong sorbent of PBTs and affects the fate and transport of these contaminants in the environment, particularly regarding flux at the sediment-water interface (107-110). In the examples above, porewater concentrations have been estimated from distribution coefficients or linear free energy relationships, expect for ref. (106), where it was directly measured using a passive sampler technique.

Passive sampler techniques allow direct measurement of the freely dissolved porewater concentration in sediment. As Mayer et al. (111) described, solid-phase microextraction (SPME), which is a passive sampler technique, is an equilibrium extraction. The dissolved chemical is allowed to come to equilibrium with the sampling phase, and the measurement endpoint is the freely dissolved concentration. There are different types of techniques (112), and also different materials used, such as poly-dimethylsiloxane (PDMS) coated fibers (113-115) and polyoxymethlylene (POM) sheets (86, 116, 117). This technique is a major advancement in environmental monitoring and modeling, particularly for applications where the truly dissolved phase controls the environmental fate or toxicity. Bioaccumulation studies are an example (61, 86). Many investigators state that only truly dissolved PBTs in sediment porewater are available for biological uptake from benthic organisms. For such studies of sparingly soluble compounds, like PCBs, the passive sampler method is a useful tool.

It is not clear, however, if passive sampler measurements are also appropriate for determining the magnitude and direction of PBT fluxes from sediment porewaters, which includes PBTs associated with colloidal material and dissolved organic carbon (DOC).

The aim of this investigation were i) to measure freely dissolved porewater PCB concentration from a highly contaminated sediment from IHSC using a passive sampler technique (PDMS-fiber), ii) to compare these values with those obtained using a one parameter linear free energy relationship, and iii) to evaluate which approach is the correct one for determining the sediment-water soluble flux of PCB congeners in Indiana Harbor.

5.3 Methods and Materials

5.3.1 Sediment Sampling

Sediment was collected in Indiana Harbor, Lake Michigan on May 8th 2009 from aboard the U.S. Environmental Protection Agency's R/V Mudpuppy in IHSC. The sediment used in this study was described as Core 2 elsewhere (see Chapter IV). This study used sediment collected from the top 30-60 cm of Core 2.

5.3.2 Bulk Sediment Concentration

Details of the analytical method are described elsewhere (56). Briefly, wet sediment (~3 g) was homogenized with combusted diatomaceous earth (7 – 15 g d. w.). Surrogate standard consisted of 500 ng of PCB14 (3,5-dichlorobiphenyl), d-PCB65 (2,3,5,6-tetrachlorabiphenyl-d5) and PCB166 (2,3,4,4',5,6-hexachlorobiphenyl) were added. Pressurized fluid extraction (Accelerated Solvent Extractor, Dionex ASE-300) was employed to extract the samples, using an acetone:hexane solution (1:1). After the extracted solution was concentrated, sulfuric acid (~2 mL) was added to the solution and mixed. This step was repeated twice. The top layer was collected and concentrated again untill 5 mL. The solution was then passed through Pasteur pipettes filled with combusted and acidified silica gel and eluted with hexane. The solution was reduced to approximately 0.5 mL and 100 ng of PCB204 (2,2',3,4,4',5,6,6'-octachlorobiphenyl) was spiked as internal standard. PCB were quantified using a modification of U.S. EPA method 1668B (90) that utilized tandem mass spectrometry GC/MS/MS (Quattro Micro GC, Micromass MS Technologies) in multiple reaction monitoring mode to quantify all 209 congeners in 161 individual or coeluting congener peaks. Total organic carbon (TOC) was analyzed by Minnesota Valley Testing Laboratories. Inc (SW-846 Method SW 9060).

5.3.3 Porewater Concentration from Bulk Sediment Concentration

The porewater concentration was calculated as a function of the bulk PCB concentration measurements, the solid-water distribution coefficient ($K_{PCBi\,d}$, L kg^{-1}) and the organic carbon base partition coefficient determined from a one-parameter linear free energy relationship (op-LFER) developed by Nguyen et al. (66) ($R^2 = 0.97$ and an absolute average value of the difference between measured and fitted values of 0.21). The following equations summaries the steps described above (eqs 5-2 to 5-4).

$$log(K_{PCBi\,oc}) = alog(K_{PCBi\,ow}) - b \qquad (5\text{-}2)$$

$$K_{PCBi\,d} = K_{PCBi\,oc} f_{oc} \qquad (5\text{-}3)$$

$$C_{PCBi\,pw} = \frac{C_{PCBi\,s}}{K_{PCBi\,d}}\left(10^6 \frac{g\,L}{kg\,m^3}\right) \qquad (5\text{-}4)$$

where $K_{PCBi\ ow}$ is the octanol-water partition coefficient for the i^{th} PCB (L kg^{-1}) (4), a = 0.94 ± 0.02 and b = -0.42 ± 0.12 are the parameters of the op-LFER (66), $K_{PCBi\ oc}$ is the sediment-porewater distribution coefficient normalized to the organic carbon for the i^{th} PCB (L kg^{-1} oc) , *foc* is the organic carbon fraction (kg oc kg^{-1}), $K_{PCBi\ d}$ is the solid-water distribution coefficient for the i^{th} PCB (L kg^{-1}), $C_{PCBi\ s}$ is the sediment concentration for the i^{th} PCB (ng g^{-1} d.w.), and $C_{PCBi\ pw}$ is the porewater concentration in the sediment for the i^{th} PCB (ng m^{-3}). No temperature correction was carried out to the $K_{PCBi\ ow}$ because all the experiments were conducted at 25 °C.

5.3.4 PDMS-fiber

New glass fibers with a 210 µm inner diameter and a 10 µm coating of poly-dimethylsiloxane (PDMS) were provided by Dr. Danny Reible, University of Texas at Austin. The calculated polymer volume is 6.9 µL PDMS per meter of fiber.

5.3.5 Porewater Concentration from PDMS-fibers

The PDMS-fibers were cleaned of non-polar contamination using hexane for 24 h. Then they were rinsed with acetone and deionized water. Fibers were ready for isotherm experiments (see below). After equilibration time was completed, the fibers were removed from the sediment. The fibers were cleaned with deionized water to ensure no particles remained. The fibers were set into an insert in a GC vial and 100 µL hexane was added. The vial stood for 24 h to allow equilibration between the fibers and the hexane. Fifty ng of PCB14 (3,5-dichlorobiphenyl), d-PCB65 (2,3,5,6-tetrachlorabiphenyl-d5), PCB166 (2,3,4,4’,5,6-hexachlorobiphenyl), 9.2 ng of d-PCB30 (2,4,6-trichlorobiphenyl-d5), and 9.3 ng of PCB204 (2,2’,3,4,4’,5,6,6’-octachlorobiphenyl) were used as internal standards and injected into the GC vials. Quantification was carried out as described above.

5.3.6 Isotherm Experiments

Approximately 15 g of wet sediment were slurried with 5 g of distilled water in 25 mL glass vials. Thirty pieces of 1 cm fiber were put into the 25 mL glass vials and shaken horizontally at 190 rpm and 25° C for 15, 30, 45 and 60 days. After the time was completed, the 30 pieces of fiber were collected and cleaned as mentioned above, and were divided into 3 sets of 10 units. For each time, triplicate PDMS-fibers were collected. The porewater concentration of freely dissolved PCBs in the sediment was calculated as follow (eq 5-5)

$$C_{PCBi\,pw} = \frac{m_{PCBi\,f}}{V_{fiber}K_{PCBi\,fiber/w}} \qquad (5\text{-}5)$$

where $C_{PCBi\,pw}$ is the porewater concentration for the ith PCB (ng L^{-1}), $m_{PCBi\,f}$ is the mass in the fiber for the ith PCB determined by the GS/MS/MS (ng), V_{fiber} is the polymer fiber volume (L) and $K_{PCBi\,fiber/w}$ is the fiber–water equilibrium partitioning coefficient for the ith PCB (no units). The fiber–water equilibrium coefficient can be determined by the following op-LFER equation (eq 5-6), which was provided by Dr. Reible (unpublished experiments).

$$log\,(K_{PCBi\,fiber/w}) = 1.03log(K_{PCBi\,ow}) - 0.938 \qquad (5\text{-}6)$$

where $K_{PCBi\,ow}$ is the octanol–water partition coefficient for the ith PCB (no units) (4). The $K_{PCBi\,fiber/w}$ values for PCB congeners ranged from $10^{3.70}$ to $10^{7.50}$ for PCB1 and PCB209, respectively (Table D-1, Appendix D). These values are very similar to those reported elsewhere. Differences between our estimate fiber–water equilibrium partitioning coefficient and previous studies (113-115, 118-120) do not exceed 0.65 log units. This outcome is remarkable, given the different coating thicknesses (7, 15 and 30 µm), values were obtained from experimental data, and different methods employed. The uptake of PCBs into the fiber can be depicted according to a one-compartment model (111, 115, 121, 122) (eq 5-7)

$$m_{PCBi\,f}(t) = C_{PCBi\,pw} K_{PCBi\,fiber/w} V_{fiber}\left(1 - e^{(-k_{PCBi} \times t)}\right) \tag{5-7}$$

where $m_{PCBi\,f}(t)$ is the mass for the ith PCB (ng) in the fiber as function of time, $C_{PCBi\,pw}$ is the porewater concentration for the ith PCB (ng L^{-1}), k_{PCBi} is the exchange rate coefficient for the ith PCB (d^{-1}), and t is time (d). Time to reach 90% of equilibrium in the fiber ($t_{90\%}$) can be obtained from ln(10)/k_{PCBi} (d).

5.3.7 Quality Assurance and Control

Quality control and assurance was evaluated through surrogate recoveries, laboratory blanks, detection limits, and replicates. Surrogate recovery of PCB14, d-PCB65 and PCB166 were 49%, 51% and 75%, respectively. Surrogate recoveries were used to correct mass congeners as follows: PCB14 from PCB1 to PCB39, d-PCB65 from PCB40 to PCB127 and PCB166 from PCB128 to PCB209. Laboratory blanks contained < 2% of total mass of PCBs detected in the sample. Limit of quantification (LOQ) for each congener in the bulk sediment concentration was obtained as 6 times the standard deviation from 3 laboratory blanks. All congeners detected were above the LOQ, so no blank correction method was needed. Laboratory PDMS-fiber blank contained < 4% of total mass of PCBs detected in the samples (only PCB207 and PCB209). If the measured congener mass was less than the mass detected in the blank, the value was substituted with zeros. In addition, if the congener was detected more than 67% of the time (8/12) in the isotherm experiments, the mass was left as measured otherwise it was filled with zeros. Only 55 individual or coeluting congeners of 161 are reported for the PDMS-fiber experiments.

5.4 Results and discussion

5.4.1 Bulk sediment

The concentration of ΣPCBs in the bulk sediment was 5400 ng g^{-1} d.w. Although the sediment sample is 30 cm below the sediment-water surface, this value is comparable with the values reported from surficial sediment samples collected in 2006 and reported by Martinez et al. (56). The congener profile distribution (Figure 5-1) shows that the tri- and hexachlorobiphenyls groups represent more than 90% of the total PCBs by mass measured in the bulk sediment.

The organic carbon content was 3.3% (kg oc kg^{-1}). Total PCB porewater concentration calculated from the bulk sediment (eqs 2 to 4) yielded 1390 ng L^{-1} (Table D-1 in Appendix D). The congener profile distribution of the porewater shows that most of the congeners are grouped in the di- to the tretrachlorobiphenyls (> 90% in mass) (Figure 5-1). Although the bulk sediment congener profile resembles Aroclor 1248 ($\cos\theta = 0.90$, (78, 79, 93)), this similarity is not as strong for the calculated porewater concentration profile ($\cos\theta = 0.72$). This outcome shows the effect of $K_{PCBi\ ow}$ in estimating $K_{PCBi\ d}$ and the porewater concentration, which increases the relative proportion of the low chlorinated congeners (low $K_{PCBi\ ow}$, low $K_{PCBi\ d}$, high $C_{PCBi\ pw}$), and reduces that of the high chlorinated congeners.

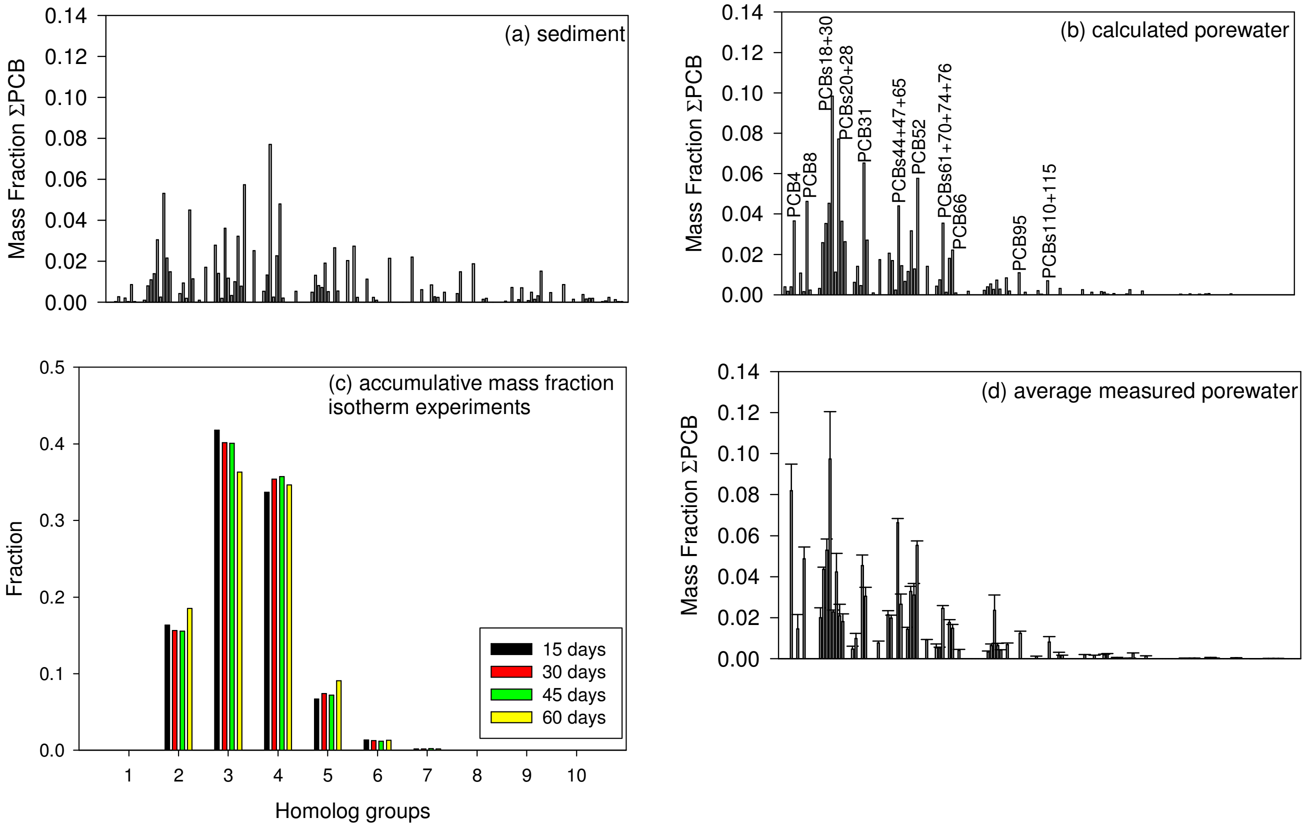


Figure 5-1 PCBs in Indiana Harbor sediment expressed as a fraction of total PCBs detected. Panel (a) Bulk sediment PCBs, determined by direct measurement; (b) Sediment porewater PCBs, calculated using eq 5-2; (c) Sediment porewater PCB homolog groups, measured using PDMS-fibers equilibrated for 15, 30, 45, and 60 days; (d) Average sediment porewater PCBs, measured using PDMS-fibers. The error bars represents one standard deviation about mean

5.4.2 Isotherm Results

The time necessary to reach equilibrium between the PDMS-fiber and the porewater concentration from the isotherm experiments was less than 20 days for the ΣPCBs (Figure 5-2). The same trend is observed for all the other congeners, expect for coeluting congeners PCBs85+116+117, where 60 days was not enough to equilibrate. For most congeners, there was no statistical significance in the results for 20 day exposures and longer (Figure 5-2). These results are shorter or similar to what has been reported for individual congeners and using the same PDMS-fiber, but with different coating thickness (111, 113). However, if $t_{90\%}$ is calculated for the total PCBs and the individual congeners, in general, 1 day is sufficient to gain equilibrium. This peculiar result could be explained due to the fact that our experiments were not designed to obtain the exchange rate coefficient (no values between 0 and 15 days). However, we did observe statistically significant decreases in the mass during the experiments for some congeners, such as PCBs26+29 ($p < 0.005$) and PCB187 ($p < 0.005$). This suggests the lost of mass through volatilization (head space in the vial), dechlorination (113) or other processes. Our sediment was not poisoned to avoid biotransformation so it is possible, although unlikely, that microbial transformations occurred.

5.4.3 Measured Porewater Concentration

Porewater concentration was determined from the average of the four isotherm experiments. The fiber-water equilibrium partitioning coefficient is a key parameter in the calculation of the porewater concentration and was provided by Prof. Danny Reible. Using this coefficient, total PCB porewater concentration determined from the SPME measurements and equation 6 were 110 ± 7.30 ng L^{-1}. This is 13 times less or 8% of what we predicted using op-LERF. Figure 5-3 shows the calculated versus the measured porewater concentrations. This result is unsurprising. Many studies in the last 15 years have reported that porewater concentrations calculated using the octanol-water partition coefficient in an op-LFER overestimate the dissolved-phase porewater concentrations by as much as three orders of magnitude (95, 116, 123-125).

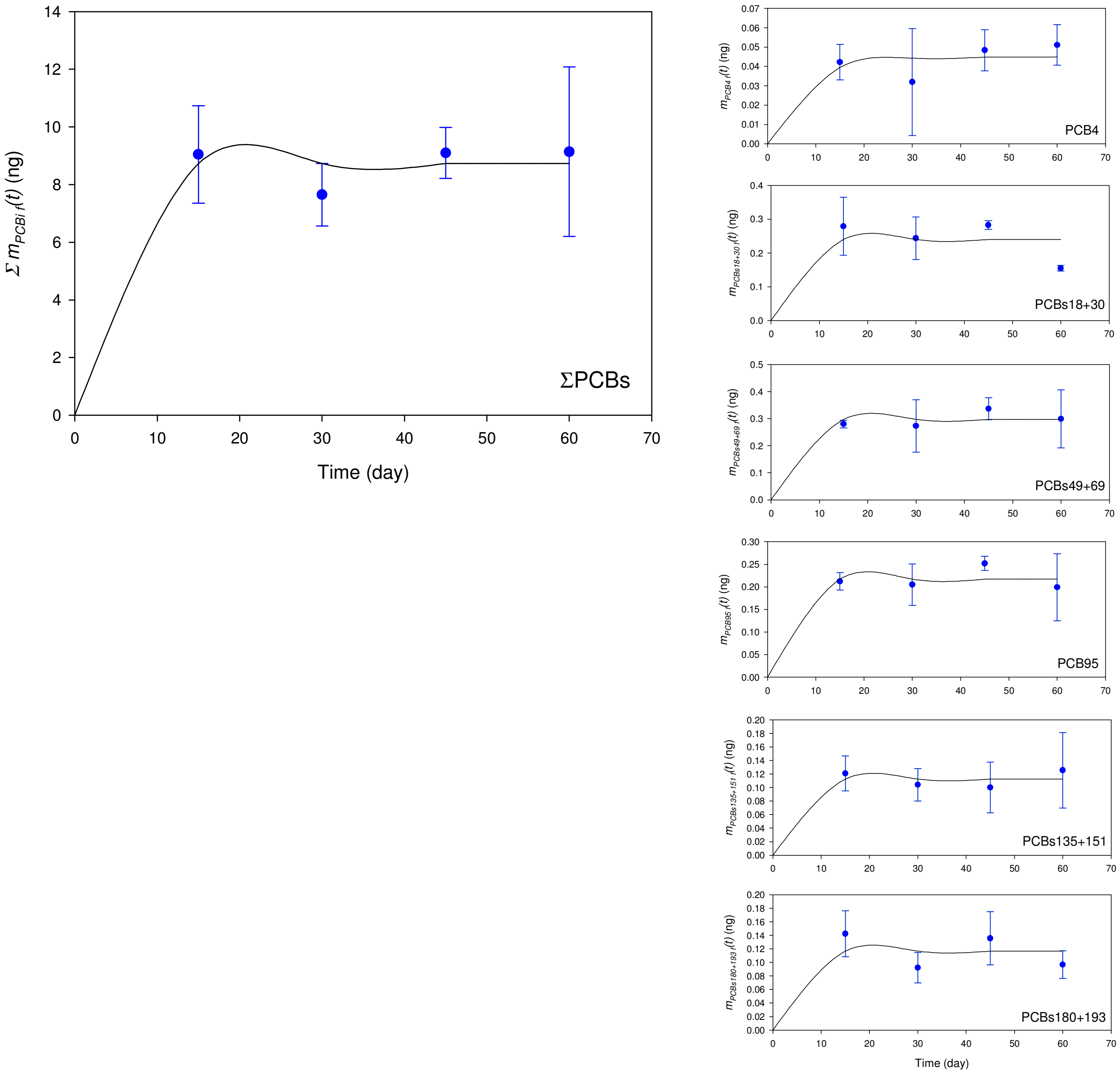


Figure 5-2 Mass of PCBs sorbed to the PDMS-fiber versus time exposure in the sediment. Experiments were carried out in triplicate and under agitation. The error bars represent one standard deviation. The fitting curve was obtained using a one-compartment model (eq 5-7)

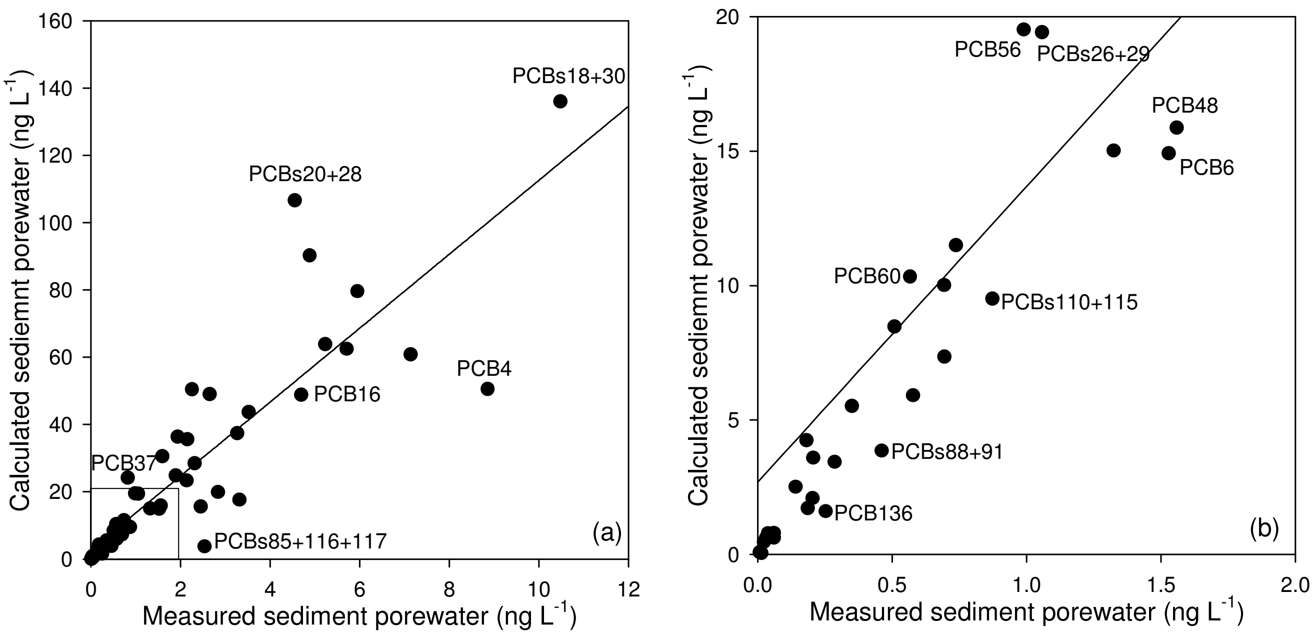


Figure 5-3 Panel (a) shows the calculated versus measured sediment porewater concentrations. Panel (b) shows a zoom of panel (a). The line represents the linear regression between both concentrations ($R^2 = 0.80$)

Most of the congeners detected using PDMS-fibers are in the di- to tetrachlorobiphenyls homolog groups (> 90% in mass). The average congener profile is presented in Figure 5-1. This congener profile is very similar to the porewater PCB profile calculated from the bulk sediment ($\cos\theta = 0.91$). Moreover, the difference between each congener fraction (congener mass to total congeners mass ratio) in the measured and calculated porewater concentrations is less than 5%. A good linear regression was found between these two concentrations ($R^2 = 0.80$). The ratio measured:calculated porewater concentrations are very constant, 10.00 ± 10.00%, with the exception of PCBs 85+116+117 and PCB202, where their values were 68.00 and 36.00%, respectively (Table D-1 in Appendix D). All these findings suggest that the resulting signatures from both methods are similar. No relationship was found between the ratio and $K_{PCBi\ ow}$.

5.4.4 Implications: Freely versus Dissolved Porewater Concentrations

This study has shown that the porewater concentrations of PCBs calculated from well-regarded empirical op-LFER and chemical flux models (including our own (81)) are much larger than porewater concentrations determined using a passive sampler technique (SPME). It is now clear to us that our calculated sediment porewater concentrations values overestimate the freely dissolved concentration of PCBs in sediment porewaters. ***Could our previous flux predictions be overestimated?*** Several other investigators have also noticed and addressed this discrepancy. First, Cornelissen et al. (86) reported that the freely dissolved concentration gradients between the surficial sediment porewater and overlying water concentrations will only provide the diffusive flux, and not the total flux. Lick (102) also showed that the diffusive flux, or what he called "mass transfer approximation" does not include processes such as molecular or Brownian diffusions or bioturbation. Although he addressed this question, he does not specifically discuss the chemical phases involved in the equations. Second, field studies of soluble sediment-water fluxes such as Connolly et al. (83) and Erickson et al. (64) have used field empirical relationships to estimate the sediment porewater concentration. Their experimental $K_{PCBi\,oc}$ are very similar to our values obtained from the op-LFER we used (< 0.004 log units). Laboratory studies of soluble sediment-water fluxes have empirical obtained $K_{PCBi\,oc}$ (101) or used estimated values through an op-LFER (104, 105) of $K_{PCBi\,oc}$. Their values of $K_{PCBi\,oc}$ are also similar to ours values (< 0.15 log units). All this information, especially the field and laboratory studies, suggest that our calculated porewater is appropriate (see eqs 2 to 4) at least for the estimation of the soluble sediment-water fluxes. Indeed, Thibodeaux (36) clearly states that to estimate the soluble flux under steady flows, the DOC fraction has to be included, and not only the freely dissolved concentration. The fraction of PCBs bound to DOC in sediment porewater could be as high as 70%, which would completely account for the difference between the op-LFER and our PDMS-fiber measurements (108).

It is clear that freely dissolved concentration is a better indicator of bioavailable contamination in sediments, and this value should be used in assessing environmental risk and exposure (126, 127). Although this analysis supports the idea that the freely dissolved porewater concentration is not the appropriate parameter for estimating the soluble sediment-water flux, it is not clear if indeed the values obtained from an op-LFER are the correct for the determination of soluble PCB flux from quiescient sediments. Therefore, there remains a need to develop and understand the *effective* porewater concentration to be used in the soluble sediment-water flux estimations.

CHAPTER VI: SUMMARY AND RECOMMENDATION OF FUTURE WORK

6.1 Summary

This research has comprehensively analyzed and evaluated polychlorinated biphenyl congeners in air, surficial water, sediment and sediment porewater of Indiana Harbor and Ship Canal, East Chicago, Indiana. Approximately 130 samples were collected throughout two field campaigns, including 60 surficial sediments, 10 dissolved-phase water, 7 suspended particulates water, 16 gas-phase air, and 2 sediment cores that consisted of 34 sections samples. Moreover, 4 isotherm experiments of sediment porewater were carried out, as 12 additional experiments. Tandem mass spectrometry (GC/MS/MS) in multiple reaction monitoring mode was used to identify and quantify PCB congeners, providing a high level of selectivity and sensitivity in complex environmental matrices, including sediment. Approximately 160 individual congeners or coeluting congeners were detected in each sample. Hence, we built a matrix of 22240 high quality data points (160 congeners x 139 samples-experiments).

Concentration of PCBs in surficial sediment in IHSC ranged from 53 to 35000 ng g^{-1} d.w. and are comparable to other PCB concentrations at contaminated tributaries in the United States, most of them (although not IHSC) established by law as Superfund sites. The PCB congener signal (congener profile) strongly resembles the original commercial mixture Aroclor 1248 (Chapter II).

Estimates of the release of PCBs from sediments to water and from water to air, showed that contaminated sediments of IHSC are currently a significant source of PCBs into the water and overlying air, as well as a tributary loading to Lake Michigan. The PCB signature in surficial sediment, water, and air support our determination that the contaminated sediment is a major source of PCBs into the water and air above it (Chapter III).

Two core samples showed that PCB concentrations are above the threshold limit to designate IHSC as a Superfund site (≥ 50 ppm). Both cores showed important difference regarding total PCB concentrations, vertical distribution and congener signatures. With the help of the PCB fate model developed in Chapter III, we have estimated the possible effects of PCB release post dredging operations. PCB release from sediment depends heavily on the PCB concentration in the surficial sediment left after dredging. For example, if the PCB concentration in the surficial sediment left is 89000 ng g^{-1} d.w., there will be a increase in relation to the base line (described in chapters III and IV) of 1500%, 510% and 170%, emissions from the sediment to the water, water to the overlying air, and the tributary load to Lake Michigan, respectively (Chapter IV). However and in particular for the airborne PCB emissions, this analysis only includes the emissions generated from the navigational water of IHSC but does not include the emissions generated from the sediments that will be disposed in the CDF. As we have shown in Chapter IV, if they dredge a 3 m sediment layer they will leave a quite low PCB concentration in the surficial sediment (Scenario II, Chapter IV), which translates to low emissions. But the mass of sediment disposed will be higher and perhaps the emissions will be higher from the CDF.

SPME passive sampler technique was successfully utilized to determine the freely dissolved PCB sediment porewater concentration. Isotherm experiments showed that less than 20 days were enough to achieve equilibrium between the PDMS-fiber and the sediment porewater concentration. These values represent 8% of the concentration calculated using a one parameter linear free energy relationship (op-LFER). However, the freely dissolved porewater concentration is not necessarily the correct parameter required for the prediction of the sediment-water soluble flux. Currently, op-LFER values are the more appropriately applied for predicting PCBs soluble release from contaminated sediments. Therefore, we do not recommend the passive sampler technique (SPME) for this purpose (Chapter V).

6.2 Recommendation of Future Work

Our study showed that gas-phase PCBs are emitted from the IHSC. However, we do not know if this emission is large relative to other regional sources. One of the next steps to following in this research could be to evaluate impact of the airborne PCB emissions from IHSC on the local atmosphere of East Chicago, Indiana. Because we already found out that IHSC is a source of PCBs to the overlying air (Chapter III) and there is a air sampling collection occurring in East Chicago (128), it may be possible to evaluate the relative importance of the IHSC emissions to concentrations of airborne PCBs in the community .

Dredging can increase the release of PCBs from the sediment to the water and from the water to the overlaying air, as well as the tributary load to Lake Michigan (Chapter IV). Therefore monitoring the air, water and sediment during and after the dredging project is executed is essential. Long-term monitoring data collected during and after dredging would provide valuable information, which then could be used to improve our knowledge on the effects of dredging a highly contaminated sediment, as well as improve the dredging operations to minimize the release of PCBs (85).

The confined disposal facility could be also an excellent place to evaluate the fate of PCBs. There is uncertainty in how the CDF is going to perform in controlling the release of PCBs into the environment. Passive sampler techniques *in situ* could be applied at the CDF for air, water and sediment monitoring. We have the knowledge of passive techniques for air and sediment, so only water passive sampling will need development. It is important to mention that the model developed in Chapter III can only be applied to a system similar to the IHSC, and not to a system such as the CDF. The air-water and sediment-water soluble release model parts were developed for a dynamic system, where a water flow is involved. In the case of the CDF, even though the Army Corps of Engineers is planning to fill with water the dikes after they have disposed the sediment, will not have a water flow. Therefore the mathematical approach developed for the air-water and sediment-water exchanges are not appropriate for the CDF. Hence field measurements at the CDF will provide useful information to better understand this particular system.

Although we have evaluated the PCB signature in both cores and found highly weathered profiles (Chapter IV), a microbiological approach such as bacterial community assessment in the sediment, could provide a better assessment of the specific type of weathering process occurring in the sediment.

Black carbon content in the sediment samples will also be interesting to determine. Impacted harbor sediments are well known to contain sub-products of combustion, such as black carbon. These compounds act as sorbent for PCBs and compete with organic carbon. This information will allow us to better predict the sediment porewater PCB concentration from bulk concentration and compare it to the values obtained through the passive sampler technique.

Finally and perhaps the issue that could have a major impact in water quality models, will be the determination of the effective sediment porewater concentration needed for predicting the sediment-water soluble flux of PBTs (Chapter V). Currently, it is not clear which concentration or phases in the sediment porewater should be included in the sediment-water exchange equation.

APPENDIX A: SUPPLEMENTAL INFORMATION CHAPTER II

Information Referenced in Chapter II: Tables and Figures

Table A-1 Location and total concentration of PCBs (ng g^{-1} d. w.) of surficial sediments samples of IHSC

Sample	**Location [a]**		**ΣPCB**
ID	**Latitude**	**Longitude**	**(ng g^{-1} d.w.)**
1	41° 40.445	87°26.513	740
2	41°40.567	87°26.552	160
3	41°40.618	87°26.331	2,100
4	41°40.337	87°26.436	3,000
5	41°40.372	87°26.291	58
6	41°40.087	87°26.100	3,700
7	41°40.051	87°26.161	4,800
8	41°40.019	87°26.210	4,500
9	41°39.958	87°26.264	4,500
10	41°40.347	87°26.339	53
11	41°40.260	87°26.224	7,200
12	41°40.233	87°26.289	4,800
13	41°40.169	87°26.403	690
14	41°40.105	87°26.531	1,200
15	41°39.849	87°26.761	4,600
16	41°39.659	87°27.090	4,200
17	41°39.635	87°27.069	7,200
18	41°39.668	87°27.027	1,700
19	41°39.777	87°26.902	4,400
20	41°39.841	87°26.840	4,800
21	41°39.916	87°26.745	24,000
22	41°39.571	87°27.206	5,300
23	41°39.569	87°27.181	10,000
24	41°39.520	87°27.240	7,800
25	41°39.498	87°27.328	5,800
26	41°39.425	87°27.377	9,300
27	41°39.441	87°27.382	8,400
28	41°39.323	87°27.508	15,000
29	41°39.390	87°27.425	8,000
30	41°39.343	87°27.542	6,200
31	41°39.305	87°27.580	4,300
32	41°39.286	87°27.558	5,500
33	41°39.251	87°27.633	27,000
34	41°39.215	87°27.722	8,800
35	41°39.151	87°27.746	10,400
36	41°39.089	87°27.827	8,500

Table A-1 continued

Sample	**Location [a]**		**ΣPCB**
ID	**Latitude**	**Longitude**	**(ng g^{-1} d.w.)**
37	41°39.109	87°27.863	8,700
38	41°39.055	87°27.960	9,400
39	41°39.024	87°27.919	8,300
40	41°38.982	87°27.931	6,600
41	41°39.006	87°28.014	10,000
42	41°38.958	87°28.080	4,800
43	41°38.943	87°28.069	6,800
44	41°38.424	87°28.282	6,000
45	41°38.497	87°28.249	10,000
46	41°38.497	87°28.284	5,900
47	41°38.539	87°28.272	5,200
48	41°38.601	87°28.250	8,000
49	41°38.710	87°28.272	9,400
50	41°38.717	87°28.298	33,000
51	41°38.754	87°28.312	11,000
52	41°38.805	87°28.385	5,000
53	41°38.767	87°28.364	9,800
54	41°38.805	87°28.447	5,100
55	41°38.782	87°28.442	9,500
56	41°38.793	87°28.543	6,800
57	41°38.797	87°28.820	6,900
58	41°38.805	87°28.822	6,600
59	41°38.809	87°28.257	8,100
60	41°38.884	87°28.149	140

[a] Geographic Coordinate System: North America Datum 1983.

Table A-2 Arithmetic mean and standard deviation of IHSC samples. PCB congeners order obtained in the quantification method.

Order	Congener (32)	Arithmetic mean (ng g^{-1} d.w.)	Standard Deviation (ng g^{-1} d.w.)
	Monochlorinated biphenyls		
1	PCB 1	2.700	9.200
2	PCB 2	1.400	2.400
3	PCB 3	5.000	23.000
	Dichlorinated biphenyls		
4	PCB 4	35.000	76.000
5	PCB 5	3.500	28.000
6	PCB 6	22.000	29.000
7	PCB 7	2.700	6.300
8	PCB 8	73.000	140.000
9	PCB 9	3.900	8.800
10	PCB 10	1.500	4.700
11	PCB 11	5.700	7.000
12	PCBs 12+13	10.000	12.000
13	PCB 15	54.000	63.000
	Trichlorinated biphenyls		
14	PCB 16	120.000	190.000
15	PCB 17	130.000	170.000
16	PCBs 30+18	260.000	350.000
17	PCB 19	34.000	64.000
18	PCBs 28+20	440.000	470.000
19	PCBs 21+33	160.000	230.000
20	PCB 22	110.000	130.000
21	PCB 23	1.200	0.990
22	PCB 24	7.100	23.000
23	PCB 25	46.000	44.000
24	PCBs 26+29	76.000	70.000
25	PCB 27	18.000	23.000
26	PCB 31	360.000	400.000
27	PCB 32	120.000	150.000
28	PCB 34	1.700	1.900
29	PCB 35	3.700	3.900
30	PCB 36	1.100	3.700
31	PCB 37	100.000	100.000
32	PCB 38	0.650	2.000
33	PCB 39	1.200	1.700

Table A-2 continued

Order	Congener	Arithmetic mean (ng g^{-1} d.w.)	Standard Deviation (ng g^{-1} d.w.)
	Tetrachlorinated biphenyls		
34	PCBs 40+41+71	250.000	250.000
35	PCB 42	150.000	130.000
36	PCB 43	15.000	15.000
37	PCBs 45+51	150.000	190.000
38	PCB 46	38.000	42.000
39	PCB 48	90.000	88.000
40	PCBs 49+69	300.000	260.000
41	PCBs 50+53	83.000	85.000
42	PCB 52	490.000	450.000
43	PCB 54	0.840	1.300
44	PCB 55	46.000	200.000
45	PCB 56	170.000	150.000
46	PCB 57	2.200	3.300
47	PCB 58	0.240	0.780
48	PCBs 59+62+75	36.000	32.000
49	PCB 60	100.000	120.000
50	PCBs 61+70+74+76	650.000	690.000
51	PCB 63	16.000	14.000
52	PCB 64	200.000	170.000
53	PCB 66	340.000	310.000
54	PCB 67	11.000	11.000
55	PCB 68	7.300	10.000
56	PCB 72	1.600	2.000
57	PCB 73	48.000	200.000
58	PCB 77	36.000	30.000
59	PCB 78	0.013	0.100
60	PCB 79	0.170	0.790
61	PCB 80	3.500	24.000
62	PCB 81	0.560	1.200
	Pentachlorinated biphenyls		
63	PCB 82	44.000	37.000
64	PCBs 83+99	110.000	100.000
65	PCB 84	76.000	65.000
66	PCBs 85+116+117	45.000	36.000
67	PCBs 86+87+109+97+119+125	140.000	120.000
68	PCBs 88+91	49.000	50.000
69	PCB 89	9.900	14.000
70	PCBs 90+101+113	170.000	140.000
71	PCB 92	32.000	23.000

Table A-2 continued

Order	Congener	Arithmetic mean (ng g^{-1} d.w.)	Standard Deviation (ng g^{-1} d.w.)
72	PCBs 93+100	8.400	31.000
73	PCB 94	1.800	2.000
74	PCB 95	160.000	140.000
75	PCB 96	4.300	4.200
76	PCBs 98+102	16.000	15.000
77	PCB 103	1.200	1.500
78	PCB 104	0.017	0.092
79	PCB 105	84.000	70.000
80	PCB 106	1.100	8.200
81	PCB 107	12.000	12.000
82	PCBs 108+124	5.500	5.500
83	PCBs 110+115	230.000	190.000
84	PCB 111	0.002	0.016
85	PCB 112	12.000	51.000
86	PCB 114	5.600	4.900
87	PCB 118	160.000	120.000
88	PCB 120	0.043	0.160
89	PCB 121	0.083	0.700
90	PCB 122	2.400	2.300
91	PCB 123	3.500	9.200
92	PCB 126	11.000	58.000
93	PCB 127	0.240	1.600
	Hexachlorinated biphenyls		
94	PCBs 129+138+160+163	87.000	55.000
95	PCB 130	4.000	3.400
96	PCB 131	1.200	4.600
97	PCB 132	29.000	21.000
98	PCB 133	0.990	1.800
99	PCBs 134+143	2.600	3.100
100	PCBs 135+151	30.000	21.000
101	PCB 136	13.000	9.400
102	PCBs 137+164	9.700	7.400
103	PCBs 139+140	2.200	12.000
104	PCB 141	16.000	16.000
105	PCB 142	0.750	6.400
106	PCB 144	4.300	3.500
107	PCB 145	1.200	6.200
108	PCB 146	12.000	8.400
109	PCBs 147+149	70.000	47.000
110	PCB 148	0.100	0.710

Table A-2 continued

Order	**Congener**	**Arithmetic mean (ng g^{-1} d.w.)**	**Standard Deviation (ng g^{-1} d.w.)**
111	PCB 150	0.012	0.075
112	PCB 152	4.400	24.000
113	PCBs 153+168	64.000	44.000
114	PCB 154	0.300	0.710
115	PCB 155	0.001	0.008
116	PCBs 156+157	9.000	8.700
117	PCB 158	8.400	5.600
118	PCB 159	0.830	3.200
119	PCB 161	0.430	2.300
120	PCB 162	0.250	2.100
121	PCB 165	0.009	0.039
122	PCB 167	2.100	2.200
123	PCB 169	0.970	1.700
	Heptachlorinated biphenyls		
124	PCB 170	21.000	14.000
125	PCBs 171+173	7.000	4.500
126	PCB 172	3.400	3.000
127	PCB 174	20.000	14.000
128	PCB 175	0.380	0.760
129	PCB 176	2.600	2.200
130	PCB 177	14.000	8.500
131	PCB 178	4.200	3.400
132	PCB 179	10.000	6.100
133	PCBs 180+193	49.000	30.000
134	PCB 181	0.058	0.270
135	PCB 182	0.029	0.170
136	PCB 183	11.000	9.000
137	PCB 184	0.063	0.300
138	PCB 185	2.900	8.100
139	PCB 186	0.390	3.300
140	PCB 187	31.000	19.000
141	PCB 188	0.034	0.140
142	PCB 189	0.200	0.500
143	PCB 190	3.500	3.000
144	PCB 191	0.540	2.100
145	PCB 192	0.350	2.800
	Octachlorinated biphenyls		
146	PCB 194	11.000	7.000
147	PCB 195	3.300	3.100
148	PCB 196	5.200	4.400

Table A-2 continued

Order	**Congener**	**Arithmetic mean (ng g^{-1} d.w.)**	**Standard Deviation (ng g^{-1} d.w.)**
149	PCB 197	0.200	1.200
150	PCBs 198+199	13.000	8.700
151	PCB 200	0.880	1.100
152	PCB 201	1.200	1.300
153	PCB 202	1.900	1.800
154	PCB 203	6.900	5.400
155	PCB 205	0.150	0.310
	Nonachlorinated biphenyls		
156	PCB 206	4.400	3.700
157	PCB 207	0.360	0.750
158	PCB 208	1.000	1.300
	Decachlorinated biphenyls		
159	PCB 209	1.100	2.200

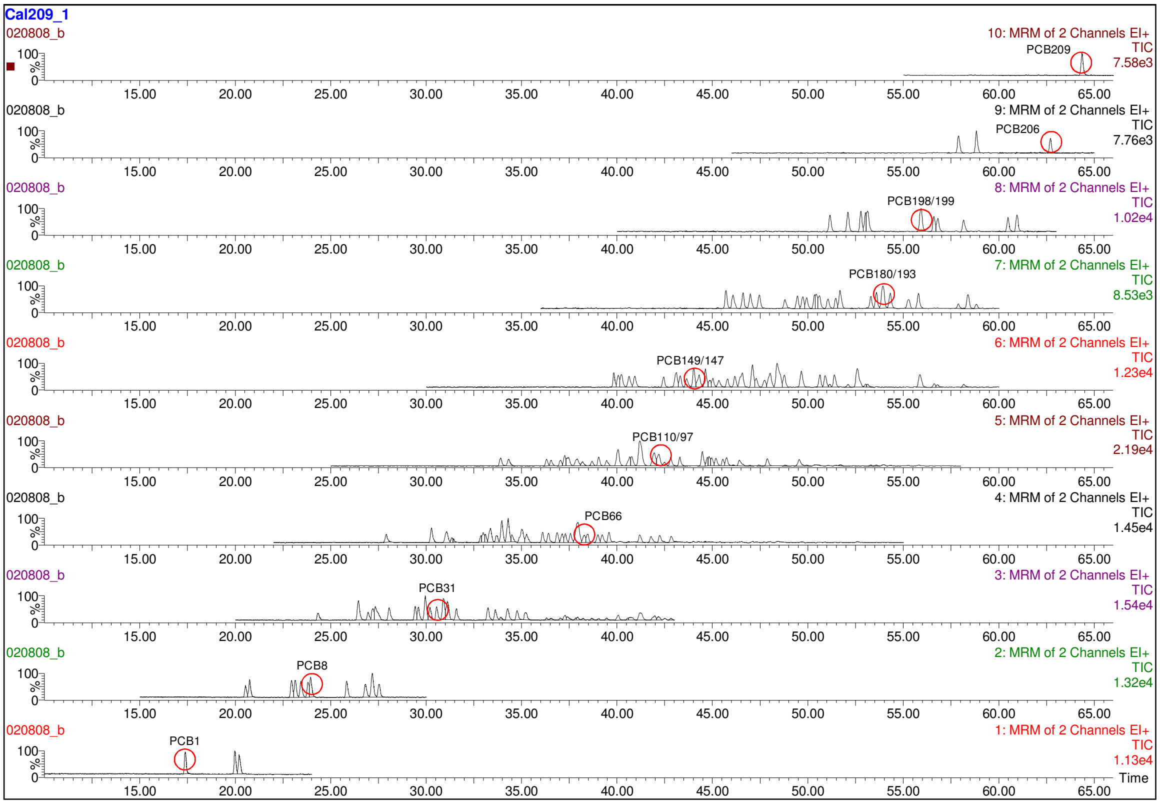


Figure A-1 Multiple reaction monitoring (MRM) chromatogram. The chromatogram shows the 10 homolog groups of PCBs, from monochlorinated biphenyls at the bottom to decachlorinated biphenyl at the top. The top figure shows the calibration standard and the bottom represents a sediment sample. For reference, PCBs 1, 8, 31, 66, 97+110, 147+149, 180+193, 198+199 and 206 have been highlighted in both chromatograms. PCB 209 has been also highlighted in the calibration standard chromatogram

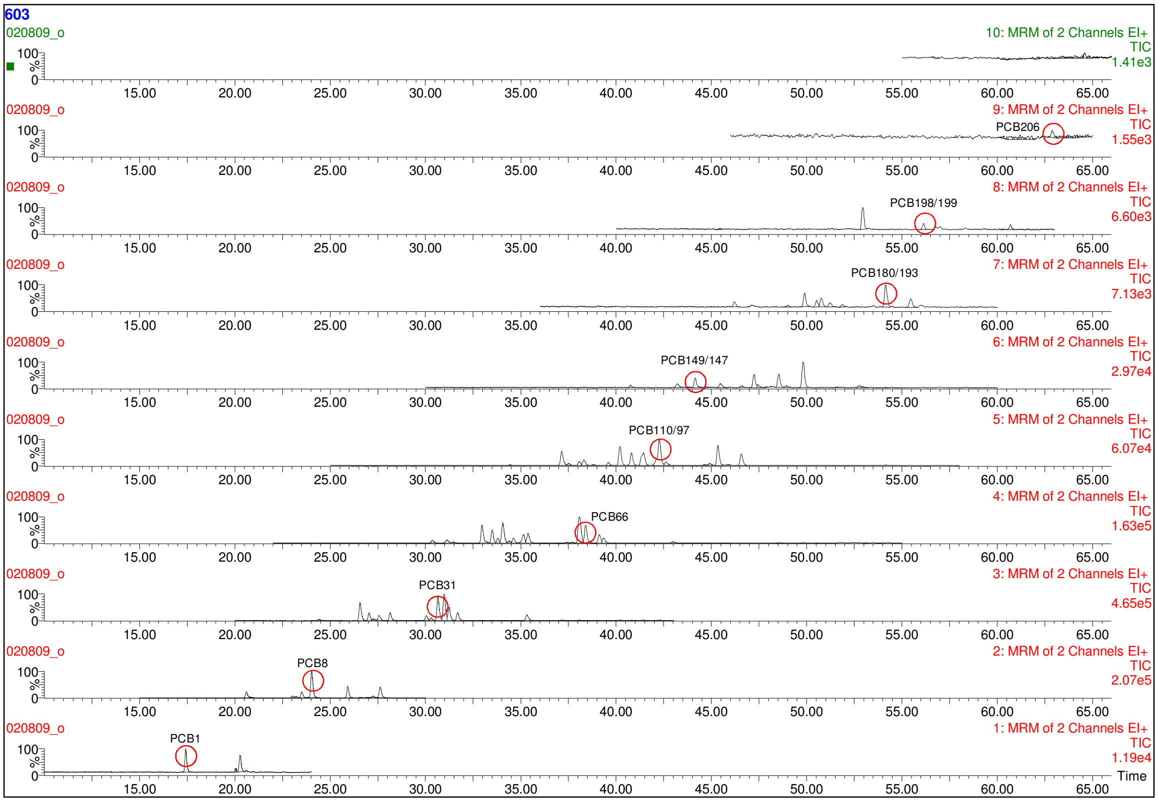


Figure A-1 continued

Additional Information: Sample and Standard Reference Material Concentrations Chromatograms and Field Photographs

Table A-3 Concentration of PCB congeners in surficial sediment IHSC

Table A-4 Concentration of PCB congeners in Standard Reference Material® 1944 (lab batch # SRM2)

Figure A-2 Labeled chromatograms for 209 PCB congeners using GC/MS/MS (32). Chromatograms are divided into homolog groups (129)

Figure A-3 Photographs of IHSC 2006 field campaign

Table A-3 Concentration of PCB congeners in surficial sediment IHSC

Sample ID	**1**	**2-1** [a]	**2-2** [a]	**2-3** [a]	**3**
Collection date	08/07/06	08/07/06	08/07/06	08/07/06	08/07/06
Lab batch #	3	4	7	8	3
PCB14 % recovery	70	77	53	58	163
PCB65 % recovery	93	91	63	71	146
PCB166 % recovery	69	85	70	83	88
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	33	18	23	21	30
Total organic carbon (%) [b]	1.44	0.43	0.43	0.43	4.15
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.00	0.00	0.00	0.02	0.72
2	0.83	0.63	0.01	0.01	2.76
3	0.00	0.00	0.00	0.06	0.99
4	1.77	0.70	0.65	0.48	6.21
5	0.00	0.00	0.00	0.00	0.00
6	1.70	0.50	0.00	0.32	5.33
7	0.40	0.19	0.00	0.00	1.19
8	7.69	2.35	2.04	1.63	26.92
9	0.47	0.16	0.00	0.00	1.11
10	0.00	0.00	0.00	0.00	0.29
11	2.65	0.48	0.37	0.34	2.46
12+13	0.88	0.27	0.41	0.00	2.79
15	9.16	2.48	2.89	2.85	26.17
16	6.62	1.90	1.81	1.88	25.16
17	5.87	1.92	2.68	2.09	23.42
18+30	13.53	4.06	5.22	4.54	54.92
19	1.41	0.38	0.62	0.47	7.18
20+28	39.38	11.33	14.65	13.54	121.46
21+33	13.23	3.80	4.70	4.24	42.42
22	10.55	3.01	4.19	3.72	30.48
23	1.24	0.61	1.14	0.75	2.01
24	0.00	0.00	0.00	0.00	0.00
25	4.38	1.24	1.27	1.08	9.86
26+29	6.01	1.53	2.23	1.99	17.77
27	1.77	0.50	0.61	0.54	5.60
31	26.58	7.35	10.97	9.14	81.51
32	7.02	2.06	2.69	2.37	32.03
34	0.00	0.00	0.00	0.00	0.57
35	0.67	0.16	0.26	0.00	0.00
36	0.00	0.00	0.00	0.00	0.00
37	15.01	3.47	5.17	4.94	35.49
38	0.00	0.00	0.00	0.00	0.00
39	0.00	0.00	0.00	3.39	0.00
40+41+71	21.40	3.80	6.42	4.94	62.50
42	12.86	2.21	2.21	2.26	40.22
43	1.52	0.00	0.46	0.00	7.30
45+51	9.06	0.00	4.42	1.74	30.53
46	3.39	0.70	0.00	0.62	9.93
48	6.47	1.17	0.00	1.34	22.69
49+69	23.25	3.72	4.57	4.10	79.53
50+53	6.81	1.42	1.81	1.51	23.55
52	55.74	8.06	8.60	6.96	181.81

Table A-3 continued

Sample ID Congener #	1 ng g $^{-1}$ d.w.	2-1 [a] ng g $^{-1}$ d.w.	2-2 [a] ng g $^{-1}$ d.w.	2-3 [a] ng g $^{-1}$ d.w.	3 ng g $^{-1}$ d.w.
54	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	0.00	0.00	0.00
56	18.77	4.19	4.64	4.81	47.54
57	0.00	9.99	0.00	11.46	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	4.35	0.59	0.93	0.75	10.44
60	8.68	1.91	2.43	2.36	21.06
61+70+74+76	50.70	1.34	13.00	0.00	133.78
63	1.42	0.26	0.49	0.00	3.54
64	19.74	3.15	4.31	3.90	53.98
66	43.86	8.74	9.46	7.66	107.61
67	1.20	0.29	0.00	0.00	3.02
68	16.27	7.47	0.52	0.45	20.31
72	0.00	0.00	0.00	0.00	0.00
73	4.01	1.48	0.00	0.00	0.00
77	4.88	1.04	0.00	1.27	10.33
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	4.52	0.91	1.02	1.14	10.60
83+99	16.76	2.38	2.51	3.64	35.25
84	8.69	2.01	1.84	2.28	18.09
85+116+117	10.94	3.46	0.00	4.82	17.24
86+87+97+109+119+125	0.00	2.67	1.73	1.69	41.91
88+91	5.75	1.09	1.36	1.10	12.54
89	0.00	0.00	0.00	0.00	2.79
90+101+113	21.54	3.24	3.72	4.10	47.42
92	3.85	0.70	0.88	0.00	9.19
93+100	0.00	0.00	0.00	0.00	0.00
94	0.00	0.00	0.29	0.00	0.96
95	19.47	3.80	4.96	4.20	45.90
96	0.37	0.00	0.00	0.00	1.13
98+102	2.39	0.24	0.00	0.00	5.66
103	0.00	0.00	0.06	0.00	0.00
104	0.00	0.00	0.08	0.00	0.00
105	10.02	1.96	1.86	2.31	25.84
106	0.00	0.00	0.00	0.00	0.00
107	1.08	0.00	0.46	0.00	4.27
108+124	0.67	0.00	0.00	0.15	1.58
110+115	28.50	5.66	6.45	6.48	62.80
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	0.71	0.00	0.17	0.00	1.91
118	19.45	3.58	2.98	4.00	49.19
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.00	0.00	0.08	0.00	0.66
123	0.00	0.26	0.00	0.00	0.00
126	4.50	2.56	2.59	2.21	7.31
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	14.92	3.38	2.59	2.82	36.18
130	1.02	0.00	0.27	0.00	1.79

Table A-3 continued

Sample ID	**1**	**2-1 [a]**	**2-2 [a]**	**2-3 [a]**	**3**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
131	0.00	0.00	0.00	0.00	0.00
132	0.00	1.06	1.21	1.49	11.46
133	0.00	0.00	5.02	0.00	0.00
134+143	0.00	0.00	0.00	0.00	1.31
135+151	2.73	0.93	0.86	1.37	12.64
136	3.72	0.39	0.35	0.36	4.58
137+164	2.22	0.55	0.00	0.00	3.14
139+140	0.00	0.00	0.00	0.00	0.00
141	2.04	0.56	0.65	0.70	6.83
142	0.00	0.00	0.00	0.00	0.00
144	0.92	0.00	0.00	0.00	1.85
145	0.00	0.00	0.00	0.00	0.00
146	1.97	0.50	0.49	0.50	4.77
147+149	12.08	2.60	0.00	2.61	28.64
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	10.32	2.36	2.57	2.18	26.51
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	1.36	3.92	0.09	0.00	3.07
158	1.50	0.28	0.30	0.00	3.72
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	0.00	0.00	0.05	0.11	1.44
169	0.00	0.00	0.00	0.00	0.00
170	3.54	0.78	0.71	1.11	9.37
171+173	1.55	0.20	0.16	0.52	3.26
172	0.00	0.18	0.00	0.00	1.66
174	3.06	0.72	0.64	1.13	9.74
175	0.00	0.00	0.00	0.14	0.00
176	0.65	0.15	0.17	0.00	1.20
177	2.07	0.41	0.62	0.48	5.30
178	1.13	0.13	0.19	0.27	2.20
179	1.75	0.29	0.34	0.43	4.03
180+193	7.95	1.42	1.51	1.31	21.39
181	0.00	0.00	0.00	0.05	0.00
182	0.00	0.00	0.00	0.00	0.00
183	1.65	0.55	0.52	0.54	5.85
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	5.14	1.21	0.83	1.21	14.15
188	0.00	0.00	0.13	0.01	0.00
189	0.00	0.00	0.00	0.01	0.00
190	0.00	0.00	0.00	0.12	1.97
191	0.00	0.00	0.14	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	1.90	0.44	0.62	0.00	4.76
195	0.00	0.19	0.00	0.00	2.05
196	0.00	0.28	0.21	0.00	2.95

Table A-3 continued

Sample ID	**1**	**2-1** [a]	**2-2** [a]	**2-3** [a]	**3**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
197	0.00	0.00	0.00	0.00	0.00
198+199	2.07	0.41	0.00	0.00	5.11
200	0.00	0.08	0.00	0.00	0.00
201	0.00	0.07	0.00	0.00	0.00
202	0.00	0.10	0.09	0.00	0.99
203	1.22	0.27	0.00	0.00	5.30
205	0.00	0.00	0.00	0.00	0.50
206	0.00	0.15	0.00	0.11	2.08
207	0.00	0.06	0.00	0.00	0.00
208	0.00	0.08	0.00	0.00	0.00
209	0.00	0.18	0.06	0.11	0.71
Total	**740.89**	**171.98**	**183.26**	**174.31**	**2091.23**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**4**	**5**	**6**	**7**	**8**
Collection date	08/07/06	08/07/06	08/07/06	08/07/06	08/07/06
Lab batch #	8	11	4	3	3
PCB14 % recovery	49	58	168	191	138
PCB65 % recovery	75	81	217	194	226
PCB166 % recovery	65	99	96	74	102
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	48	13	32	33	35
Total organic carbon (%)	4.38	2.30	4.00	4.39	3.75
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.71	0.15	1.15	2.28	0.00
2	0.29	0.09	1.88	3.37	2.10
3	1.24	0.00	1.54	3.01	0.00
4	6.58	0.00	14.12	24.11	9.83
5	0.00	0.00	0.40	0.92	0.00
6	6.17	0.00	10.57	17.67	9.40
7	0.73	0.00	1.68	2.66	1.80
8	25.04	0.00	56.86	84.69	44.81
9	1.04	0.00	2.35	3.73	1.91
10	0.34	0.00	0.61	1.10	0.00
11	4.49	0.00	1.77	4.21	5.12
12+13	3.67	0.00	4.23	7.53	5.85
15	32.77	0.00	43.16	67.69	45.67
16	33.57	0.00	0.00	100.69	68.85
17	37.04	0.00	60.57	87.74	54.35
18+30	80.62	2.59	134.97	200.65	128.70
19	7.11	0.00	15.12	24.34	12.72
20+28	194.40	2.96	247.24	332.86	273.05
21+33	60.20	2.24	98.54	128.14	96.99
22	54.38	2.17	68.53	88.23	75.01
23	1.51	0.00	1.17	1.79	2.17
24	1.13	0.00	39.02	0.00	0.00
25	16.04	0.00	18.76	28.25	22.54
26+29	29.02	0.00	38.29	52.49	42.06
27	7.74	0.00	12.52	18.78	12.90
31	135.71	3.57	177.10	236.66	183.86
32	39.35	0.76	61.90	99.69	57.65
34	0.43	0.00	0.72	0.94	1.10
35	3.17	0.00	1.92	2.45	2.84
36	0.86	0.00	1.26	0.00	1.74
37	66.91	1.35	64.98	76.59	81.41
38	0.00	0.00	0.00	0.00	0.00
39	1.87	0.00	0.73	0.00	0.00
40+41+71	100.16	0.00	111.13	139.68	150.67
42	49.86	0.00	74.40	93.72	89.78
43	7.48	0.00	13.42	18.39	15.60
45+51	35.12	0.00	52.03	76.38	66.68
46	12.02	0.00	17.04	23.11	20.72
48	34.04	0.00	48.86	58.00	55.55
49+69	108.39	0.00	145.65	187.88	174.31
50+53	26.44	0.00	40.66	60.08	46.37
52	183.34	5.14	314.02	417.33	380.75
54	0.67	0.00	0.74	1.23	0.00
55	2.57	0.00	2.74	2.72	3.79
56	83.59	0.00	93.40	99.30	108.74

Table A-3 continued

Sample ID **Congener #**	**4** **ng g^{-1} d.w.**	**5** **ng g^{-1} d.w.**	**6** **ng g^{-1} d.w.**	**7** **ng g^{-1} d.w.**	**8** **ng g^{-1} d.w.**
57	0.00	0.00	2.59	1.89	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	16.51	0.00	20.31	24.95	24.28
60	47.01	0.00	46.51	51.97	56.63
61+70+74+76	258.09	3.19	279.13	318.02	335.42
63	7.47	0.00	7.23	8.29	9.14
64	85.26	0.00	91.23	123.10	126.39
66	158.25	0.00	207.50	233.17	252.02
67	5.34	0.00	7.49	8.28	8.66
68	1.48	0.00	13.76	16.57	25.42
72	1.11	0.00	0.96	1.10	0.00
73	18.31	0.00	0.00	0.00	6.33
77	0.00	0.00	19.01	20.50	23.71
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	22.87	0.00	18.60	20.56	23.05
83+99	72.74	1.82	55.12	66.30	82.04
84	37.78	1.38	29.46	37.81	42.52
85+116+117	37.29	4.18	24.34	30.44	37.50
86+87+97+109+119+125	37.12	3.58	64.84	76.44	86.03
88+91	21.87	0.00	22.41	25.22	29.80
89	4.04	0.00	3.29	4.54	4.78
90+101+113	95.04	3.86	76.75	91.92	109.85
92	17.56	0.97	13.55	17.62	21.03
93+100	2.55	0.00	1.80	2.51	0.00
94	1.27	0.00	1.70	1.79	0.00
95	74.89	4.26	68.25	90.08	99.50
96	2.12	0.00	2.23	2.68	3.11
98+102	7.01	0.00	6.14	7.43	7.87
103	1.06	0.00	0.86	1.31	0.00
104	0.00	0.00	0.00	0.00	0.00
105	40.05	2.43	37.11	41.71	43.19
106	0.00	1.15	0.00	0.00	0.00
107	8.67	0.00	6.34	7.14	7.50
108+124	3.52	0.00	2.39	3.10	3.67
110+115	119.20	0.00	89.35	109.36	123.26
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	3.17	1.70	2.68	2.75	3.13
118	82.93	0.00	69.78	80.71	87.51
120	0.17	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	1.71	0.00	1.49	1.62	0.00
123	0.00	0.00	0.00	0.00	2.69
126	0.00	0.00	5.24	5.61	6.63
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	58.13	1.63	45.86	50.88	57.91
130	3.16	0.00	2.52	3.16	4.66
131	0.44	0.49	0.00	0.00	0.00
132	21.05	0.00	16.05	17.86	19.85
133	0.00	0.00	0.00	0.00	0.00

Table A-3 continued

Sample ID **Congener #**	**4** **ng g $^{-1}$ d.w.**	**5** **ng g $^{-1}$ d.w.**	**6** **ng g $^{-1}$ d.w.**	**7** **ng g $^{-1}$ d.w.**	**8** **ng g $^{-1}$ d.w.**
134+143	3.67	0.00	1.81	0.00	2.69
135+151	22.79	0.00	17.58	11.25	13.11
136	8.61	0.00	6.48	15.36	20.24
137+164	5.26	1.18	4.70	8.48	8.96
139+140	1.19	0.00	0.00	0.94	0.00
141	10.57	0.00	6.15	10.61	11.67
142	0.00	0.00	0.00	0.00	0.00
144	3.89	0.00	2.25	3.20	3.45
145	0.00	0.00	0.00	0.00	0.00
146	8.24	0.00	5.95	7.78	9.52
147+149	52.18	1.27	38.51	46.56	53.38
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	50.39	0.00	33.67	40.52	45.88
154	0.00	0.00	0.00	0.57	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	4.75	3.88	3.88	3.99	5.77
158	5.91	0.00	4.58	4.96	5.34
159	0.00	0.00	0.00	0.00	4.07
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	1.93	0.00	1.60	1.72	0.00
169	8.85	0.00	0.00	0.84	0.00
170	12.80	0.00	10.86	11.96	11.87
171+173	5.44	0.00	3.41	5.26	5.98
172	2.67	0.00	2.00	2.25	0.00
174	19.95	0.68	9.22	11.44	13.30
175	1.08	0.00	0.00	0.00	0.00
176	2.17	0.00	1.71	1.74	3.16
177	10.49	0.27	7.49	7.82	8.79
178	3.72	0.00	2.51	3.19	0.00
179	8.06	0.86	5.38	7.29	8.80
180+193	33.92	0.00	25.86	27.54	30.33
181	0.00	0.23	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	11.72	0.00	5.26	6.56	7.28
184	0.00	0.59	0.00	0.00	0.00
185	0.00	0.91	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	21.88	0.00	18.02	20.53	23.30
188	0.00	0.34	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	2.65	0.79	2.39	3.03	3.33
191	0.78	0.00	0.00	0.00	0.00
192	0.00	0.19	0.00	0.00	0.00
194	7.01	0.00	6.31	7.20	6.10
195	2.64	0.00	2.10	2.57	0.00
196	4.70	0.00	4.35	4.23	4.11
197	0.00	0.00	0.00	0.00	0.00
198+199	9.19	0.00	7.60	7.68	7.11
200	1.14	0.00	0.00	0.79	0.00

Table A-3 continued

Sample ID **Congener #**	**4** **ng g $^{-1}$ d.w.**	**5** **ng g $^{-1}$ d.w.**	**6** **ng g $^{-1}$ d.w.**	**7** **ng g $^{-1}$ d.w.**	**8** **ng g $^{-1}$ d.w.**
201	1.95	0.00	1.07	0.96	0.00
202	2.08	0.00	1.42	1.44	0.00
203	5.39	0.00	5.38	6.37	3.29
205	0.12	0.00	0.00	0.00	0.00
206	1.85	1.17	3.01	3.28	0.00
207	0.00	0.66	0.00	0.00	0.00
208	0.89	0.00	0.00	0.00	0.00
209	0.52	0.19	0.00	0.00	0.00
Total	**3237.10**	**64.87**	**3714.07**	**4789.39**	**4453.32**

Table A-3 continued

Sample ID	**9**	**10**	**11**	**12**	**13**
Collection date	08/07/06	08/07/06	08/08/06	08/08/06	08/08/06
Lab batch #	4	4	11	4	10
PCB14 % recovery	190	90	70	148	79
PCB65 % recovery	160	108	333	147	90
PCB166 % recovery	84	91	86	87	90
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	35	15	30	30	30
Total organic carbon (%)	4.28	1.29	4.19	4.26	2.00
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	2.34	0.00	1.75	4.22	0.04
2	3.08	0.81	0.40	2.37	0.17
3	2.71	0.00	1.07	4.30	0.00
4	40.77	0.43	75.31	77.12	1.21
5	1.35	0.00	0.00	0.00	0.00
6	24.52	0.32	32.68	25.28	2.65
7	3.51	0.25	2.57	4.47	0.00
8	144.42	1.07	186.09	190.56	9.01
9	5.95	0.09	8.85	5.20	0.00
10	1.43	0.00	2.33	0.00	0.00
11	3.33	0.18	3.44	0.87	0.00
12+13	6.66	0.00	5.75	5.94	0.00
15	68.44	0.37	85.80	77.62	12.32
16	116.83	0.82	238.57	118.54	8.96
17	103.87	0.78	251.34	123.77	8.35
18+30	216.87	1.74	534.68	275.56	19.88
19	35.76	0.24	58.28	59.95	2.34
20+28	325.55	2.19	672.25	0.00	46.64
21+33	178.96	1.17	388.19	710.10	16.44
22	95.05	0.69	245.04	111.85	11.76
23	1.77	0.73	0.00	0.88	0.00
24	0.00	0.00	0.00	0.00	0.00
25	24.92	0.66	42.02	0.00	4.72
26+29	52.27	0.31	118.35	59.85	6.57
27	18.27	0.18	40.13	0.00	0.00
31	242.82	1.75	640.49	277.90	32.32
32	104.97	0.59	203.08	131.46	7.25
34	0.96	0.00	1.63	0.42	0.00
35	2.84	0.00	5.68	0.00	0.00
36	1.04	0.00	0.00	0.00	0.00
37	74.62	0.58	193.44	94.80	19.20
38	0.00	0.00	0.00	5.51	0.79
39	0.64	0.00	0.00	1.54	0.00
40+41+71	104.79	0.89	259.84	0.00	15.23
42	68.43	0.49	100.16	65.28	0.00
43	13.09	0.00	13.24	0.00	0.00
45+51	68.94	0.00	132.80	110.46	7.84
46	22.35	0.00	29.75	0.00	6.30
48	46.79	0.36	95.64	0.00	4.70
49+69	137.28	0.90	224.42	107.25	16.02
50+53	52.18	0.33	72.13	65.33	12.27
52	282.64	1.64	387.33	0.00	40.14
54	1.73	0.00	0.00	1.40	0.00
55	3.40	0.00	0.00	226.24	0.00
56	80.32	0.64	157.78	115.09	19.36

Table A-3 continued

Sample ID	**9**	**10**	**11**	**12**	**13**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
57	1.95	2.03	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	18.97	0.00	35.65	0.00	0.00
60	42.47	0.32	102.74	50.39	8.16
61+70+74+76	257.94	0.00	598.78	404.35	36.55
63	6.11	0.00	12.86	6.47	0.00
64	81.11	0.69	170.14	82.94	11.19
66	181.97	1.46	319.38	0.00	20.61
67	7.40	0.00	12.07	0.00	0.00
68	17.96	10.37	0.00	10.55	0.00
72	0.91	0.00	0.00	0.00	0.00
73	0.00	1.73	0.00	273.46	0.00
77	17.39	0.00	36.31	24.38	0.00
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	16.54	0.00	24.37	20.78	5.69
83+99	48.97	0.64	0.00	0.00	16.61
84	30.02	0.41	39.68	35.92	13.26
85+116+117	24.24	0.00	28.66	0.00	0.00
86+87+97+109+119+125	57.58	0.62	99.23	74.09	9.37
88+91	22.03	0.00	17.28	32.02	6.50
89	3.84	0.00	4.61	3.58	0.00
90+101+113	74.26	0.92	92.35	81.11	23.12
92	14.77	0.00	16.02	15.40	5.91
93+100	3.11	0.00	0.00	0.00	0.00
94	1.91	0.00	0.00	0.00	0.00
95	73.15	0.93	83.39	87.88	30.67
96	2.43	0.00	1.57	2.46	1.95
98+102	6.71	0.00	7.71	0.00	0.00
103	1.48	0.62	1.15	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	32.54	0.00	62.28	47.58	9.25
106	0.00	0.00	0.00	0.00	0.00
107	4.36	0.00	8.40	0.00	0.00
108+124	2.58	0.00	2.97	3.70	0.00
110+115	85.43	0.00	117.99	131.77	42.21
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	39.57	0.00
114	2.06	0.00	4.28	2.40	0.00
118	61.44	0.72	87.76	81.73	15.21
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	1.30	0.00	0.00	0.00	1.87
123	1.57	0.00	0.00	7.85	0.00
126	7.60	3.14	0.00	6.14	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	62.83	0.45	42.58	0.00	22.01
130	2.85	0.00	0.00	2.26	0.00
131	1.17	0.00	0.00	0.00	0.00
132	21.09	0.00	15.42	18.25	11.48
133	0.94	0.00	0.00	0.00	0.00

Table A-3 continued

Sample ID	**9**	**10**	**11**	**12**	**13**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
134+143	2.70	0.00	0.00	0.00	0.00
135+151	26.79	0.00	15.53	17.49	0.00
136	9.14	0.00	6.13	6.13	0.00
137+164	6.27	0.00	2.49	5.05	0.00
139+140	0.83	0.00	0.00	0.00	0.00
141	9.42	0.00	11.70	0.00	0.00
142	0.00	0.00	0.00	0.00	0.00
144	3.74	0.00	0.00	2.03	0.00
145	0.00	0.00	0.00	0.00	0.00
146	9.83	0.00	5.65	6.79	0.00
147+149	55.32	0.50	38.09	40.51	20.71
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	49.64	0.30	34.83	44.68	17.63
154	0.68	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	5.78	4.89	4.99	12.85	0.00
158	6.64	0.00	4.56	4.84	0.00
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	2.31	0.00	0.00	2.03	0.00
169	1.63	0.00	0.00	0.99	0.00
170	20.93	0.05	13.45	10.87	0.00
171+173	6.92	0.00	2.92	3.59	2.53
172	4.01	0.00	0.00	1.95	2.56
174	16.27	0.07	12.98	11.39	4.36
175	0.95	0.00	0.00	0.00	0.85
176	2.58	0.07	1.13	1.21	1.20
177	12.70	0.04	5.18	6.26	0.00
178	4.07	0.09	2.22	2.69	0.00
179	8.41	0.07	6.33	5.00	0.00
180+193	47.82	0.12	29.12	26.53	15.28
181	0.00	0.03	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.99
183	9.43	0.06	9.70	0.00	0.74
184	0.00	0.07	0.00	0.00	0.51
185	0.00	0.06	0.00	9.01	0.00
186	0.00	0.00	0.00	0.00	1.07
187	29.40	0.32	15.66	17.97	8.63
188	0.00	0.00	0.00	0.00	0.00
189	1.17	0.08	0.00	0.00	0.00
190	4.56	0.00	3.61	1.97	0.00
191	0.90	0.05	0.00	0.00	1.74
192	0.00	0.05	0.00	0.00	1.03
194	12.28	0.00	6.38	5.59	1.55
195	4.19	0.00	1.93	2.35	0.00
196	5.64	0.00	0.00	4.51	0.00
197	0.00	0.00	0.00	0.00	0.00
198+199	12.90	0.00	10.49	7.45	0.00
200	1.21	0.00	0.00	0.79	0.00

Table A-3 continued

Sample ID **Congener #**	**9** **ng g $^{-1}$ d.w.**	**10** **ng g $^{-1}$ d.w.**	**11** **ng g $^{-1}$ d.w.**	**12** **ng g $^{-1}$ d.w.**	**13** **ng g $^{-1}$ d.w.**
201	1.34	0.00	0.00	0.68	0.00
202	1.98	0.00	1.53	1.35	0.00
203	9.16	0.00	0.00	5.20	0.00
205	0.00	0.00	0.47	0.00	0.00
206	5.10	0.00	5.35	2.99	2.75
207	0.00	0.00	0.67	0.00	0.00
208	1.45	0.00	2.29	0.00	2.82
209	1.18	0.00	1.51	0.82	0.11
Total	**4508.72**	**53.18**	**7814.81**	**4881.68**	**711.20**

Table A-3 continued

Sample ID	**14**	**15**	**16-1** [a]	**16-2** [a]	**16-3** [a]
Collection date	08/08/06	08/08/06	08/08/06	08/08/06	08/08/06
Lab batch #	1	3	1	7	8
PCB14 % recovery	80	119	92	64	51
PCB65 % recovery	113	177	229	100	91
PCB166 % recovery	97	85	90	82	66
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	18	28	29	27	23
Total organic carbon (%) [b]	2.33	3.75	4.73	4.73	4.73
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.00	0.42	0.00	0.30	0.31
2	0.20	2.05	0.00	0.20	0.17
3	0.15	1.22	0.00	0.47	0.50
4	1.68	7.22	0.00	2.65	2.52
5	0.00	0.00	13.25	0.00	0.00
6	1.36	7.11	0.00	2.81	2.36
7	0.00	1.36	0.00	0.36	0.00
8	8.66	28.30	0.00	8.83	7.68
9	0.32	1.51	0.00	0.51	0.34
10	0.00	0.00	0.00	0.06	0.10
11	0.67	2.33	0.00	2.31	0.25
12+13	1.12	4.22	0.78	1.58	1.59
15	8.80	30.74	5.75	11.27	12.91
16	15.74	45.21	72.83	26.68	27.83
17	12.32	39.62	77.75	29.00	29.98
18+30	0.00	93.04	0.00	79.37	79.79
19	2.78	8.18	33.24	5.74	5.12
20+28	69.83	200.03	413.37	130.87	140.92
21+33	27.52	65.09	217.40	41.23	33.78
22	19.37	51.69	124.91	0.00	32.17
23	0.50	1.82	0.81	1.20	1.06
24	0.00	0.00	0.00	0.36	0.35
25	5.30	19.75	9.76	7.54	7.28
26+29	9.80	33.78	28.83	17.43	17.92
27	2.40	8.97	8.37	4.70	4.96
31	49.32	150.16	463.43	123.45	121.18
32	13.18	41.81	107.54	28.44	30.13
34	0.00	0.92	0.68	0.31	0.44
35	0.83	1.85	0.97	0.92	1.61
36	0.00	0.00	0.00	31.42	0.76
37	22.26	55.27	84.32	34.53	40.20
38	0.00	0.44	0.51	0.11	0.36
39	0.00	0.00	0.96	1.09	0.89
40+41+71	29.96	117.70	358.77	100.12	105.46
42	20.06	75.01	252.07	46.87	49.74
43	2.67	14.35	25.05	5.41	7.99
45+51	16.18	65.47	125.44	90.33	37.19
46	5.34	17.12	50.01	12.64	12.62
48	11.46	48.83	124.62	36.91	39.24
49+69	35.79	157.37	449.32	102.72	112.18
50+53	11.32	45.16	99.28	26.20	26.46
52	76.22	354.54	700.30	177.59	189.43
54	0.00	2.33	1.49	0.47	0.00
55	0.00	2.83	890.74	2.34	0.00
56	30.97	95.02	0.00	75.76	86.07

Table A-3 continued

Sample ID	**14**	**15**	**16-1** [a]	**16-2** [a]	**16-3** [a]
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
57	0.00	2.80	3.49	0.64	0.41
58	0.00	0.00	0.00	4.38	0.29
59+62+75	5.20	19.26	46.83	14.14	14.72
60	14.56	49.31	0.00	46.00	56.02
61+70+74+76	91.97	304.39	1313.88	256.55	300.46
63	2.17	8.82	25.59	6.49	6.80
64	27.25	106.90	291.04	77.68	88.45
66	63.25	225.11	0.00	143.08	168.93
67	2.21	7.30	15.39	0.00	4.65
68	7.97	22.37	14.25	0.99	1.04
72	0.00	1.20	1.78	0.58	0.50
73	0.00	0.00	0.00	0.00	148.57
77	6.50	18.77	0.00	12.42	18.28
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.30
82	10.28	23.06	74.30	16.60	20.89
83+99	20.34	72.22	0.00	39.95	69.43
84	14.85	39.89	126.34	27.63	33.86
85+116+117	13.16	32.27	90.10	24.76	30.96
86+87+97+109+119+125	28.81	84.41	242.58	28.20	35.60
88+91	9.03	28.00	61.32	18.44	20.99
89	2.23	4.50	17.48	3.09	3.79
90+101+113	34.95	134.16	0.00	65.71	81.25
92	6.25	22.74	33.77	12.14	14.12
93+100	0.00	4.65	0.00	1.72	2.32
94	0.00	2.98	3.08	1.40	1.46
95	30.06	115.98	199.09	56.54	66.70
96	0.71	2.56	5.61	1.66	1.86
98+102	3.74	8.20	26.23	5.98	7.80
103	0.00	2.09	1.43	0.69	1.91
104	0.00	0.00	0.00	0.01	0.00
105	16.39	40.09	157.84	31.43	38.13
106	0.00	0.00	0.00	0.00	0.00
107	2.29	6.47	0.00	4.16	8.58
108+124	0.82	0.00	0.00	2.20	3.33
110+115	48.33	127.09	310.70	79.89	106.60
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	144.59	0.00	0.00
114	1.08	3.12	9.91	2.27	3.18
118	29.15	87.65	261.52	53.80	74.12
120	0.00	0.00	0.00	0.23	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.69	1.45	4.88	1.13	1.78
123	0.92	2.49	24.24	1.36	0.00
126	3.60	0.00	0.00	3.88	4.31
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	26.37	134.14	55.29	55.30	41.27
130	1.41	4.84	3.26	1.94	2.10
131	0.00	0.00	1.50	0.54	0.00
132	7.85	40.82	21.46	12.44	15.42
133	0.00	1.82	0.00	1.55	1.27

Table A-3 continued

Sample ID	**14**	**15**	**16-1** [a]	**16-2** [a]	**16-3** [a]
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
134+143	0.00	0.00	0.00	2.12	2.49
135+151	9.17	32.25	19.23	15.96	15.74
136	3.10	47.20	7.75	4.95	6.08
137+164	2.78	17.89	6.68	6.87	3.17
139+140	0.00	0.00	1.08	0.74	0.00
141	5.33	32.11	11.68	10.65	8.03
142	0.00	0.00	0.00	0.00	0.80
144	1.16	9.07	2.91	2.74	2.19
145	0.00	0.00	0.00	0.00	0.00
146	3.69	19.67	6.37	6.81	5.84
147+149	21.13	132.35	48.82	34.50	37.85
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	21.63	129.59	41.04	44.91	35.96
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.07	0.00
156+157	2.00	8.02	6.18	4.09	10.68
158	2.52	12.01	5.62	5.11	3.98
159	0.00	0.00	0.00	0.26	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.12	0.00
165	0.00	0.00	0.00	0.12	0.16
167	0.66	3.96	1.98	1.80	1.38
169	0.36	2.66	0.00	4.78	0.68
170	6.28	47.82	10.75	25.91	9.56
171+173	2.82	18.00	4.18	8.13	3.77
172	1.17	8.13	2.03	4.35	1.91
174	5.98	42.08	15.33	22.91	13.34
175	0.00	2.89	0.00	0.80	0.76
176	0.94	8.10	1.38	3.04	2.27
177	4.34	28.19	7.44	14.42	7.76
178	1.57	9.77	2.76	4.76	3.07
179	3.47	24.85	5.53	8.40	5.93
180+193	13.51	107.36	27.40	57.28	24.82
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	3.47	27.73	8.09	15.59	9.06
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	10.03	69.39	17.93	26.76	17.10
188	0.00	0.00	0.00	0.00	0.00
189	0.00	1.81	0.00	1.03	0.42
190	1.31	10.73	3.52	5.24	1.68
191	0.00	2.43	0.62	1.04	0.57
192	0.00	0.00	0.00	0.00	24.88
194	3.40	23.02	9.53	13.01	4.35
195	1.50	10.07	3.61	5.62	1.89
196	1.73	12.11	3.11	7.13	2.59
197	0.00	0.00	0.00	0.46	0.00
198+199	4.06	22.62	9.99	12.54	6.17
200	0.63	3.72	0.00	1.69	0.63

Table A-3 continued

Sample ID **Congener #**	**14** **ng g $^{-1}$ d.w.**	**15** **ng g $^{-1}$ d.w.**	**16-1 [a]** **ng g $^{-1}$ d.w.**	**16-2 [a]** **ng g $^{-1}$ d.w.**	**16-3 [a]** **ng g $^{-1}$ d.w.**
201	0.00	3.02	0.88	1.58	1.01
202	1.22	3.59	1.77	2.02	1.52
203	2.65	13.96	5.11	8.10	2.14
205	0.00	0.00	0.00	0.73	0.15
206	1.39	0.00	3.18	3.34	0.69
207	0.00	0.00	0.36	0.74	0.00
208	0.00	0.00	0.54	0.99	0.62
209	0.31	0.00	0.69	0.60	0.35
Total	**1193.79**	**4641.94**	**8636.36**	**2797.51**	**3058.31**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**16-4** [a]	**17-1** [a]	**17-2** [a]	**18-1** [a]	**18-2** [a]
Collection date	08/08/06	08/08/06	08/08/06	08/08/06	08/08/06
Lab batch #	9	1	4	3	7
PCB14 % recovery	55	124	176	101	77
PCB65 % recovery	134	169	260	152	107
PCB166 % recovery	75	96	101	79	93
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	26	32	33	24	20
Total organic carbon (%) [b]	4.73	6.19	6.19	4.84	4.84
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.37	0.00	1.54	0.48	0.30
2	0.23	1.56	2.51	1.12	0.18
3	0.47	1.28	2.69	0.49	0.23
4	3.19	10.07	18.10	3.12	3.16
5	0.00	0.00	0.22	0.00	0.00
6	2.58	8.82	13.36	3.02	3.14
7	0.35	1.23	1.47	0.72	0.42
8	9.18	35.49	46.44	11.56	9.84
9	0.45	1.60	2.23	0.62	0.51
10	0.16	0.00	0.64	0.00	0.22
11	2.04	2.43	4.15	1.18	2.98
12+13	1.82	6.14	7.88	1.99	2.26
15	12.89	40.83	59.89	13.33	13.39
16	30.57	87.21	88.77	19.79	15.65
17	34.68	80.94	87.85	17.54	18.06
18+30	92.28	0.00	211.40	39.55	41.72
19	6.09	18.93	21.40	3.20	3.59
20+28	158.20	391.56	394.39	88.64	87.43
21+33	48.98	106.36	94.97	27.21	23.89
22	41.48	89.98	89.12	23.57	24.53
23	0.43	2.19	0.87	1.19	0.86
24	0.00	0.00	0.00	0.00	0.44
25	8.09	37.17	35.65	9.19	8.74
26+29	20.00	68.06	70.17	15.23	15.31
27	5.25	16.28	15.24	3.84	3.52
31	149.01	285.33	292.37	66.18	68.03
32	33.10	80.91	102.02	17.66	17.69
34	0.52	1.52	1.47	0.34	0.25
35	1.68	4.11	3.05	0.96	1.01
36	0.14	0.00	0.00	0.00	0.00
37	43.03	0.00	86.98	24.34	25.84
38	0.26	0.00	0.55	0.00	0.18
39	3.27	0.00	1.19	0.00	0.16
40+41+71	104.74	229.06	194.37	66.38	54.95
42	48.50	160.09	134.28	41.71	27.02
43	7.75	22.52	25.73	6.65	4.80
45+51	35.48	112.53	95.24	28.82	54.94
46	11.81	33.24	30.30	8.54	6.08
48	37.26	88.06	79.22	26.62	20.02
49+69	109.26	302.20	283.98	85.27	61.64
50+53	27.28	76.15	79.39	23.05	15.78
52	196.92	611.74	605.07	177.84	101.29
54	0.38	0.00	1.30	0.00	0.39
55	2.10	1.95	0.00	0.00	1.62
56	86.46	173.14	164.79	53.06	39.72

Table A-3 continued

Sample ID **Congener #**	**16-4** [a] **ng g^{-1} d.w.**	**17-1** [a] **ng g^{-1} d.w.**	**17-2** [a] **ng g^{-1} d.w.**	**18-1** [a] **ng g^{-1} d.w.**	**18-2** [a] **ng g^{-1} d.w.**
57	0.64	1.95	2.99	0.00	0.46
58	0.10	0.00	0.00	0.00	0.00
59+62+75	14.26	37.30	28.07	11.58	8.97
60	54.01	86.78	82.35	28.03	21.63
61+70+74+76	294.68	631.70	554.11	169.38	131.72
63	7.28	15.11	14.94	5.02	3.95
64	84.45	202.38	173.53	62.07	43.50
66	163.06	404.07	386.82	124.02	74.64
67	4.32	12.91	13.24	4.11	2.48
68	0.55	29.74	15.89	19.53	0.60
72	0.63	2.29	2.31	0.00	0.65
73	0.00	6.14	0.00	4.78	0.00
77	16.09	35.66	34.59	11.52	7.93
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.46	0.00	0.00	0.00	0.00
82	21.24	50.90	34.63	11.61	9.46
83+99	64.96	221.14	117.29	38.38	24.13
84	30.37	84.58	58.75	21.04	16.20
85+116+117	27.40	66.61	42.34	20.15	14.91
86+87+97+109+119+125	33.29	164.23	137.75	42.34	16.84
88+91	22.89	52.07	41.08	13.66	10.69
89	3.74	9.84	7.77	2.22	1.69
90+101+113	75.47	204.93	154.57	52.55	40.94
92	13.19	36.54	30.39	9.99	7.98
93+100	1.67	0.00	14.86	3.35	1.82
94	1.11	4.13	2.58	1.06	0.87
95	62.95	180.17	135.49	45.19	36.76
96	1.92	5.02	4.59	1.22	0.96
98+102	6.70	21.64	0.00	4.11	3.85
103	0.67	2.67	2.01	0.00	0.91
104	0.00	0.00	0.00	0.00	0.11
105	42.86	96.25	77.31	22.87	17.55
106	0.00	0.00	0.00	0.00	0.08
107	8.42	15.79	13.60	3.99	2.76
108+124	3.08	6.24	4.92	1.71	1.34
110+115	98.13	253.33	192.11	61.66	48.04
111	0.00	0.00	0.00	0.00	0.15
112	0.00	0.00	0.00	0.00	0.00
114	3.27	6.50	4.86	2.01	1.27
118	74.25	178.63	145.23	43.67	33.64
120	0.08	0.00	0.00	0.00	0.09
121	0.00	0.00	0.00	0.00	0.00
122	1.42	2.88	1.99	0.69	0.74
123	0.00	0.00	0.00	0.00	0.89
126	2.34	14.57	9.52	6.11	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	33.87	132.94	123.75	33.61	22.58
130	1.71	0.00	5.08	1.61	1.25
131	0.43	0.00	1.66	0.00	0.00
132	10.77	42.72	38.08	9.93	7.05
133	0.47	1.89	1.67	0.90	1.21

Table A-3 continued

Sample ID **Congener #**	**16-4** [a] **ng g^{-1} d.w.**	**17-1** [a] **ng g^{-1} d.w.**	**17-2** [a] **ng g^{-1} d.w.**	**18-1** [a] **ng g^{-1} d.w.**	**18-2** [a] **ng g^{-1} d.w.**
134+143	1.90	6.29	5.08	0.00	0.00
135+151	11.79	48.51	47.39	7.18	8.57
136	4.24	18.37	14.31	9.25	3.55
137+164	4.02	13.44	10.85	4.96	2.70
139+140	0.70	0.00	1.24	0.00	0.21
141	6.02	25.56	25.36	5.06	4.07
142	0.00	0.00	0.00	0.00	0.00
144	1.81	6.44	5.86	1.90	1.26
145	0.00	0.00	0.00	0.00	0.00
146	4.65	17.39	16.17	5.07	3.37
147+149	26.14	111.04	100.80	31.57	19.80
148	0.00	0.00	0.00	0.00	0.06
150	0.00	0.00	0.00	0.00	0.02
152	0.00	0.00	0.00	0.00	0.00
153+168	26.96	109.56	106.39	28.48	19.28
154	0.37	0.00	1.02	0.67	0.36
155	0.00	0.00	0.00	0.00	0.00
156+157	2.89	13.11	11.23	2.10	0.18
158	3.03	12.49	12.26	3.06	2.16
159	0.00	0.00	0.00	0.00	0.10
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.13
165	0.00	0.00	0.00	0.00	0.07
167	1.06	4.27	3.76	0.00	0.87
169	0.63	2.78	2.83	0.82	0.00
170	7.94	33.62	46.00	12.32	5.61
171+173	3.55	14.12	15.29	4.88	2.21
172	1.37	7.23	7.77	2.30	1.28
174	9.30	32.35	42.56	10.56	7.03
175	0.48	1.43	1.68	0.00	0.00
176	1.18	4.76	5.72	1.82	1.09
177	5.75	23.68	26.27	7.28	4.06
178	2.18	8.46	8.64	3.00	0.00
179	4.20	16.40	17.12	6.33	3.06
180+193	19.26	77.28	102.12	29.64	13.50
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	5.81	18.53	27.69	7.00	3.80
184	0.10	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	11.07	55.36	63.96	18.90	7.61
188	0.00	0.00	0.00	0.00	0.00
189	0.00	1.44	2.03	0.00	0.00
190	1.84	8.40	9.30	3.02	1.18
191	0.00	1.25	1.33	0.00	0.29
192	0.00	0.00	0.00	0.00	0.00
194	5.11	23.96	23.28	8.02	3.01
195	1.52	7.41	8.96	3.09	1.06
196	2.78	12.07	14.87	4.14	1.76
197	0.00	0.00	0.00	0.00	0.00
198+199	6.44	32.16	21.78	7.37	0.00
200	0.92	0.00	2.61	1.04	0.33

Table A-3 continued

Sample ID **Congener #**	**16-4** [a] **ng g $^{-1}$ d.w.**	**17-1** [a] **ng g $^{-1}$ d.w.**	**17-2** [a] **ng g $^{-1}$ d.w.**	**18-1** [a] **ng g $^{-1}$ d.w.**	**18-2** [a] **ng g $^{-1}$ d.w.**
201	0.95	3.63	2.50	0.99	0.55
202	1.26	7.16	4.17	1.81	0.87
203	3.51	21.05	18.98	4.79	2.34
205	0.16	0.00	0.00	0.00	0.16
206	2.63	17.49	6.97	2.26	1.32
207	0.48	2.46	0.00	0.00	0.00
208	0.83	4.15	1.34	0.00	0.46
209	0.52	2.88	1.75	0.00	0.35
Total	**2865.26**	**7340.89**	**7014.24**	**2050.34**	**1534.78**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**18-3** [a]	**18-4** [a]	**19**	**20**	**21-1** [a]
Collection date	08/08/06	08/08/06	08/09/06	08/09/06	08/09/06
Lab batch #	8	9	10	10	8
PCB14 % recovery	55	55	82	65	61
PCB65 % recovery	81	106	178	135	261
PCB166 % recovery	74	72	93	71	61
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	32	28	43	40	37
Total organic carbon (%) [b]	4.84	4.84	5.65	6.40	5.75
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.35	0.32	0.67	0.00	3.63
2	0.16	0.08	0.00	0.00	1.49
3	0.47	0.49	0.00	0.00	2.72
4	2.88	3.22	4.84	4.90	126.89
5	0.00	0.16	0.00	0.00	0.00
6	2.80	3.21	4.91	5.55	36.91
7	0.00	0.48	0.00	0.00	3.64
8	9.84	10.10	19.90	19.68	202.84
9	0.51	0.65	0.00	0.00	10.08
10	0.00	0.17	0.00	0.22	3.81
11	1.21	2.92	34.36	9.81	4.32
12+13	2.21	2.49	2.87	0.00	9.73
15	13.88	15.34	33.82	32.50	99.75
16	17.30	17.51	34.06	40.25	480.06
17	19.26	20.75	45.40	46.28	415.64
18+30	44.92	45.38	107.46	113.17	1137.78
19	3.33	3.63	7.42	9.47	92.72
20+28	98.20	103.61	234.89	236.91	1193.49
21+33	27.68	30.43	66.62	70.46	549.35
22	27.92	28.90	62.52	60.93	370.08
23	0.94	0.38	0.00	0.00	1.56
24	0.52	0.00	0.00	0.00	0.00
25	9.31	9.44	21.38	14.51	58.57
26+29	16.60	17.66	40.35	37.54	189.07
27	3.83	4.07	11.78	5.94	58.33
31	73.08	80.79	172.83	169.70	1192.26
32	19.01	19.89	44.52	49.25	376.14
34	0.37	0.35	0.00	0.00	4.12
35	1.38	1.53	0.00	0.00	9.47
36	0.23	0.37	0.00	0.00	0.51
37	30.46	32.97	64.86	62.58	253.47
38	0.07	0.00	0.00	0.00	1.15
39	0.52	0.76	0.00	0.00	4.48
40+41+71	57.21	53.82	136.67	153.45	831.00
42	27.27	27.87	75.69	88.51	404.53
43	4.46	4.43	17.21	0.00	72.45
45+51	20.38	20.68	61.92	60.33	408.54
46	6.35	6.24	0.00	4.18	117.62
48	18.82	19.81	53.13	47.83	373.70
49+69	61.76	63.68	169.92	158.96	938.67
50+53	14.23	14.62	39.04	53.32	285.79
52	100.00	109.41	323.77	366.83	1600.34
54	0.34	0.25	0.00	0.00	5.24
55	0.00	1.51	0.00	0.00	0.00
56	44.24	47.60	120.26	120.71	502.67

Table A-3 continued

Sample ID **Congener #**	**18-3** [a] **ng g^{-1} d.w.**	**18-4** [a] **ng g^{-1} d.w.**	**19** **ng g^{-1} d.w.**	**20** **ng g^{-1} d.w.**	**21-1** [a] **ng g^{-1} d.w.**
57	0.00	0.00	0.00	0.00	5.15
58	0.00	0.00	0.00	0.00	3.67
59+62+75	8.62	8.96	26.89	20.94	120.17
60	26.16	27.12	62.33	63.80	332.83
61+70+74+76	148.55	154.21	351.50	377.23	2288.75
63	4.33	4.25	11.55	10.89	48.68
64	44.57	46.71	111.79	124.59	623.57
66	84.80	87.82	203.47	212.80	1014.47
67	2.99	2.78	5.24	0.00	30.48
68	1.28	0.62	0.00	0.00	3.21
72	0.29	0.64	0.00	0.00	4.29
73	0.00	0.00	0.00	0.00	0.00
77	11.02	9.68	24.04	21.08	83.96
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	12.25	13.07	29.28	28.89	111.70
83+99	37.64	39.33	94.07	108.93	396.04
84	19.01	19.37	38.36	52.77	220.77
85+116+117	19.57	15.93	0.00	0.00	136.15
86+87+97+109+119+125	18.77	20.08	104.98	109.06	214.24
88+91	11.63	13.58	34.80	51.89	154.32
89	2.09	2.09	0.00	4.37	28.23
90+101+113	46.37	50.83	130.76	156.12	482.77
92	8.82	9.14	24.90	33.31	82.16
93+100	2.09	2.95	37.80	21.29	9.86
94	0.00	0.72	0.00	0.00	6.66
95	40.36	40.68	107.10	130.68	470.74
96	0.80	1.30	0.00	1.65	15.61
98+102	4.99	0.00	13.30	8.40	54.53
103	0.00	0.74	0.00	0.00	5.74
104	0.00	0.00	0.00	0.00	0.00
105	21.88	25.80	51.12	54.03	181.92
106	0.00	0.00	0.00	0.00	0.00
107	3.75	4.27	0.00	0.00	36.51
108+124	2.17	1.91	0.00	0.00	17.33
110+115	61.25	64.81	183.05	191.42	608.08
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	1.97	1.93	2.39	4.98	15.92
118	43.12	46.11	91.19	95.87	351.48
120	0.00	0.08	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	1.13	1.09	0.00	0.00	5.66
123	1.48	0.00	11.82	0.00	0.00
126	3.19	2.68	0.00	11.72	5.46
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	29.56	33.33	86.10	121.34	134.44
130	1.16	2.13	0.00	0.00	9.52
131	0.00	0.73	0.00	0.00	1.77
132	11.44	11.54	23.74	42.09	57.25
133	0.65	0.59	0.00	0.00	1.91

Table A-3 continued

Sample ID **Congener #**	**18-3** [a] **ng g^{-1} d.w.**	**18-4** [a] **ng g^{-1} d.w.**	**19** **ng g^{-1} d.w.**	**20** **ng g^{-1} d.w.**	**21-1** [a] **ng g^{-1} d.w.**
134+143	1.29	1.84	0.00	0.00	8.91
135+151	10.37	13.03	31.73	53.07	63.08
136	4.65	4.47	11.26	17.31	26.25
137+164	2.25	3.28	3.82	0.00	15.39
139+140	0.00	0.62	0.00	0.00	3.07
141	5.48	6.21	0.00	31.11	29.10
142	0.00	0.00	0.00	0.00	0.00
144	2.00	2.30	5.35	3.88	10.73
145	0.00	0.00	0.00	0.00	0.00
146	4.19	4.43	0.00	28.49	0.00
147+149	25.16	28.40	89.53	122.50	123.86
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.09	0.00	0.00	0.00
152	0.00	0.00	0.00	105.34	0.00
153+168	24.52	29.19	86.85	0.00	106.27
154	0.00	0.54	4.81	2.14	0.54
155	0.00	0.00	0.00	0.00	0.00
156+157	1.72	2.11	6.41	0.00	26.06
158	2.91	3.33	8.63	9.49	13.53
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	16.18
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	1.15	1.22	0.00	0.00	5.65
169	0.00	0.00	0.00	0.00	0.00
170	7.11	8.63	32.33	48.01	0.00
171+173	3.09	3.34	5.89	10.31	9.40
172	1.99	1.32	9.77	7.26	5.49
174	9.13	9.84	24.99	37.24	38.07
175	0.00	0.66	0.00	0.00	0.68
176	1.35	1.67	0.00	7.30	4.39
177	5.34	5.93	23.85	30.30	17.36
178	2.31	2.53	8.61	12.45	9.14
179	3.82	4.83	17.47	21.25	14.79
180+193	17.16	19.53	94.71	94.68	67.86
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	6.10	7.13	21.97	27.40	20.25
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.71	0.00
187	11.72	12.67	41.75	51.48	41.16
188	0.00	0.12	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	1.73	2.04	11.79	0.00	5.92
191	0.00	0.00	0.00	0.00	18.56
192	0.00	0.00	0.00	0.00	0.00
194	3.93	3.70	30.66	24.85	11.91
195	1.92	1.64	9.02	0.00	5.15
196	2.07	2.22	16.08	6.64	9.36
197	0.00	0.00	0.00	0.00	0.00
198+199	4.98	5.91	30.66	24.45	18.43
200	0.54	0.47	2.67	0.00	1.57

Table A-3 continued

Sample ID **Congener #**	**18-3 [a]** **ng g $^{-1}$ d.w.**	**18-4 [a]** **ng g $^{-1}$ d.w.**	**19** **ng g $^{-1}$ d.w.**	**20** **ng g $^{-1}$ d.w.**	**21-1 [a]** **ng g $^{-1}$ d.w.**
201	0.70	0.66	3.12	0.00	2.28
202	0.66	1.15	0.00	0.00	4.12
203	2.87	3.12	15.85	13.87	8.97
205	0.00	0.34	0.00	1.49	0.30
206	1.36	1.27	13.90	9.00	4.29
207	0.00	0.00	0.87	2.02	0.00
208	0.55	0.55	3.28	0.00	0.00
209	0.28	0.29	0.03	0.00	1.54
Total	**1700.47**	**1800.15**	**4542.33**	**4907.95**	**21580.23**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**21-2** [a]	**21-3** [a]	**21-4** [a]	**22**	**23**
Collection date	08/09/06	08/09/06	08/09/06	08/09/06	08/09/06
Lab batch #	7	1	9	1	3
PCB14 % recovery	74	126	66	125	133
PCB65 % recovery	303	349	266	215	241
PCB166 % recovery	74	86	59	98	81
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	41	31	44	30	32
Total organic carbon (%) [b]	5.75	5.75	5.75	3.73	5.62
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	4.58	3.74	3.90	0.68	6.48
2	1.59	2.88	1.54	0.55	4.89
3	2.54	0.00	2.82	0.69	4.97
4	173.57	209.68	126.65	6.90	86.15
5	0.00	0.00	251.53	0.00	3.52
6	48.55	45.10	37.89	1.10	46.54
7	5.31	29.18	3.24	0.86	7.68
8	286.44	316.65	0.07	7.75	241.14
9	13.27	0.00	10.36	0.39	12.69
10	5.61	2.92	4.16	31.42	4.00
11	4.72	0.00	2.33	1.78	2.55
12+13	7.90	9.81	9.54	4.68	15.09
15	113.28	111.16	95.93	29.12	113.95
16	550.27	932.92	382.27	61.03	309.85
17	515.49	883.35	355.32	54.26	241.33
18+30	1368.31	0.00	951.19	0.00	0.00
19	144.47	423.32	88.16	12.01	79.07
20+28	1288.11	2177.16	994.35	276.75	0.00
21+33	707.57	728.13	452.39	81.27	0.00
22	417.47	0.00	315.80	69.93	247.35
23	3.05	4.31	0.95	1.11	2.61
24	0.00	0.00	0.00	0.00	0.00
25	70.05	0.00	49.64	27.11	51.00
26+29	205.13	181.41	158.72	46.75	0.00
27	73.13	0.00	53.20	11.64	40.91
31	1438.37	1850.86	1021.94	200.51	675.47
32	392.33	854.77	289.77	61.26	253.75
34	4.89	0.00	3.32	0.97	2.56
35	7.86	0.00	9.32	2.45	7.07
36	3.14	4.76	5.65	0.00	0.00
37	248.95	376.66	223.63	69.78	191.65
38	0.18	17.04	2.48	0.00	1.13
39	2.19	11.51	4.85	0.65	1.25
40+41+71	845.55	1412.05	758.40	187.31	398.42
42	448.63	766.28	355.03	134.46	242.18
43	0.00	0.00	50.93	19.72	48.12
45+51	1058.04	650.43	373.33	87.17	189.40
46	132.67	239.36	109.57	27.22	64.71
48	329.54	0.00	314.96	70.31	165.62
49+69	914.64	1344.37	823.70	241.80	476.93
50+53	318.29	519.25	279.76	59.86	135.84
52	1659.74	2247.14	0.00	496.15	1032.08
54	5.10	5.90	4.17	0.00	1.93
55	0.00	1502.59	0.00	3.91	9.13
56	517.73	0.00	486.84	141.85	284.02

Table A-3 continued

Sample ID	**21-2** [a]	**21-3** [a]	**21-4** [a]	**22**	**23**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
57	4.68	5.52	2.91	3.39	5.17
58	1.93	0.00	0.00	0.00	0.00
59+62+75	109.96	0.00	113.51	31.01	61.96
60	293.26	795.44	293.39	72.49	164.46
61+70+74+76	2118.40	4117.64	2028.55	479.41	1015.04
63	43.71	47.52	42.70	13.76	24.49
64	589.89	664.39	567.93	166.17	318.48
66	959.93	0.00	921.22	318.44	679.62
67	26.63	0.00	24.21	10.73	20.30
68	0.00	27.74	2.10	18.93	26.44
72	0.00	0.00	4.36	1.90	2.88
73	0.00	0.00	1130.62	0.00	0.00
77	78.11	109.54	76.82	26.78	55.34
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	196.98	0.00	0.00	0.00
81	5.38	0.00	0.00	2.04	4.05
82	108.20	210.62	103.70	41.08	55.37
83+99	257.15	0.00	347.00	91.49	158.72
84	194.24	388.00	187.84	68.84	97.44
85+116+117	0.00	0.00	128.06	49.77	70.64
86+87+97+109+119+125	421.68	695.85	203.77	131.38	195.34
88+91	141.52	360.36	141.49	41.24	62.23
89	23.57	48.94	26.11	9.29	13.76
90+101+113	425.09	714.36	433.23	151.28	205.58
92	72.73	103.77	79.94	27.79	38.75
93+100	0.00	0.00	0.00	2.59	0.00
94	5.25	0.00	6.80	2.67	4.38
95	400.05	774.06	432.78	134.25	202.23
96	14.61	23.30	13.92	3.65	6.49
98+102	47.37	70.56	53.87	13.73	24.45
103	2.89	0.00	4.29	1.80	2.43
104	0.00	0.00	0.00	0.00	0.00
105	197.97	384.90	189.02	69.90	110.13
106	0.00	73.63	0.00	0.00	0.00
107	34.55	0.00	0.00	9.97	16.39
108+124	15.45	31.72	19.21	4.85	7.23
110+115	644.58	1132.42	548.95	197.60	253.15
111	0.00	0.00	0.00	0.00	0.00
112	0.00	398.43	0.00	0.00	0.00
114	12.75	21.53	14.99	4.71	7.16
118	327.17	649.32	338.28	129.24	191.99
120	0.00	0.00	0.73	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	4.14	0.00	7.09	2.51	4.09
123	0.00	0.00	36.66	3.35	0.00
126	5.80	18.49	9.18	0.00	8.39
127	0.00	0.00	0.00	7.68	0.00
129+138+160+163	133.83	265.75	133.36	66.81	69.16
130	8.54	13.34	7.45	4.08	4.87
131	1.68	0.00	3.19	1.97	0.00
132	52.02	102.42	48.34	23.21	27.40
133	4.82	0.00	1.38	0.00	0.00

Table A-3 continued

Sample ID **Congener #**	**21-2** [a] **ng g^{-1} d.w.**	**21-3** [a] **ng g^{-1} d.w.**	**21-4** [a] **ng g^{-1} d.w.**	**22** **ng g^{-1} d.w.**	**23** **ng g^{-1} d.w.**
134+143	5.00	0.00	8.71	0.00	0.00
135+151	53.61	96.15	53.76	26.30	13.90
136	20.64	39.79	23.11	9.32	22.14
137+164	28.47	26.60	14.78	7.76	13.33
139+140	2.66	0.00	3.08	0.00	1.28
141	23.29	0.00	26.62	12.15	0.00
142	0.00	0.00	0.00	0.00	0.00
144	8.91	12.78	10.63	3.33	4.10
145	0.00	0.00	0.00	0.00	0.00
146	18.37	34.36	17.23	0.00	9.64
147+149	111.52	256.65	113.80	57.53	60.67
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.50	0.00	0.00	0.00	0.00
153+168	104.66	245.27	98.49	51.99	46.06
154	0.00	0.00	0.59	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	22.39	46.99	23.55	7.09	6.92
158	12.42	22.12	11.19	6.48	7.86
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	7.28	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	5.03	8.90	4.55	1.94	2.30
169	0.00	0.00	0.00	0.00	1.16
170	25.24	53.50	21.50	12.13	11.75
171+173	9.51	17.07	9.34	5.16	4.86
172	5.74	10.20	5.84	2.79	2.54
174	34.13	65.23	29.84	13.28	12.40
175	0.00	0.00	0.00	0.00	0.00
176	3.78	8.07	4.26	2.13	2.24
177	15.02	34.47	17.97	8.81	7.26
178	5.48	8.85	5.57	3.52	3.10
179	13.53	25.32	14.08	7.38	6.79
180+193	66.21	114.38	64.14	29.68	28.98
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	17.34	38.42	17.63	7.24	7.15
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	36.23	80.32	34.31	22.81	22.58
188	0.21	0.00	0.12	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	5.13	14.25	4.10	2.99	2.29
191	0.00	0.00	1.53	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	13.44	32.63	12.51	7.68	7.93
195	4.22	14.58	4.39	2.82	2.84
196	9.47	17.30	7.41	3.61	5.13
197	0.00	5.09	0.00	0.00	0.00
198+199	17.01	38.30	19.09	9.77	8.89
200	1.85	0.00	1.45	1.26	0.00

Table A-3 continued

Sample ID **Congener #**	**21-2** [a] **ng g $^{-1}$ d.w.**	**21-3** [a] **ng g $^{-1}$ d.w.**	**21-4** [a] **ng g $^{-1}$ d.w.**	**22** **ng g $^{-1}$ d.w.**	**23** **ng g $^{-1}$ d.w.**
201	1.55	4.70	2.29	1.63	0.00
202	3.81	8.60	3.32	2.36	1.58
203	10.68	25.58	8.61	4.55	7.88
205	0.61	0.00	1.28	0.00	0.00
206	6.29	17.61	6.43	4.65	4.43
207	0.00	0.00	0.00	0.00	0.00
208	1.38	4.42	2.36	1.02	0.00
209	1.17	3.35	1.40	1.31	0.00
Total	**22854.30**	**31743.10**	**18909.40**	**5324.68**	**10258.97**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**24-1** [a]	**24-2** [a]	**25**	**26**	**27-1** [a]
Collection date	08/09/06	08/09/06	08/09/06	08/09/06	08/09/06
Lab batch #	1	7	3	8	3
PCB14 % recovery	136	75	181	58	140
PCB65 % recovery	208	146	245	164	180
PCB166 % recovery	102	76	83	76	65
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	36	54	31	49	40
Total organic carbon (%) [b]	5.03	5.03	4.97	5.55	1.88
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.00	2.03	2.40	2.09	2.58
2	0.59	0.90	3.17	0.74	5.21
3	0.91	3.08	3.49	2.82	3.76
4	5.33	17.06	15.86	21.38	19.36
5	0.00	0.00	0.64	0.00	0.55
6	6.06	16.60	15.67	20.40	18.85
7	0.70	1.80	2.06	1.73	3.01
8	21.19	42.37	49.58	44.39	53.42
9	0.98	2.35	2.38	2.40	2.77
10	0.00	0.78	0.72	0.74	0.93
11	11.25	25.18	4.74	14.62	9.48
12+13	5.30	11.57	10.72	13.62	13.21
15	28.60	67.24	65.84	68.87	72.94
16	48.62	83.13	71.70	118.00	114.05
17	47.88	97.90	65.88	139.94	106.36
18+30	0.00	235.21	160.30	321.67	256.75
19	10.10	21.19	23.58	27.00	25.67
20+28	258.62	472.69	330.73	624.94	512.94
21+33	60.61	112.33	88.16	150.79	124.48
22	60.30	122.39	81.50	162.04	122.46
23	1.41	1.55	1.81	1.44	2.56
24	0.00	1.76	0.00	2.12	0.00
25	29.81	53.51	36.95	71.32	59.36
26+29	47.36	91.46	62.72	129.70	97.78
27	9.95	20.55	19.44	24.37	23.71
31	181.44	360.86	240.74	501.27	368.52
32	53.75	100.89	80.01	128.53	129.90
34	1.09	1.58	1.35	2.78	2.41
35	2.55	6.11	2.86	7.15	3.43
36	1.18	3.97	0.00	3.14	3.07
37	72.66	131.45	82.27	161.23	102.86
38	0.00	0.34	0.58	0.97	0.83
39	0.00	3.17	0.00	2.83	1.15
40+41+71	185.79	364.63	182.19	354.10	255.35
42	130.51	190.64	126.65	171.77	174.85
43	19.05	29.08	22.35	21.23	36.35
45+51	881.88	351.22	126.51	124.55	122.06
46	24.98	43.99	42.17	43.65	162.39
48	64.32	129.29	61.19	126.50	108.60
49+69	251.97	425.69	275.46	395.87	380.19
50+53	57.13	102.16	105.46	94.73	2.11
52	499.62	725.48	677.78	655.08	47.24
54	0.00	1.34	1.53	1.18	0.00
55	357.67	0.00	2.44	9.13	4.29
56	142.20	259.36	108.16	263.39	155.75

Table A-3 continued

Sample ID **Congener #**	**24-1** [a] **ng g^{-1} d.w.**	**24-2** [a] **ng g^{-1} d.w.**	**25** **ng g^{-1} d.w.**	**26** **ng g^{-1} d.w.**	**27-1** [a] **ng g^{-1} d.w.**
57	3.71	4.11	3.37	3.80	4.66
58	0.00	2.91	0.00	0.00	0.00
59+62+75	27.74	59.33	37.14	53.94	43.86
60	69.74	142.29	53.39	151.10	84.71
61+70+74+76	502.78	888.34	339.13	923.50	531.02
63	12.65	26.54	10.04	25.48	16.53
64	168.53	306.25	157.22	289.00	225.21
66	0.00	496.34	258.32	504.51	376.22
67	12.90	19.72	8.28	16.61	0.00
68	22.76	3.03	18.29	2.65	22.51
72	2.03	4.46	1.87	3.41	2.52
73	0.00	0.00	0.00	0.00	695.58
77	27.38	48.45	28.55	55.92	37.67
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	2.46	1.81	0.00	0.00	0.00
82	44.40	64.08	35.36	68.96	40.73
83+99	105.14	170.52	106.30	225.75	120.24
84	75.45	116.25	66.82	115.89	67.53
85+116+117	60.01	87.84	45.72	93.86	55.10
86+87+97+109+119+125	147.13	111.73	122.32	121.51	140.69
88+91	47.05	77.33	41.96	69.51	43.50
89	8.77	12.33	9.15	12.88	7.27
90+101+113	170.74	279.63	140.85	278.01	150.96
92	32.99	54.37	27.66	50.85	28.21
93+100	0.00	6.10	3.20	5.94	3.31
94	2.88	3.91	3.11	4.09	2.91
95	155.91	241.95	153.81	233.97	152.90
96	4.05	7.15	5.02	6.75	5.71
98+102	18.58	26.08	14.50	25.08	12.95
103	1.97	2.96	1.69	2.77	1.93
104	0.00	0.00	0.00	0.00	0.00
105	78.66	112.48	58.31	116.72	85.34
106	0.00	0.00	0.00	0.00	0.00
107	13.74	22.89	0.00	26.71	14.44
108+124	5.60	9.16	4.42	9.77	5.71
110+115	215.99	338.47	182.34	353.80	201.01
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	5.44	8.97	3.54	9.46	6.00
118	147.69	213.07	116.34	246.31	163.02
120	0.00	0.00	0.00	0.45	0.00
121	0.00	0.00	0.00	0.00	0.00
122	3.04	5.05	2.87	4.40	3.31
123	0.00	0.00	12.42	0.00	0.00
126	9.89	525.61	6.02	0.00	8.75
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	82.10	122.67	67.29	116.00	79.48
130	4.47	6.18	3.49	6.22	5.06
131	0.00	1.41	0.92	2.38	40.26
132	29.76	43.69	23.33	46.79	0.00
133	0.00	4.17	0.99	1.73	0.00

Table A-3 continued

Sample ID	**24-1** [a]	**24-2** [a]	**25**	**26**	**27-1** [a]
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
134+143	0.00	6.74	2.86	7.30	2.91
135+151	31.53	47.71	13.20	47.97	15.32
136	12.23	20.25	19.65	17.39	19.92
137+164	8.27	19.85	10.41	11.55	12.53
139+140	1.56	1.84	1.18	3.16	0.00
141	14.68	21.57	12.56	20.58	12.88
142	0.00	0.00	0.00	0.00	0.00
144	4.56	7.75	3.71	7.10	4.04
145	0.00	0.00	0.00	0.00	0.00
146	11.74	17.62	9.41	15.18	10.66
147+149	1.96	106.08	59.01	107.33	65.23
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.63	0.00	0.00	0.00
152	0.00	0.00	0.00	0.28	0.00
153+168	66.26	97.03	51.51	92.63	58.80
154	0.00	1.64	0.65	1.17	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	7.76	9.17	5.85	12.27	7.15
158	8.31	11.17	6.09	11.65	7.61
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	2.74	3.09	2.20	0.00	2.86
169	0.00	1.44	1.32	1.31	1.40
170	15.31	24.25	14.45	23.65	19.17
171+173	6.17	8.84	5.51	9.74	7.52
172	3.60	3.72	2.97	5.37	3.32
174	16.53	27.76	12.79	32.03	15.96
175	0.00	1.78	0.00	1.52	0.00
176	3.00	4.56	2.24	4.58	2.44
177	10.89	17.00	9.08	20.00	11.24
178	3.80	7.48	3.62	7.34	4.05
179	9.52	15.00	7.76	14.20	9.54
180+193	35.84	58.33	32.90	62.38	41.40
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	9.12	19.78	7.60	19.98	9.86
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	28.70	38.89	26.13	42.16	30.94
188	0.00	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.85	0.00
190	3.63	4.32	3.36	4.07	4.08
191	0.00	0.00	0.61	0.92	0.00
192	0.00	0.00	0.00	0.00	0.00
194	9.60	13.11	9.79	12.24	13.55
195	4.40	5.02	2.84	4.04	4.32
196	5.40	7.35	4.37	8.65	5.27
197	0.00	0.00	0.00	0.71	0.00
198+199	10.50	17.46	10.64	18.53	15.08
200	1.55	1.45	1.30	2.74	0.00

Table A-3 continued

Sample ID **Congener #**	**24-1 [a]** **ng g $^{-1}$ d.w.**	**24-2 [a]** **ng g $^{-1}$ d.w.**	**25** **ng g $^{-1}$ d.w.**	**26** **ng g $^{-1}$ d.w.**	**27-1 [a]** **ng g $^{-1}$ d.w.**
201	1.71	2.36	1.30	3.05	1.51
202	2.84	3.27	2.33	4.48	2.36
203	7.35	9.38	7.11	8.96	10.21
205	0.00	0.40	0.00	0.42	0.00
206	4.75	5.33	5.46	3.41	6.95
207	0.00	0.00	0.00	0.80	0.00
208	1.04	1.96	1.20	1.79	0.00
209	18.75	1.65	1.79	0.92	2.80
Total	**6293.13**	**10089.54**	**5811.84**	**9999.08**	**7643.18**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**27-2 [a]**	**28-1 [a]**	**28-2 [a]**	**29**	**30**
Collection date	08/09/06	08/09/06	08/09/06	08/09/06	08/09/06
Lab batch #	7	7	3	5	5
PCB14 % recovery	77	76	116	91	77
PCB65 % recovery	154	186	197	112	127
PCB166 % recovery	75	73	73	58	66
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	43	50	39	43	33
Total organic carbon (%) [b]	1.88	5.47	5.47	4.85	5.35
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	1.07	2.76	0.00	1.11	0.94
2	0.54	1.27	7.61	0.57	0.39
3	1.93	4.66	5.85	1.55	1.43
4	11.33	46.92	41.72	11.08	8.84
5	0.00	1.04	0.00	0.00	0.00
6	18.85	52.81	49.42	14.16	7.95
7	1.19	3.59	5.35	1.10	0.93
8	28.20	96.61	107.68	39.10	24.36
9	1.80	5.24	6.24	1.98	1.16
10	0.42	1.53	1.45	0.00	0.00
11	35.83	10.24	3.37	10.57	6.18
12+13	14.55	44.89	44.53	9.87	5.66
15	47.43	98.63	101.27	41.04	31.76
16	62.33	198.89	239.79	82.20	51.84
17	87.16	265.47	239.90	80.07	55.97
18+30	196.65	536.63	499.01	172.77	124.34
19	17.17	51.55	48.26	14.56	12.12
20+28	496.21	970.64	1027.29	324.38	277.28
21+33	83.47	247.14	305.51	78.74	60.24
22	107.35	231.82	240.21	□7.15	59.54
23	1.74	2.47	4.41	1.11	1.17
24	1.24	3.93	0.00	0.00	0.00
25	139.41	175.14	173.35	40.26	29.52
26+29	185.23	185.87	180.13	63.57	46.63
27	15.88	40.37	41.68	16.12	13.73
31	369.36	796.34	782.58	216.30	178.47
32	82.60	198.04	240.33	68.26	53.56
34	3.22	8.27	7.08	1.79	1.06
35	7.18	9.24	11.63	2.56	2.85
36	2.48	4.90	0.00	0.00	0.00
37	96.72	155.77	179.93	52.83	59.30
38	1.11	1.66	1.56	0.00	0.00
39	2.82	3.59	2.69	0.00	0.00
40+41+71	339.17	566.06	469.29	234.90	203.89
42	197.05	303.37	310.66	157.02	137.02
43	29.35	32.10	64.70	22.92	15.29
45+51	349.52	666.69	224.03	114.07	90.36
46	41.95	82.04	71.97	34.74	30.28
48	111.79	230.49	209.77	105.76	83.34
49+69	454.28	701.59	643.45	350.43	289.45
50+53	101.81	203.14	176.20	92.06	66.54
52	747.66	1202.30	1416.11	572.02	455.61
54	1.10	3.25	0.00	0.00	0.00
55	0.00	0.00	9.20	5.83	5.86
56	206.80	354.56	330.59	182.51	160.08

Table A-3 continued

Sample ID **Congener #**	**27-2** [a] **ng g^{-1} d.w.**	**28-1** [a] **ng g^{-1} d.w.**	**28-2** [a] **ng g^{-1} d.w.**	**29** **ng g^{-1} d.w.**	**30** **ng g^{-1} d.w.**
57	3.47	4.07	9.41	0.00	0.00
58	0.92	1.09	0.00	0.00	0.00
59+62+75	53.82	90.00	77.53	41.71	37.25
60	113.29	149.93	141.12	95.31	81.19
61+70+74+76	739.07	1299.05	1231.70	629.95	523.78
63	25.89	34.15	35.63	20.95	15.73
64	301.27	457.79	423.53	218.62	191.83
66	403.07	656.13	779.29	460.76	402.76
67	21.28	26.03	34.62	15.97	12.60
68	3.91	3.48	49.69	0.00	0.00
72	4.61	5.31	6.46	0.00	2.38
73	0.00	0.00	0.00	0.00	0.00
77	47.65	70.87	63.30	44.53	34.71
78	0.00	0.00	0.00	0.00	0.00
79	0.00	1.24	0.00	0.00	0.00
80	0.00	0.54	0.00	0.00	0.00
81	1.06	3.11	0.00	0.00	0.00
82	55.76	77.27	67.30	51.46	46.68
83+99	160.64	223.26	225.62	153.88	132.81
84	114.96	149.96	134.06	78.99	70.84
85+116+117	79.87	106.70	94.36	65.32	57.71
86+87+97+109+119+125	107.14	152.74	253.32	178.28	155.10
88+91	72.54	112.01	79.74	57.36	50.16
89	12.77	100.55	16.19	9.55	8.23
90+101+113	259.45	361.64	298.84	194.32	174.18
92	50.68	67.96	52.53	37.48	34.68
93+100	0.00	6.99	0.00	0.00	0.00
94	3.86	4.84	6.77	0.00	0.00
95	225.92	314.93	279.34	175.53	144.63
96	0.00	10.55	9.44	5.72	4.11
98+102	26.89	34.57	31.98	14.26	13.60
103	9.11	3.38	0.00	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	109.71	146.78	135.97	102.41	84.37
106	0.87	1.47	0.00	0.00	0.00
107	17.36	30.94	25.71	20.44	18.07
108+124	9.02	11.33	0.00	0.00	7.09
110+115	332.02	448.31	363.67	264.55	220.33
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	9.32	9.54	10.51	7.89	7.76
118	211.44	300.51	284.95	204.26	165.87
120	0.00	1.07	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	4.15	5.82	5.43	0.00	3.31
123	5.59	0.00	0.00	0.00	0.00
126	7.09	8.82	15.05	0.00	7.85
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	106.05	166.07	126.37	113.88	93.35
130	5.51	9.90	7.17	7.40	7.06
131	1.43	0.00	0.00	0.00	0.00
132	39.16	61.19	47.71	40.26	31.33
133	4.08	5.40	0.00	0.00	0.00

Table A-3 continued

Sample ID	**27-2 [a]**	**28-1 [a]**	**28-2 [a]**	**29**	**30**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
134+143	5.05	0.00	9.43	0.00	0.00
135+151	41.47	0.00	24.58	41.22	33.97
136	15.15	24.09	35.83	13.52	12.44
137+164	12.65	31.36	24.10	11.09	10.88
139+140	1.98	2.75	0.00	0.00	0.00
141	18.66	31.82	17.79	21.44	15.97
142	0.00	0.00	0.00	0.00	0.00
144	5.16	0.00	8.06	7.27	3.99
145	0.00	47.54	0.00	0.00	0.00
146	15.37	24.93	17.91	15.33	11.83
147+149	89.27	138.13	109.48	89.46	73.82
148	0.00	2.17	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	85.24	132.48	91.61	89.81	72.66
154	1.50	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	10.64	16.06	13.29	11.25	0.00
158	10.60	15.42	14.02	11.34	9.19
159	0.00	0.00	0.00	0.00	9.85
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	18.36
165	0.00	0.28	0.00	0.00	0.00
167	4.03	5.59	4.64	0.00	0.00
169	1.86	8.78	0.00	0.00	0.00
170	22.15	34.17	28.34	26.39	19.38
171+173	7.68	13.55	10.26	9.94	6.81
172	4.87	6.89	7.15	0.00	0.00
174	25.50	44.98	23.23	21.56	17.23
175	0.94	0.00	0.00	0.00	0.00
176	3.45	6.82	4.78	0.00	0.00
177	15.17	23.96	15.82	19.40	16.44
178	5.44	10.99	6.50	0.00	0.00
179	11.65	19.56	12.90	13.92	9.61
180+193	55.69	91.56	59.49	64.62	48.64
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	16.32	26.96	13.73	14.57	9.00
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	33.76	54.41	42.63	45.93	30.47
188	0.00	0.00	0.00	0.00	0.00
189	0.78	1.36	0.00	0.00	0.00
190	4.54	7.91	6.36	0.00	0.00
191	1.29	1.24	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	13.25	17.31	17.18	15.59	9.02
195	4.71	8.37	0.00	0.00	0.00
196	8.00	11.02	9.73	0.00	0.00
197	0.00	0.00	0.00	0.00	0.00
198+199	15.52	25.50	18.18	15.28	12.20
200	1.89	4.34	0.00	0.00	0.00

Table A-3 continued

Sample ID **Congener #**	**27-2** [a] **ng g $^{-1}$ d.w.**	**28-1** [a] **ng g $^{-1}$ d.w.**	**28-2** [a] **ng g $^{-1}$ d.w.**	**29** **ng g $^{-1}$ d.w.**	**30** **ng g $^{-1}$ d.w.**
201	2.02	3.05	0.00	0.00	0.00
202	3.29	5.81	0.00	0.00	0.00
203	10.80	13.56	16.36	0.00	0.00
205	0.33	0.30	0.00	0.00	0.00
206	6.72	7.29	10.15	4.43	0.00
207	1.27	1.99	0.00	0.00	0.00
208	1.98	2.29	0.00	0.00	0.00
209	1.37	1.98	0.00	0.00	0.00
Total	**9063.65**	**15469.34**	**14623.62**	**7161.50**	**5948.01**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**31**	**32-1** [a]	**32-2** [a]	**33**	**34**
Collection date	08/10/06	08/10/06	08/10/06	08/10/06	08/10/06
Lab batch #	5	7	5	5	4
PCB14 % recovery	58	68	67	76	129
PCB65 % recovery	114	142	139	560	196
PCB166 % recovery	60	75	63	101	81
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	32	35	29	34	35
Total organic carbon (%) [b]	6.51	3.51	3.51	6.88	5.70
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.75	1.49	1.15	73.16	4.23
2	0.30	0.68	0.39	18.76	3.60
3	1.25	2.52	1.81	27.86	8.23
4	6.04	11.05	6.50	519.09	45.39
5	0.00	0.00	0.00	0.00	0.00
6	5.31	11.38	5.81	142.50	38.62
7	0.55	1.16	0.57	19.15	3.83
8	19.74	28.06	20.78	856.75	94.31
9	0.87	1.62	1.03	49.19	2.79
10	0.00	0.68	0.00	15.65	0.00
11	5.53	8.28	0.85	10.96	0.00
12+13	4.16	7.62	4.53	36.80	12.07
15	25.75	44.75	23.70	247.26	71.40
16	35.98	51.80	31.50	924.67	157.87
17	36.35	62.08	32.81	706.14	208.12
18+30	83.76	148.40	75.52	1617.96	339.08
19	12.83	21.92	12.60	335.99	40.17
20+28	186.09	294.24	165.10	1979.62	977.31
21+33	44.64	68.27	41.53	1243.74	0.00
22	41.87	75.98	35.92	559.67	177.71
23	0.60	1.06	0.59	1.45	3.07
24	0.00	1.60	0.00	104.93	0.00
25	18.19	32.91	16.77	89.73	98.18
26+29	30.37	58.44	27.14	232.09	78.66
27	10.97	16.25	10.24	0.00	0.00
31	118.56	224.65	104.53	1628.18	368.22
32	37.58	65.44	34.89	814.15	140.84
34	0.58	1.43	0.51	4.86	0.00
35	1.87	4.36	1.70	13.25	0.00
36	0.00	2.17	0.00	0.00	1.11
37	45.32	83.73	40.88	429.42	139.50
38	0.00	0.53	0.66	2.29	0.00
39	0.00	2.25	0.00	4.79	0.00
40+41+71	130.56	234.58	127.26	834.73	152.06
42	89.74	140.78	104.94	493.20	144.68
43	8.66	0.00	9.42	57.49	0.00
45+51	75.07	311.85	81.67	338.35	113.75
46	24.13	41.32	26.23	116.01	85.12
48	45.18	74.22	43.36	354.57	0.00
49+69	181.50	296.30	198.93	957.28	211.47
50+53	57.54	90.52	61.18	242.22	108.93
52	317.35	558.61	356.49	0.00	660.91
54	0.00	1.35	0.00	4.01	2.26
55	3.38	0.00	1.94	0.00	0.00
56	97.99	154.41	89.00	671.98	293.13

Table A-3 continued

Sample ID **Congener #**	**31** **ng g^{-1} d.w.**	**32-1**[a] **ng g^{-1} d.w.**	**32-2**[a] **ng g^{-1} d.w.**	**33** **ng g^{-1} d.w.**	**34** **ng g^{-1} d.w.**
57	0.00	1.39	0.00	10.22	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	27.82	45.00	28.50	103.46	0.00
60	47.75	81.12	43.88	373.36	0.00
61+70+74+76	298.02	514.95	291.08	2692.05	572.05
63	10.02	15.02	8.24	54.49	3.77
64	116.15	191.42	111.90	672.43	302.98
66	239.79	317.66	251.27	1645.74	793.57
67	6.85	9.32	6.50	43.06	4.37
68	1.64	2.28	1.60	0.00	10.30
72	1.59	2.70	1.45	3.69	0.00
73	0.00	10.85	0.00	1185.89	0.00
77	25.58	33.78	24.71	134.10	48.09
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	5.81	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	1.52	0.00	3.38	0.00
82	40.55	49.84	41.15	163.26	0.00
83+99	112.10	135.83	122.45	434.00	0.00
84	68.93	99.55	68.65	234.79	170.91
85+116+117	47.01	67.24	48.90	165.66	0.00
86+87+97+109+119+125	129.19	90.10	139.29	554.76	152.59
88+91	42.83	62.06	45.38	158.26	0.00
89	6.53	10.31	8.43	30.82	37.69
90+101+113	143.14	228.15	155.97	544.11	170.26
92	27.61	42.76	29.16	95.83	0.00
93+100	2.93	4.05	2.67	0.00	0.00
94	2.17	4.14	2.57	8.37	3.59
95	133.21	205.11	138.47	485.95	216.46
96	3.67	6.23	4.22	13.94	5.85
98+102	12.66	21.72	13.90	52.71	0.00
103	1.81	2.37	1.52	3.75	0.91
104	0.00	0.00	0.00	0.00	0.00
105	62.52	74.59	59.21	350.61	111.31
106	0.00	0.00	0.00	0.00	0.00
107	13.01	12.18	8.86	23.74	0.00
108+124	4.72	6.89	5.17	0.00	0.00
110+115	192.08	269.42	200.97	714.67	346.15
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	66.20
114	4.02	4.94	3.84	22.70	9.86
118	118.96	150.47	121.39	580.93	228.74
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	2.89	2.96	3.15	10.83	0.00
123	0.00	4.60	4.01	56.38	31.90
126	5.11	6.31	4.63	0.00	8.13
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	90.86	102.42	90.32	260.37	112.01
130	4.42	5.26	5.46	13.71	0.00
131	0.00	1.59	0.00	6.35	0.00
132	29.97	36.50	30.95	94.50	38.88
133	0.00	3.73	0.00	2.90	0.00

Table A-3 continued

Sample ID **Congener #**	**31** **ng g^{-1} d.w.**	**32-1 [a]** **ng g^{-1} d.w.**	**32-2 [a]** **ng g^{-1} d.w.**	**33** **ng g^{-1} d.w.**	**34** **ng g^{-1} d.w.**
134+143	0.00	6.18	0.00	13.72	0.00
135+151	30.23	40.01	31.10	93.42	42.39
136	10.46	16.46	11.15	32.52	14.12
137+164	8.87	17.48	10.05	27.42	9.20
139+140	0.00	1.65	0.00	4.68	0.00
141	14.58	19.75	10.04	49.18	119.65
142	0.00	0.00	0.00	0.00	0.00
144	3.67	5.94	4.99	13.86	2.30
145	0.00	0.00	0.00	0.00	0.00
146	11.31	13.86	12.07	34.41	14.82
147+149	68.05	88.78	76.21	199.51	91.51
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.22	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	68.77	82.52	63.89	193.29	0.00
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	8.11	7.67	6.37	32.34	21.08
158	8.86	8.71	9.86	27.24	7.99
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.06	0.00	0.00	0.00
167	3.00	3.59	2.62	8.09	4.18
169	1.67	5.30	0.00	3.89	0.00
170	20.01	20.23	20.58	57.90	24.25
171+173	7.96	8.03	6.98	19.90	7.82
172	4.24	4.11	3.17	10.59	2.77
174	18.01	26.74	19.20	56.87	0.00
175	0.00	1.33	0.00	4.22	0.00
176	3.15	4.04	2.85	9.29	3.62
177	13.91	15.83	12.75	38.81	12.74
178	4.24	5.89	4.78	12.75	5.26
179	9.38	12.32	9.41	28.37	11.32
180+193	46.69	53.26	46.09	138.74	50.29
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	10.26	15.88	9.93	26.39	37.68
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	33.06	33.21	34.64	94.12	38.05
188	0.00	0.00	0.00	0.00	0.00
189	0.00	1.15	0.00	0.00	0.00
190	4.23	4.70	3.20	9.61	4.53
191	0.00	1.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	12.37	9.64	10.52	22.48	8.92
195	3.76	4.68	0.00	9.41	3.16
196	7.43	5.55	5.61	16.23	16.42
197	0.00	0.00	0.00	0.00	0.00
198+199	13.46	13.51	15.67	30.05	12.80
200	0.00	1.26	0.00	4.49	0.00

Table A-3 continued

Sample ID **Congener #**	**31** **ng g $^{-1}$ d.w.**	**32** **ng g $^{-1}$ d.w.**	**32** **ng g $^{-1}$ d.w.**	**33** **ng g $^{-1}$ d.w.**	**34** **ng g $^{-1}$ d.w.**
201	2.09	1.58	0.00	4.72	0.00
202	2.24	2.97	2.92	5.62	0.83
203	6.69	8.30	6.25	12.68	0.00
205	0.00	0.00	0.00	0.00	0.00
206	2.62	3.65	2.38	5.18	4.02
207	0.89	0.55	0.00	0.00	0.00
208	1.38	1.15	0.00	1.78	0.00
209	0.83	1.21	0.00	0.00	1.65
Total	**4351.52**	**6759.06**	**4385.59**	**30145.25**	**8806.55**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**35**	**36**	**37**	**38**	**39**
Collection date	08/10/06	08/10/06	08/10/06	08/10/06	08/10/06
Lab batch #	5	5	5	5	6
PCB14 % recovery	54	82	67	74	94
PCB65 % recovery	140	162	122	136	216
PCB166 % recovery	59	76	63	61	109
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	48	45	46	51	47
Total organic carbon (%)	5.91	7.00	5.93	5.53	5.94
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	2.66	1.37	1.52	1.64	1.46
2	0.76	0.70	0.00	0.64	0.87
3	3.95	2.39	2.44	2.34	3.07
4	29.71	17.91	17.09	14.76	17.95
5	0.00	0.00	0.00	0.00	0.39
6	47.61	19.48	20.95	17.96	25.22
7	2.65	1.65	1.30	1.70	2.26
8	88.33	50.25	52.04	51.20	47.96
9	4.56	2.40	2.80	2.04	3.20
10	1.43	0.00	0.00	0.00	0.64
11	3.96	7.68	9.58	19.38	4.37
12+13	40.48	13.04	13.68	11.28	13.76
15	65.89	48.32	49.60	44.52	61.50
16	0.00	106.18	106.04	87.43	86.66
17	165.26	105.69	101.72	94.91	111.38
18+30	329.73	222.37	225.84	202.89	224.42
19	26.09	18.60	18.30	17.08	19.12
20+28	769.04	462.32	474.18	444.59	478.36
21+33	203.89	134.66	128.20	130.47	124.94
22	162.40	103.70	104.72	100.55	124.35
23	1.52	1.42	1.65	1.50	1.30
24	89.36	0.00	0.00	0.00	0.00
25	163.44	55.20	60.83	51.82	75.47
26+29	122.93	87.90	87.64	81.62	110.28
27	27.26	21.56	20.79	18.29	18.23
31	531.01	327.32	334.66	310.87	392.07
32	141.26	84.21	85.63	78.43	99.41
34	5.61	2.13	2.30	2.04	2.72
35	7.89	4.46	4.26	4.95	4.79
36	0.00	0.00	0.00	0.00	0.00
37	108.76	89.71	90.39	85.63	124.32
38	0.00	0.00	0.00	0.00	0.43
39	3.02	0.00	0.00	0.00	0.00
40+41+71	344.49	269.42	284.15	298.93	266.43
42	232.15	181.67	192.24	198.89	180.44
43	0.00	22.86	18.48	23.67	19.70
45+51	149.71	114.06	116.48	127.67	99.91
46	48.45	37.94	40.34	39.93	35.36
48	158.97	117.78	122.42	126.86	101.89
49+69	467.43	371.91	381.84	423.12	325.17
50+53	110.16	85.54	87.53	92.85	79.87
52	730.30	577.50	596.73	637.20	536.62
54	0.00	0.00	0.00	0.00	1.31
55	12.92	8.41	0.00	8.19	4.83
56	262.37	206.87	212.11	230.47	239.01

Table A-3 continued

Sample ID **Congener #**	**35** **ng g $^{-1}$ d.w.**	**36** **ng g $^{-1}$ d.w.**	**37** **ng g $^{-1}$ d.w.**	**38** **ng g $^{-1}$ d.w.**	**39** **ng g $^{-1}$ d.w.**
57	0.00	0.00	0.00	0.00	2.54
58	0.00	0.00	0.00	0.00	1.45
59+62+75	59.54	47.03	47.90	53.87	43.84
60	119.58	115.35	119.85	124.96	134.99
61+70+74+76	1003.74	752.20	779.20	836.08	769.19
63	29.21	21.42	26.45	27.12	22.16
64	0.00	255.95	257.94	269.49	247.38
66	596.88	535.04	563.61	633.60	446.92
67	0.00	21.01	17.58	20.44	20.24
68	0.00	0.00	0.00	0.00	2.32
72	0.00	3.31	0.00	0.00	3.07
73	18.41	0.00	0.00	0.00	0.00
77	55.52	48.80	53.71	51.68	50.14
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	3.37
82	73.15	55.27	61.95	63.16	62.82
83+99	203.75	167.94	179.12	185.80	186.02
84	111.33	93.03	95.63	107.99	92.70
85+116+117	88.42	69.24	77.66	82.57	71.71
86+87+97+109+119+125	248.14	197.91	211.41	229.71	202.46
88+91	77.46	63.45	65.37	74.70	56.95
89	12.89	8.24	10.31	12.50	10.45
90+101+113	270.02	224.22	231.80	247.90	220.50
92	53.83	43.43	41.34	47.96	42.56
93+100	4.40	3.93	0.00	0.00	3.14
94	0.00	0.00	0.00	0.00	2.96
95	231.82	186.74	199.75	210.84	194.88
96	8.40	4.54	5.63	6.63	5.19
98+102	24.01	17.51	13.77	15.98	19.13
103	0.00	0.00	0.00	0.00	2.22
104	0.00	0.00	0.00	0.00	0.00
105	121.65	115.48	116.52	121.15	111.06
106	0.00	0.00	0.00	0.00	0.00
107	25.24	22.31	27.13	27.86	24.49
108+124	11.75	9.51	9.94	9.78	8.48
110+115	340.42	285.72	303.77	318.47	292.81
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	9.31	8.50	9.77	8.87	9.66
118	267.29	218.42	227.81	245.60	262.48
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	5.36	4.83	0.00	0.00	4.63
123	0.00	0.00	0.00	0.00	0.00
126	12.29	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	149.06	111.96	131.38	137.70	133.23
130	0.00	7.31	0.00	0.00	6.22
131	0.00	0.00	0.00	0.00	2.40
132	52.40	37.48	42.33	49.16	42.10
133	0.00	0.00	0.00	0.00	1.67

Table A-3 continued

Sample ID **Congener #**	**35** **ng g^{-1} d.w.**	**36** **ng g^{-1} d.w.**	**37** **ng g^{-1} d.w.**	**38** **ng g^{-1} d.w.**	**39** **ng g^{-1} d.w.**
134+143	8.56	0.00	0.00	0.00	6.52
135+151	53.86	39.81	43.05	46.54	48.16
136	18.69	15.26	16.43	13.76	14.04
137+164	16.75	14.16	13.57	22.59	13.92
139+140	0.00	0.00	0.00	0.00	1.92
141	30.18	15.74	17.25	23.80	22.57
142	0.00	0.00	0.00	0.00	0.00
144	6.32	5.67	0.00	7.20	5.77
145	0.00	0.00	0.00	0.00	0.00
146	23.12	18.20	16.99	19.37	16.94
147+149	114.62	90.90	100.96	106.39	99.28
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	106.49	86.22	89.44	103.62	96.70
154	0.00	0.00	0.00	0.00	1.28
155	0.00	0.00	0.00	0.00	0.00
156+157	13.21	0.00	10.87	13.80	12.36
158	15.37	10.87	13.08	14.90	14.86
159	0.00	13.18	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	0.00	0.00	0.00	0.00	4.58
169	0.00	0.00	0.00	0.00	2.54
170	32.81	26.74	24.39	35.98	29.35
171+173	0.00	8.70	14.48	0.00	11.40
172	0.00	0.00	0.00	0.00	5.96
174	32.18	24.16	27.56	26.97	27.28
175	0.00	0.00	0.00	0.00	0.00
176	0.00	4.21	0.00	0.00	3.84
177	24.60	17.28	21.13	21.62	19.32
178	0.00	0.00	0.00	0.00	7.02
179	15.45	14.03	11.66	14.47	13.18
180+193	74.77	58.92	66.40	73.39	68.98
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	16.47	13.19	13.71	15.64	15.02
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	29.53
187	53.78	43.09	51.11	52.49	0.00
188	0.00	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	0.00	0.00	0.00	0.00	4.90
191	0.00	0.00	0.00	0.00	1.36
192	0.00	0.00	0.00	0.00	0.00
194	14.09	15.51	16.67	17.29	14.55
195	0.00	0.00	0.00	0.00	5.78
196	0.00	0.00	0.00	0.00	8.76
197	0.00	0.00	0.00	0.00	0.00
198+199	23.75	17.16	19.39	21.75	19.20
200	0.00	0.00	0.00	0.00	2.46

Table A-3 continued

Sample ID **Congener #**	**35** **ng g $^{-1}$ d.w.**	**36** **ng g $^{-1}$ d.w.**	**37** **ng g $^{-1}$ d.w.**	**38** **ng g $^{-1}$ d.w.**	**39** **ng g $^{-1}$ d.w.**
201	0.00	0.00	0.00	0.00	2.35
202	0.00	0.00	0.00	0.00	3.28
203	11.96	0.00	0.00	0.00	10.12
205	0.00	0.00	0.00	0.00	0.00
206	0.00	3.29	0.00	0.00	4.64
207	0.00	0.00	0.00	0.00	0.00
208	0.00	1.58	0.00	0.00	1.45
209	0.00	0.97	0.00	0.00	1.61
Total	**10659.71**	**8302.47**	**8587.18**	**8961.44**	**8564.76**

Table A-3 continued

Sample ID	**40**	**41**	**42-1**[a]	**42-2**[a]	**42-3**[a]
Collection date	08/10/06	08/10/06	08/10/06	08/10/06	08/10/06
Lab batch #	6	6	8	1	4
PCB14 % recovery	95	91	135	93	59
PCB65 % recovery	224	184	140	153	138
PCB166 % recovery	104	107	91	92	70
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	27	51	27	27	33
Total organic carbon (%)[b]	6.70	6.81	4.32	4.32	4.32
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	1.25	1.58	0.99	0.00	1.09
2	0.67	0.93	4.00	0.00	0.23
3	2.59	3.69	1.38	0.00	1.40
4	19.64	17.09	9.78	4.42	12.22
5	0.00	0.52	0.43	0.00	0.51
6	33.09	26.28	11.94	6.35	13.85
7	1.77	2.57	1.77	0.00	1.35
8	49.41	55.97	34.37	18.92	33.99
9	3.12	4.28	2.11	0.00	1.90
10	0.75	0.78	0.40	0.00	0.52
11	4.49	9.73	1.26	2.11	1.90
12+13	20.84	15.73	7.45	4.63	8.77
15	57.03	73.64	28.00	18.91	41.67
16	95.47	102.73	58.91	42.45	78.18
17	119.00	134.08	59.23	44.43	87.95
18+30	238.40	269.49	130.32	0.00	195.76
19	20.63	22.03	12.14	8.58	15.47
20+28	474.33	575.28	255.97	224.15	373.64
21+33	116.15	157.95	87.41	72.80	108.13
22	124.00	155.85	64.86	59.91	101.10
23	1.24	2.15	2.19	0.00	1.21
24	0.00	0.00	0.00	0.00	1.74
25	100.27	82.37	32.45	26.34	43.38
26+29	107.02	123.54	48.86	39.47	74.73
27	17.17	19.82	10.14	8.09	15.55
31	403.43	473.74	201.13	165.49	306.02
32	97.17	114.31	63.12	42.92	77.63
34	2.99	2.90	1.09	0.00	1.90
35	6.66	6.74	2.40	2.91	4.95
36	0.00	3.42	0.00	0.00	0.00
37	100.75	158.83	53.92	56.01	96.89
38	0.57	0.91	0.00	0.00	0.67
39	2.41	2.16	0.85	0.00	1.84
40+41+71	246.63	325.13	133.87	140.37	231.29
42	173.01	225.85	89.29	91.15	116.43
43	19.69	26.30	19.22	13.95	17.83
45+51	98.95	120.40	61.96	107.52	82.46
46	33.08	42.24	19.47	18.45	27.94
48	102.08	127.71	51.79	54.54	82.09
49+69	310.54	406.37	189.50	172.36	252.11
50+53	76.83	92.23	49.08	40.33	58.96
52	507.85	657.92	414.62	359.59	428.97
54	1.17	1.37	0.00	0.00	0.79
55	6.19	0.00	0.00	0.00	6.01
56	217.30	296.97	106.27	117.00	176.85

Table A-3 continued

Sample ID	40	41	42-1 [a]	42-2 [a]	42-3 [a]
Congener #	ng g^{-1} d.w.	ng g^{-1} d.w.	ng g^{-1} d.w.	ng g^{-1} d.w.	ng g^{-1} d.w.
57	0.00	2.84	1.38	0.00	1.77
58	0.00	0.00	0.00	0.00	0.42
59+62+75	41.07	55.26	19.02	19.88	36.21
60	119.96	162.39	55.74	58.40	99.03
61+70+74+76	0.00	950.91	381.12	392.68	613.41
63	0.00	27.75	9.45	11.80	15.71
64	229.16	299.27	116.95	124.34	189.53
66	0.00	553.38	248.74	246.22	325.07
67	0.00	23.91	9.14	8.92	11.63
68	0.00	2.46	34.08	23.07	1.87
72	2.91	4.32	1.27	0.00	2.47
73	0.00	0.00	0.00	0.00	0.00
77	42.85	61.14	20.78	21.46	37.04
78	0.00	0.00	0.00	0.00	0.14
79	1.42	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	1.21	1.62	0.00	0.00	1.30
82	53.71	69.80	23.28	32.98	45.44
83+99	162.98	226.03	74.11	67.76	134.76
84	80.67	110.08	38.37	45.58	73.93
85+116+117	61.30	88.84	35.79	38.66	59.09
86+87+97+109+119+125	174.76	245.01	88.27	94.68	69.59
88+91	50.34	70.88	25.42	25.36	42.38
89	9.49	12.15	5.37	0.00	7.83
90+101+113	194.15	270.33	96.74	105.12	175.05
92	37.29	49.31	19.78	18.07	32.24
93+100	0.00	3.93	9.52	0.00	4.01
94	2.93	4.12	1.85	0.00	2.77
95	174.36	236.27	88.98	84.84	148.77
96	5.15	5.52	2.69	0.00	4.27
110+115	257.50	355.29	124.92	142.62	222.32
98+102	19.03	20.37	0.00	8.53	15.37
103	1.97	2.69	0.75	0.00	1.98
104	0.00	0.00	0.00	0.00	0.00
105	94.03	133.30	51.98	54.56	69.19
106	0.00	0.00	0.00	0.00	0.00
107	22.03	31.42	9.02	4.76	17.05
108+124	7.31	10.54	3.81	0.00	0.00
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	9.13	12.65	4.11	0.00	6.08
118	222.31	315.44	99.45	96.15	149.24
120	0.00	0.00	0.00	0.00	0.17
121	0.00	0.00	0.00	0.00	0.00
122	5.09	5.62	1.66	0.00	2.55
123	0.00	0.00	0.00	0.00	0.00
126	7.47	12.74	0.00	8.17	5.72
127	0.00	0.00	11.75	0.00	0.00
129+138+160+163	109.44	160.01	53.54	51.45	71.25
130	6.42	10.17	2.62	0.00	4.27
131	2.50	0.00	0.00	0.00	1.46
132	36.36	49.37	17.49	19.50	28.66
133	1.46	2.64	0.00	0.00	0.00

Table A-3 continued

Sample ID **Congener #**	**40** **ng g^{-1} d.w.**	**41** **ng g^{-1} d.w.**	**42-1**[a] **ng g^{-1} d.w.**	**42-2**[a] **ng g^{-1} d.w.**	**42-3**[a] **ng g^{-1} d.w.**
134+143	4.03	8.11	3.25	0.00	4.33
135+151	0.00	56.37	17.88	19.54	30.74
136	13.58	18.17	6.74	7.64	11.60
137+164	11.95	15.85	5.92	0.00	7.02
139+140	1.56	2.77	0.00	0.00	1.57
141	20.15	25.45	8.29	9.64	0.00
142	0.00	0.00	0.00	0.00	0.00
144	5.40	7.26	2.60	0.00	4.19
145	22.84	0.00	0.00	0.00	0.00
146	14.55	21.14	7.25	6.53	10.47
147+149	83.57	117.22	42.02	44.23	69.20
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	79.96	112.35	38.16	42.02	60.30
154	1.31	0.00	0.00	0.00	0.96
155	0.00	0.00	0.00	0.00	0.00
156+157	11.60	14.97	5.24	5.86	7.19
158	12.32	17.47	5.46	6.75	6.51
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	4.03	0.00	1.67	0.00	0.00
169	1.81	1.83	0.00	0.00	1.37
170	24.49	34.98	12.55	9.86	13.36
171+173	8.91	13.42	4.35	0.00	6.09
172	4.98	6.13	2.35	0.00	3.03
174	21.97	27.25	12.34	11.31	21.38
175	0.00	0.00	0.00	0.00	1.00
176	3.60	4.43	1.74	0.00	2.70
177	14.22	20.49	6.98	8.38	12.25
178	5.77	8.49	2.52	0.00	4.65
179	11.41	15.24	5.74	6.06	9.67
180+193	54.02	78.40	27.88	27.68	36.49
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	12.31	17.45	7.48	0.00	11.73
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	9.01	0.00
186	0.00	0.00	0.00	0.00	0.00
187	38.64	57.28	19.25	20.57	24.81
188	0.00	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	4.59	7.32	2.18	0.00	2.88
191	0.00	0.00	0.00	0.00	0.56
192	0.00	0.00	0.00	0.00	0.00
194	11.16	16.59	5.53	8.34	5.74
195	4.04	6.91	3.36	0.00	2.53
196	7.73	8.44	4.80	0.00	4.11
197	0.00	0.00	0.00	0.00	0.00
198+199	13.94	18.32	6.98	6.82	9.52
200	2.03	2.21	0.00	0.00	1.19

Table A-3 continued

Sample ID **Congener #**	**40** **ng g $^{-1}$ d.w.**	**41** **ng g $^{-1}$ d.w.**	**42-1 [a]** **ng g $^{-1}$ d.w.**	**42-2 [a]** **ng g $^{-1}$ d.w.**	**42-3 [a]** **ng g $^{-1}$ d.w.**
201	1.85	2.15	0.00	0.00	1.74
202	2.58	4.73	1.66	0.00	2.36
203	10.42	11.01	5.90	5.28	4.44
205	0.00	0.00	0.00	0.00	0.10
206	3.68	5.74	3.03	4.14	1.55
207	0.63	1.08	0.00	0.00	0.00
208	1.20	2.02	0.00	0.00	0.63
209	1.22	1.88	1.14	1.25	0.43
Total	**6817.42**	**10394.23**	**4395.10**	**4030.62**	**6319.29**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-3 continued

Sample ID	**43**	**44**	**45**	**46**	**47**
Collection date	08/10/06	08/10/06	08/11/06	08/11/06	08/11/06
Lab batch #	10	10	10	10	10
PCB14 % recovery	90	85	89	86	101
PCB65 % recovery	289	120	305	167	195
PCB166 % recovery	97	95	94	90	110
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	34	48	52	58	55
Total organic carbon (%)	2.38	6.37	5.45	4.03	4.67
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.12	0.53	0.19	0.72	1.46
2	0.00	0.00	0.56	0.87	0.00
3	199.95	1.21	3.29	1.88	0.57
4	15.10	9.69	28.93	15.90	10.21
5	0.00	0.00	0.00	0.00	0.00
6	28.98	15.95	32.68	18.17	18.87
7	0.00	0.00	0.00	0.00	0.00
8	47.34	27.30	51.49	30.48	26.47
9	2.96	0.00	0.00	0.00	1.93
10	0.00	0.00	0.00	0.00	0.00
11	1.57	3.42	6.09	2.63	0.00
12+13	17.44	6.09	15.37	9.22	6.27
15	77.27	39.18	74.96	37.21	35.06
16	90.70	60.89	115.35	61.02	48.18
17	105.15	69.81	145.29	73.34	56.82
18+30	237.84	169.02	323.32	158.71	136.06
19	17.40	12.77	28.49	12.82	11.43
20+28	517.18	345.86	599.07	323.37	269.24
21+33	121.55	88.77	142.80	82.25	65.35
22	106.77	92.21	142.54	87.36	66.88
23	0.00	0.00	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	0.00
25	72.39	44.45	80.80	45.27	38.82
26+29	77.73	75.22	136.34	70.97	62.55
27	22.35	16.73	30.60	16.27	13.95
31	321.00	254.20	474.06	240.71	200.42
32	89.76	69.89	122.73	67.53	56.03
34	3.05	0.00	1.92	0.00	0.42
35	4.03	0.00	5.15	0.00	2.00
36	0.00	0.00	0.00	0.00	0.00
37	79.18	82.04	137.72	77.99	68.01
38	0.00	1.45	0.00	0.00	0.46
39	0.00	0.72	0.00	0.00	0.00
40+41+71	229.88	226.72	360.08	226.47	202.27
42	124.05	109.03	192.86	119.82	112.67
43	0.00	0.00	0.00	0.00	18.95
45+51	87.35	75.22	122.50	40.09	40.49
46	34.99	21.87	53.90	25.76	26.57
48	85.61	76.41	128.77	70.12	59.56
49+69	257.96	260.60	407.46	232.13	225.64
50+53	69.21	63.52	98.98	61.76	52.57
52	633.78	557.00	906.53	493.94	472.23
54	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	0.00	0.00	0.00
56	183.82	170.73	278.23	169.71	167.41

Table A-3 continued

Sample ID	**43**	**44**	**45**	**46**	**47**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
57	1.68	0.00	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	35.16	36.92	58.36	32.74	37.03
60	76.15	92.78	150.91	103.86	87.33
61+70+74+76	588.11	518.91	907.05	519.64	438.68
63	16.66	15.31	24.88	14.38	13.52
64	189.24	175.97	296.27	188.24	166.18
66	285.40	292.89	471.86	285.59	257.92
67	10.75	8.44	15.48	0.00	0.00
68	0.00	0.00	0.00	0.00	0.00
72	0.00	0.00	0.00	9.36	0.00
73	0.00	0.00	0.00	0.00	0.00
77	34.75	35.56	70.45	43.20	30.91
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	2.77
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	1.76	0.00	0.00
82	36.60	34.23	64.86	35.47	43.02
83+99	132.55	141.99	235.18	133.31	123.16
84	57.40	68.35	107.17	69.57	30.29
85+116+117	0.00	38.51	61.65	0.00	0.00
86+87+97+109+119+125	137.48	156.01	247.07	152.08	131.97
88+91	42.19	44.92	70.67	45.60	38.61
89	8.16	5.83	10.49	0.00	0.00
90+101+113	153.33	174.02	255.72	152.93	145.13
92	30.75	30.63	51.43	29.52	33.66
93+100	0.00	0.00	0.00	0.00	0.00
94	0.00	0.00	0.00	0.00	3.10
95	163.56	174.12	255.88	163.69	149.22
96	2.83	2.19	5.80	0.00	0.00
110+115	235.93	237.35	367.76	269.86	237.98
98+102	14.93	13.23	29.78	13.82	12.72
103	0.00	0.00	0.00	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	64.49	77.75	115.12	75.21	59.03
106	0.00	0.00	0.00	0.00	0.00
107	8.13	19.25	27.68	14.85	14.50
108+124	5.66	8.61	9.23	0.00	7.35
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	4.50	0.00	7.23	6.11	0.00
118	122.70	141.36	217.32	135.62	115.34
120	0.39	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.00	1.76	3.94	0.00	0.00
123	6.70	0.00	0.00	0.00	0.00
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	63.71	83.69	129.76	90.21	69.15
130	5.51	6.14	0.00	0.00	4.55
131	0.00	0.00	0.00	0.00	0.96
132	23.15	28.17	44.15	23.45	24.42
133	0.00	0.00	0.00	0.00	0.00

Table A-3 continued

Sample ID **Congener #**	**43** **ng g^{-1} d.w.**	**44** **ng g^{-1} d.w.**	**45** **ng g^{-1} d.w.**	**46** **ng g^{-1} d.w.**	**47** **ng g^{-1} d.w.**
134+143	2.59	2.05	0.00	0.00	0.00
135+151	30.21	28.64	52.99	37.90	26.88
136	10.89	12.89	19.77	9.07	14.35
137+164	7.16	11.94	0.00	9.91	0.00
139+140	0.00	0.00	0.00	0.00	0.00
141	21.19	0.00	27.49	18.57	11.96
142	0.00	0.00	0.00	0.00	0.00
144	3.04	3.34	3.03	0.00	0.71
145	0.00	0.00	0.00	0.00	0.00
146	13.22	17.70	24.08	14.62	14.64
147+149	58.93	68.73	108.97	68.72	58.02
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	62.86	0.00
153+168	55.21	50.59	99.56	62.47	59.68
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	0.00	0.00	0.00	0.00	0.00
158	5.70	11.43	13.16	0.00	7.14
159	0.00	8.32	18.25	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	0.00	0.00	0.00	0.00	0.00
169	0.00	0.00	0.00	0.00	0.00
170	16.73	16.50	32.66	14.80	17.94
171+173	7.63	6.49	14.14	4.36	8.79
172	0.00	0.00	7.23	0.00	4.57
174	17.02	19.77	35.49	22.58	0.00
175	0.00	0.00	0.00	0.00	0.00
176	0.00	0.00	5.01	0.00	2.18
177	10.55	12.86	25.93	15.98	7.65
178	4.92	2.78	8.29	0.00	0.00
179	8.01	9.09	14.51	10.77	9.01
180+193	42.15	44.34	80.76	48.48	48.08
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	0.00	0.00	19.69	0.00	0.00
184	1.52	0.00	0.00	0.00	0.00
185	17.35	17.04	0.00	19.67	18.54
186	0.00	0.00	0.00	0.00	0.00
187	24.47	27.04	45.00	30.40	21.97
188	0.62	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	0.00	0.00	0.00	4.07	3.55
191	0.00	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	8.88	10.47	14.87	9.37	5.42
195	0.00	0.00	6.12	0.00	0.00
196	2.54	2.95	6.22	0.00	0.00
197	0.00	0.00	0.00	0.00	0.00
198+199	15.53	12.66	26.44	0.00	13.27
200	0.00	1.12	0.00	0.00	0.00

Table A-3 continued

Sample ID **Congener #**	**43** **ng g $^{-1}$ d.w.**	**44** **ng g $^{-1}$ d.w.**	**45** **ng g $^{-1}$ d.w.**	**46** **ng g $^{-1}$ d.w.**	**47** **ng g $^{-1}$ d.w.**
201	0.00	2.19	0.00	5.22	0.00
202	3.02	0.00	0.00	0.00	0.00
203	5.34	5.61	9.10	0.00	4.72
205	0.00	1.05	0.00	0.00	0.00
206	5.27	4.47	10.45	9.46	8.23
207	0.00	3.83	0.00	2.40	1.75
208	1.78	6.48	0.00	2.99	0.00
209	0.04	0.09	0.04	0.00	0.06
Total	**6923.51**	**6135.82**	**10293.22**	**5967.44**	**5223.45**

Table A-3 continued

Sample ID	**48**	**49**	**50**	**51**	**52**
Collection date	08/11/06	08/11/06	08/11/06	08/11/06	08/11/06
Lab batch #	6	6	10	8	6
PCB14 % recovery	81	100	88	57	67
PCB65 % recovery	205	241	515	151	107
PCB166 % recovery	101	114	100	70	78
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	46	50	48	50	55
Total organic carbon (%)	4.41	4.45	5.17	5.76	4.14
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	0.96	2.75	39.97	3.06	0.84
2	0.57	1.00	3.20	1.15	0.42
3	2.25	4.22	28.72	4.40	1.66
4	23.26	33.36	359.78	29.08	9.09
5	0.07	1.57	0.00	1.46	0.16
6	34.58	42.38	203.28	43.82	13.31
7	1.24	5.16	45.77	4.59	1.43
8	45.55	109.74	783.14	105.68	27.47
9	2.28	7.53	61.18	6.73	2.16
10	0.69	1.30	23.68	1.11	0.45
11	4.13	18.43	6.59	14.85	21.17
12+13	16.95	18.19	71.27	23.87	7.27
15	61.92	85.44	500.63	84.79	37.17
16	211.60	142.06	936.44	168.08	45.21
17	123.88	169.64	921.67	189.11	62.39
18+30	249.95	334.15	1960.67	406.10	127.69
19	26.12	30.35	184.30	32.60	10.92
20+28	480.54	605.85	2728.48	751.38	276.00
21+33	90.04	202.75	1210.14	252.40	75.38
22	116.51	176.13	847.22	219.42	77.98
23	0.88	1.40	4.12	1.73	1.70
24	49.23	0.00	0.00	4.16	0.44
25	72.03	83.08	208.41	95.53	37.30
26+29	115.16	127.76	453.81	149.65	57.50
27	21.23	23.33	174.14	30.06	9.65
31	101.78	517.17	2140.17	626.32	224.46
32	110.83	129.50	697.00	149.02	55.92
34	2.58	3.03	10.56	3.30	1.28
35	4.86	6.78	25.96	9.20	3.20
36	0.00	0.00	0.00	4.01	0.00
37	114.04	152.53	688.00	181.69	76.60
38	0.52	0.62	1.09	1.15	1.03
39	1.39	2.22	0.00	3.37	0.59
40+41+71	265.84	307.89	1116.92	399.83	159.67
42	182.07	199.64	568.44	194.22	110.38
43	19.24	23.14	0.00	23.79	10.56
45+51	100.89	117.01	441.33	148.37	59.22
46	34.10	41.39	174.33	53.07	20.60
48	97.00	122.21	450.29	151.52	61.44
49+69	330.86	357.10	1096.13	444.00	202.27
50+53	78.38	86.97	316.53	104.31	47.94
52	538.94	569.68	2374.12	733.71	328.08
54	1.19	1.35	0.00	1.86	0.00
55	6.24	0.00	0.00	9.79	0.00
56	215.76	271.47	900.61	306.38	150.36

Table A-3 continued

Sample ID **Congener #**	**48** **ng g^{-1} d.w.**	**49** **ng g^{-1} d.w.**	**50** **ng g^{-1} d.w.**	**51** **ng g^{-1} d.w.**	**52** **ng g^{-1} d.w.**
57	2.19	3.00	10.90	3.31	3.36
58	0.00	0.00	0.00	0.00	0.00
59+62+75	42.32	48.86	187.54	62.38	25.56
60	335.06	149.94	473.41	179.59	84.44
61+70+74+76	719.80	862.05	2727.78	1074.94	474.53
63	21.68	23.63	62.11	28.81	14.49
64	242.16	271.78	836.40	323.07	150.56
66	427.45	492.74	1458.46	568.25	273.89
67	21.13	22.70	50.92	21.34	12.62
68	2.19	2.19	0.00	3.55	1.88
72	3.71	3.18	7.83	3.60	1.68
73	0.00	0.00	0.00	0.00	0.00
77	48.25	53.82	168.98	63.17	28.72
78	0.00	0.00	0.00	0.00	0.00
79	0.00	2.70	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	1.42	1.31	0.00	1.91	0.00
82	59.16	63.28	148.72	75.05	40.48
83+99	181.13	184.28	485.23	245.29	117.72
84	89.48	95.21	244.50	128.85	58.57
85+116+117	69.79	72.97	0.00	101.42	49.93
86+87+97+109+119+125	188.68	206.51	559.45	133.31	120.62
88+91	56.33	57.43	145.84	74.70	36.57
89	8.59	10.46	38.36	15.58	5.76
90+101+113	210.27	219.55	566.18	306.10	135.13
92	40.84	44.59	99.48	58.95	26.05
93+100	3.07	0.00	0.00	6.11	0.00
94	3.29	3.39	0.00	4.57	2.17
95	185.96	197.51	599.89	260.02	120.24
96	4.89	5.28	14.52	7.41	3.06
98+102	16.57	22.25	66.34	26.09	13.68
103	2.27	2.29	0.00	3.48	1.67
104	0.00	0.00	0.00	0.00	0.00
105	104.10	111.88	286.79	127.97	67.98
106	0.00	0.00	0.00	0.00	0.00
107	24.44	24.72	65.22	28.75	16.99
108+124	9.23	8.84	19.32	10.66	5.38
110+115	287.85	296.79	872.67	389.20	183.92
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	9.89	0.00	16.92	10.85	6.21
118	250.98	261.67	487.60	264.19	162.58
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	4.68	5.30	0.00	5.56	2.88
123	0.00	0.00	0.00	0.00	0.00
126	7.86	0.00	0.00	8.63	8.19
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	122.02	137.93	221.69	126.77	81.95
130	7.40	7.06	11.93	6.62	5.17
131	2.65	2.95	0.00	3.19	0.00
132	38.74	1.73	89.54	51.12	26.96
133	1.04	0.00	1.94	1.83	0.00

Table A-3 continued

Sample ID **Congener #**	**48** **ng g $^{-1}$ d.w.**	**49** **ng g $^{-1}$ d.w.**	**50** **ng g $^{-1}$ d.w.**	**51** **ng g $^{-1}$ d.w.**	**52** **ng g $^{-1}$ d.w.**
134+143	4.26	4.35	0.00	7.53	2.55
135+151	42.80	41.86	85.30	52.72	29.56
136	14.26	14.04	35.63	20.03	8.79
137+164	13.92	13.00	1.96	14.00	8.15
139+140	1.92	2.20	7.50	2.08	0.00
141	22.17	21.20	51.47	22.88	9.84
142	0.00	57.25	0.00	0.00	0.00
144	5.34	4.89	11.00	8.52	4.16
145	0.00	0.00	0.00	0.00	0.00
146	15.23	15.37	35.21	18.52	10.59
147+149	88.68	87.93	177.21	116.61	59.06
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	173.22	0.00	0.00
153+168	87.55	85.85	0.00	102.97	54.20
154	0.00	0.00	0.00	1.71	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	12.59	0.00	41.45	12.00	7.55
158	14.44	0.00	21.81	11.32	9.38
159	0.00	12.42	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	4.00	0.00	6.82	4.20	3.79
169	1.76	1.77	0.00	1.71	0.00
170	28.24	24.37	57.06	25.22	19.49
171+173	9.22	8.12	13.60	10.67	5.90
172	5.22	5.47	0.00	6.87	4.15
174	22.58	23.20	44.70	36.93	15.68
175	0.00	0.00	0.00	1.74	0.00
176	3.64	3.79	5.18	5.43	2.71
177	17.18	16.94	26.71	21.64	13.74
178	5.50	5.52	12.88	7.31	4.40
179	11.59	12.08	16.95	16.15	9.10
180+193	61.04	55.87	103.68	63.80	42.99
181	0.00	0.00	0.00	0.55	0.00
182	0.00	0.00	0.00	0.00	0.00
183	13.36	13.31	0.00	19.64	9.76
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	44.94	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	42.60	40.74	64.92	43.70	31.54
188	0.00	0.00	0.00	0.00	0.00
189	0.00	1.75	0.00	1.59	0.00
190	5.14	5.27	7.09	4.63	3.96
191	0.84	1.28	0.00	0.99	0.00
192	0.00	0.00	0.00	0.00	0.00
194	14.25	11.36	22.71	11.97	10.06
195	6.20	4.23	7.85	5.19	2.81
196	7.55	6.37	5.44	8.49	5.71
197	0.00	0.00	0.00	0.00	0.00
198+199	17.92	14.18	28.27	18.88	11.76
200	2.16	2.28	0.00	1.63	1.65

Table A-3 continued

Sample ID **Congener #**	**48** **ng g^{-1} d.w.**	**49** **ng g^{-1} d.w.**	**50** **ng g^{-1} d.w.**	**51** **ng g^{-1} d.w.**	**52** **ng g^{-1} d.w.**
201	1.91	1.56	0.00	2.80	0.00
202	2.97	2.75	0.00	3.84	2.18
203	10.06	7.54	4.20	9.14	7.62
205	0.00	0.00	0.00	0.30	0.00
206	5.83	4.75	11.09	3.50	2.69
207	0.00	0.00	0.00	0.74	0.00
208	1.42	0.91	0.00	1.52	0.00
209	1.54	1.39	0.24	1.06	1.14
Total	**8443.58**	**9756.22**	**34910.69**	**11722.62**	**5206.64**

Table A-3 continued

Sample ID	**53**	**54**	**55**	**56**	**57**
Collection date	08/11/06	08/11/06	08/11/06	08/11/06	08/11/06
Lab batch #	6	6	11	11	11
PCB14 % recovery	105	85	83	91	74
PCB65 % recovery	270	156	465	390	374
PCB166 % recovery	110	102	100	114	116
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	50	38	44	49	44
Total organic carbon (%)	4.29	3.44	3.98	4.21	3.49
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	2.00	0.86	2.08	1.19	3.26
2	0.90	0.55	0.85	0.49	1.45
3	3.76	1.48	2.68	2.00	2.23
4	22.62	13.79	36.13	16.85	72.47
5	0.70	0.00	0.00	0.00	0.00
6	33.85	19.51	42.73	16.87	23.78
7	3.30	1.49	5.67	1.10	1.36
8	71.63	40.94	95.14	40.17	97.37
9	5.24	2.90	6.78	0.00	5.41
10	0.93	0.53	0.00	0.00	0.00
11	9.76	2.78	5.60	9.15	0.00
12+13	16.72	9.06	26.03	9.51	6.72
15	69.79	38.48	73.71	46.71	57.33
16	107.83	71.09	144.71	67.75	0.00
17	132.56	83.93	164.72	92.97	169.12
18+30	267.05	176.23	374.35	220.03	418.16
19	23.12	15.13	36.42	20.55	41.87
20+28	532.84	318.35	634.17	395.50	492.92
21+33	159.83	99.41	238.72	123.99	200.96
22	147.24	90.86	185.13	108.50	133.50
23	1.30	1.22	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	99.50
25	79.55	44.67	93.73	45.89	36.58
26+29	115.46	75.06	123.90	83.17	85.46
27	19.11	12.13	31.81	14.09	24.94
31	445.49	281.79	556.04	344.54	503.40
32	109.19	70.47	165.96	100.61	145.64
34	2.70	1.93	3.11	1.11	0.00
35	5.20	3.58	5.66	6.07	0.00
36	0.00	0.00	0.00	0.42	0.00
37	130.51	81.54	147.28	104.99	104.03
38	0.66	0.36	0.00	0.00	0.00
39	1.87	1.09	1.58	0.28	1.52
40+41+71	316.43	168.64	389.25	275.11	278.11
42	215.24	112.88	156.07	113.60	101.67
43	24.52	12.58	21.98	18.20	0.00
45+51	124.49	64.55	172.22	118.77	144.01
46	42.69	23.59	38.17	25.46	29.71
48	127.95	66.03	135.81	86.89	107.45
49+69	391.29	195.84	389.56	284.22	232.77
50+53	96.08	49.48	99.87	73.13	85.45
52	628.06	327.99	692.89	528.42	0.00
54	1.16	0.96	0.00	0.00	0.00
55	0.00	3.38	0.00	0.00	290.32
56	280.76	150.12	236.33	167.81	0.00

Table A-3 continued

Sample ID **Congener #**	**53** **ng g^{-1} d.w.**	**54** **ng g^{-1} d.w.**	**55** **ng g^{-1} d.w.**	**56** **ng g^{-1} d.w.**	**57** **ng g^{-1} d.w.**
57	4.40	1.44	0.00	17.91	0.00
58	1.55	0.00	0.00	0.00	0.00
59+62+75	51.79	27.41	52.84	34.90	29.32
60	158.15	86.23	129.87	100.61	145.24
61+70+74+76	907.46	478.29	935.59	615.97	27.94
63	27.40	13.96	19.58	0.00	0.00
64	286.38	154.44	268.20	201.83	170.89
66	517.08	275.46	482.25	344.98	578.29
67	25.00	11.50	13.51	0.00	0.00
68	2.68	1.75	0.00	11.65	0.00
72	3.38	1.57	0.00	3.12	0.00
73	0.00	0.00	0.00	0.00	349.34
77	57.60	27.55	57.68	38.41	30.52
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	80.11
81	4.67	0.00	0.00	0.00	0.00
82	68.44	37.44	59.45	49.44	43.85
83+99	209.97	102.10	144.07	0.00	0.00
84	104.76	53.46	86.12	72.98	65.45
85+116+117	77.67	45.45	72.03	56.65	49.10
86+87+97+109+119+125	220.86	114.89	102.37	176.50	185.62
88+91	64.16	32.71	42.80	31.91	29.88
89	11.65	5.61	12.61	8.81	0.00
90+101+113	248.33	123.67	233.96	173.91	176.18
92	46.68	23.25	36.81	29.23	30.31
93+100	0.00	1.77	0.00	5.78	157.71
94	3.53	1.57	3.07	0.00	0.00
95	222.40	113.81	195.59	156.84	4.59
96	5.94	3.01	5.37	3.54	2.06
98+102	24.75	9.34	23.33	16.07	15.51
103	2.34	1.21	0.00	2.48	0.00
104	0.00	0.00	0.52	0.00	0.63
105	119.15	65.36	127.40	104.07	111.86
106	0.00	0.00	0.00	5.10	3.89
107	28.87	14.00	0.00	0.00	0.00
108+124	9.30	5.19	8.56	7.34	9.05
110+115	325.55	166.92	309.00	250.56	243.51
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	95.48
114	0.00	6.48	9.18	5.61	5.83
118	279.82	145.56	212.49	164.13	175.19
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.41	0.00	6.25
122	5.53	3.85	5.35	4.28	4.56
123	0.00	0.00	19.43	12.99	15.76
126	0.00	6.56	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	136.86	69.95	118.24	93.37	123.91
130	7.73	3.87	6.13	6.73	6.07
131	2.53	0.00	3.13	0.00	0.00
132	44.16	23.28	37.66	33.82	41.07
133	1.67	0.00	2.50	1.67	0.00

Table A-3 continued

Sample ID **Congener #**	**53** **ng g^{-1} d.w.**	**54** **ng g^{-1} d.w.**	**55** **ng g^{-1} d.w.**	**56** **ng g^{-1} d.w.**	**57** **ng g^{-1} d.w.**
134+143	7.81	2.90	3.64	3.80	2.63
135+151	49.28	24.48	33.67	29.30	40.88
136	16.71	8.06	13.74	12.82	13.54
137+164	14.67	7.35	17.92	10.44	16.22
139+140	108.98	0.00	0.99	0.44	2.40
141	22.45	13.23	25.02	18.47	29.62
142	0.00	0.00	0.00	0.00	0.00
144	6.43	3.00	3.74	6.45	8.83
145	0.00	0.00	0.00	0.00	0.00
146	17.54	8.48	0.00	16.19	16.86
147+149	0.00	53.02	78.53	69.94	107.31
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	97.77	50.18	86.03	76.80	101.73
154	1.13	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	13.23	7.09	13.72	13.84	7.93
158	14.14	7.41	13.14	9.57	14.04
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	10.92	0.00	0.00
162	0.00	0.00	0.00	0.82	0.00
165	0.00	0.00	0.00	0.00	0.00
167	4.68	2.61	5.13	3.25	3.54
169	2.31	0.00	0.00	0.00	2.58
170	26.84	15.64	35.46	29.03	47.75
171+173	10.75	4.91	8.33	7.42	9.70
172	6.08	2.42	8.25	5.64	11.99
174	24.76	14.05	36.35	23.41	50.62
175	1.40	0.00	0.00	0.00	2.10
176	3.95	2.00	4.32	4.33	3.02
177	17.51	9.80	14.16	14.38	23.48
178	5.95	3.25	5.92	7.78	8.37
179	14.30	7.50	14.83	11.76	18.90
180+193	62.51	33.86	65.91	63.00	100.88
181	0.00	0.00	0.00	0.00	1.15
182	0.00	0.00	0.00	0.00	0.00
183	14.15	8.11	0.00	0.00	0.00
184	0.00	0.00	0.00	0.00	2.15
185	0.00	0.00	22.23	17.96	28.53
186	0.00	0.00	0.00	0.00	0.00
187	46.36	26.26	37.09	30.22	50.45
188	0.00	0.00	0.00	0.00	0.98
189	0.00	0.00	0.00	0.00	0.00
190	5.08	3.37	3.36	4.45	6.04
191	1.00	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	1.00
194	12.35	7.06	15.65	12.72	19.26
195	5.46	2.99	4.13	4.73	8.82
196	9.64	5.51	6.68	7.64	9.49
197	0.00	0.00	0.00	0.56	0.00
198+199	15.91	8.49	22.27	13.59	24.74
200	2.40	1.60	0.00	0.00	2.12

Table A-3 continued

Sample ID **Congener #**	**53** **ng g $^{-1}$ d.w.**	**54** **ng g $^{-1}$ d.w.**	**55** **ng g $^{-1}$ d.w.**	**56** **ng g $^{-1}$ d.w.**	**57** **ng g $^{-1}$ d.w.**
201	2.06	1.10	0.00	0.00	4.06
202	3.70	2.12	2.38	3.10	3.11
203	12.50	6.97	12.01	8.89	15.45
205	0.00	0.00	0.55	1.15	0.31
206	4.42	2.33	6.34	6.95	10.60
207	0.00	0.00	1.11	0.00	2.61
208	1.68	1.11	4.29	0.00	4.60
209	1.54	0.83	2.68	2.82	4.56
Total	**9781.02**	**5356.20**	**10014.42**	**6962.93**	**7858.41**

Table A-3 continued

Sample ID	**58-1** [a]	**58-2** [a]	**59**	**60-1** [a]	**60-2** [a]
Collection date	08/11/06	08/11/06	08/11/06	08/11/06	08/11/06
Lab batch #	7	1	11	6	8
PCB14 % recovery	51	191	97	95	68
PCB65 % recovery	102	221	531	99	70
PCB166 % recovery	67	84	130	100	59
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	35	21	42	34	37
Total organic carbon (%) [b]	5.49	5.49	4.52	3.82	3.82
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	1.52	1.47	1.67	0.00	0.00
2	1.28	0.60	1.33	0.00	0.00
3	1.32	1.40	2.88	0.00	1.69
4	33.26	41.93	23.30	0.84	1.27
5	0.00	0.00	0.00	1.35	0.00
6	20.02	18.22	34.15	0.61	0.00
7	2.30	0.92	0.00	0.00	0.00
8	70.73	53.73	70.29	0.00	2.03
9	4.87	2.29	4.06	0.00	0.00
10	1.73	2.08	0.00	0.00	0.00
11	2.19	1.19	8.91	0.00	0.00
12+13	10.77	9.58	17.18	2.87	0.00
15	39.56	51.88	61.40	0.84	1.40
16	171.37	0.00	0.00	2.06	2.83
17	174.68	160.14	145.13	2.38	2.97
18+30	0.00	397.51	316.89	4.86	6.82
19	71.96	42.42	24.39	0.00	1.10
20+28	432.90	484.39	552.81	6.28	7.92
21+33	182.75	167.75	187.20	2.43	3.20
22	105.13	126.79	160.37	1.82	2.76
23	0.00	1.86	0.00	0.33	0.98
24	0.00	85.90	76.48	0.00	0.00
25	61.94	64.01	74.65	1.16	0.12
26+29	63.58	90.94	123.86	0.13	2.14
27	24.56	28.66	26.42	0.31	0.00
31	316.44	458.97	492.25	5.27	5.68
32	219.49	139.77	129.76	1.92	2.49
34	0.00	2.23	3.81	0.56	0.00
35	1.85	5.30	4.42	1.03	0.55
36	0.00	3.30	0.00	0.56	0.60
37	57.48	80.28	145.11	13.66	12.76
38	0.00	0.19	0.00	0.76	0.00
39	0.00	2.67	0.65	1.40	1.13
40+41+71	218.95	232.51	363.79	3.19	5.14
42	155.61	114.54	148.90	0.00	2.08
43	17.43	20.30	24.70	0.00	0.00
45+51	153.07	318.48	91.96	1.84	2.36
46	77.61	40.16	33.50	0.00	0.00
48	61.08	91.68	121.52	0.00	1.83
49+69	406.17	274.49	359.43	4.34	6.36
50+53	162.88	104.05	82.39	1.37	1.92
52	467.64	513.60	634.09	0.00	9.95
54	4.13	1.07	0.00	0.00	0.00
55	218.13	3.97	0.00	4.24	5.24
56	82.18	131.04	193.14	2.74	2.65

Table A-3 continued

Sample ID **Congener #**	**58-1 ^{a}** **ng g $^{-1}$ d.w.**	**58-2 ^{a}** **ng g $^{-1}$ d.w.**	**59** **ng g $^{-1}$ d.w.**	**60-1 ^{a}** **ng g $^{-1}$ d.w.**	**60-2 ^{a}** **ng g $^{-1}$ d.w.**
57	0.00	0.97	0.00	0.00	0.00
58	0.00	0.71	0.00	0.00	0.00
59+62+75	21.42	34.99	54.05	0.00	0.00
60	40.22	73.83	118.72	1.49	0.00
61+70+74+76	498.47	464.96	786.47	8.53	10.01
63	9.96	13.49	20.89	0.00	0.00
64	141.41	168.42	250.78	3.08	5.01
66	0.00	219.53	427.81	0.00	0.00
67	7.63	8.21	14.46	0.00	0.00
68	13.59	0.00	0.00	0.88	0.00
72	0.00	0.88	0.00	0.00	0.00
73	0.00	0.00	0.00	5.64	0.00
77	10.81	32.23	51.21	0.00	0.00
78	0.00	0.89	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.93	0.00	0.00	0.00
82	18.17	38.69	55.81	0.00	0.00
83+99	0.00	88.52	0.00	0.00	0.00
84	67.88	51.53	86.12	3.31	2.17
85+116+117	21.60	47.26	68.46	5.67	5.99
86+87+97+109+119+125	88.49	Ķ□□□□	79.42	0.00	0.00
88+91	61.97	34.08	45.92	0.00	1.33
89	0.00	6.27	14.05	0.00	0.00
90+101+113	102.71	141.37	209.32	0.00	2.28
92	24.80	25.62	37.47	0.00	0.00
93+100	0.00	119.29	194.16	0.00	2.07
94	0.00	0.00	0.00	0.00	0.00
95	119.94	0.00	0.00	0.00	0.00
96	5.05	4.36	0.00	0.00	0.19
98+102	14.62	11.64	13.77	0.00	0.00
103	0.00	0.19	0.00	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	61.78	81.06	118.06	0.00	0.72
106	0.00	0.00	0.00	0.00	0.00
107	6.83	14.32	0.00	0.00	0.48
108+124	2.67	5.21	7.54	0.00	0.00
110+115	120.16	203.06	298.82	0.00	3.42
111	0.00	0.00	0.00	0.00	0.00
112	60.24	0.00	120.62	1.15	0.00
114	4.19	6.06	0.00	0.00	0.00
118	95.32	147.07	203.59	0.00	2.75
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.00	2.61	0.00	0.00	0.40
123	0.00	0.00	16.60	0.00	0.23
126	5.67	4.51	0.00	0.00	4.70
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	104.77	110.35	108.99	0.17	1.41
130	6.51	6.98	0.00	0.31	0.00
131	0.00	1.73	0.00	0.28	0.00
132	25.59	35.79	0.00	0.93	0.00
133	0.00	2.26	11.30	0.00	0.00

Table A-3 continued

Sample ID	**58-1** [a]	**58-2** [a]	**59**	**60-1** [a]	**60-2** [a]
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
134+143	6.06	5.26	5.55	0.00	0.00
135+151	30.65	34.46	34.70	0.33	0.00
136	0.00	12.68	0.00	0.16	0.00
137+164	12.66	19.67	9.11	0.22	0.00
139+140	0.00	1.32	0.00	0.18	0.00
141	18.71	22.04	38.18	0.45	0.00
142	0.00	0.00	1.88	0.00	0.00
144	4.34	4.56	17.11	0.06	0.00
145	12.41	0.00	14.92	0.00	0.00
146	12.24	13.17	0.00	0.13	0.00
147+149	74.48	80.27	78.65	0.90	0.82
148	0.00	0.00	5.97	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	12.68	0.09	0.00
153+168	75.86	82.68	75.22	0.00	0.00
154	0.00	0.47	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	19.37	10.66	15.22	8.68	9.74
158	9.84	9.73	10.02	0.00	0.00
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.37
165	0.00	0.00	0.00	0.00	0.00
167	5.00	3.89	5.62	0.00	0.00
169	2.51	1.38	0.00	0.00	0.00
170	30.09	26.91	29.68	0.47	0.37
171+173	12.29	10.37	7.39	0.27	0.47
172	6.32	5.30	0.00	0.03	0.00
174	34.98	34.58	0.00	0.29	0.00
175	0.00	1.60	0.00	0.00	0.00
176	3.00	4.77	0.00	0.00	0.00
177	17.12	19.79	16.62	0.50	0.00
178	5.65	6.03	0.00	0.24	0.23
179	9.33	12.87	13.32	0.03	0.31
180+193	65.81	73.07	57.26	0.62	0.20
181	0.00	0.00	1.98	0.45	0.18
182	0.00	0.00	0.00	0.08	1.22
183	17.97	19.25	19.42	0.16	0.12
184	0.00	0.00	0.00	0.08	0.00
185	0.00	0.00	26.84	0.00	0.00
186	0.00	0.00	0.00	0.00	0.12
187	39.85	39.62	33.24	0.96	0.24
188	0.00	0.00	0.00	0.11	0.06
189	0.00	0.83	0.00	0.00	0.00
190	8.39	6.37	3.67	0.28	0.00
191	0.00	1.10	0.00	0.11	0.00
192	0.00	0.00	0.00	0.14	0.48
194	19.98	13.04	11.47	0.00	0.73
195	8.23	5.89	7.36	0.00	0.00
196	7.58	8.23	0.00	0.00	0.00
197	0.00	0.00	9.01	0.00	0.00
198+199	18.75	18.57	0.00	0.00	0.00
200	0.00	3.46	0.00	0.00	0.00

Table A-3 continued

Sample ID	**58-1** [a]	**58-2** [a]	**59**	**60-1** [a]	**60-2** [a]
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
201	0.00	1.97	0.00	0.00	0.00
202	2.82	4.33	0.00	0.00	0.00
203	8.81	10.30	7.32	0.00	0.00
205	0.00	0.69	0.00	0.00	0.41
206	8.06	5.42	5.50	0.50	0.27
207	0.00	0.87	0.00	0.04	0.00
208	0.00	2.47	0.00	0.00	0.00
209	2.75	1.86	1.86	0.33	0.47
Total	**6472.92**	**7280.23**	**8733.99**	**119.55**	**157.96**

[a] Duplicates were from the same homogenized sediment sample but extracted and reanalyzed more than once.

[b] Total organic carbon (%) was measured in only one sample.

Table A-4 Concentration of PCB congeners in Standard Reference Material® 1944 (lab batch # SRM2)

Sample ID	**SRM1**	**SRM2**	**SRM3**	**SRM4**	**SRM5**	**SRM6**	**Arithmetic mean**	**Standard deviation**
PCB14 % recovery	85	120	104	108	113	126		
PCB65 % recovery	76	91	92	92	95	106		
PCB166 % recovery	73	72	72	76	69	79		
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng	100 ng		
Water content	1 %	1 %	1 %	1 %	1 %	1 %		
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
8	21.20	20.51	23.73	23.61	24.71	24.11	22.98	1.70
18	46.59	40.37	45.31	45.29	45.87	44.82	44.71	2.21
28	99.83	83.39	94.36	91.27	87.07	87.00	90.49	5.95
31	81.81	70.86	78.63	76.76	72.14	73.09	75.55	4.24
49	45.58	59.02	56.49	50.61	57.34	56.94	54.33	5.16
52	78.34	106.72	105.17	95.51	111.45	101.81	99.84	11.79
66	40.14	41.37	44.90	41.24	56.48	47.82	45.33	6.17
87	14.54	16.46	39.44	17.78	45.74	41.75	29.28	14.45
95	25.72	30.11	30.69	30.75	36.08	30.62	30.66	3.29
99	42.40	44.55	46.24	43.04	52.81	45.18	45.70	3.75
90+101	53.82	58.08	58.79	59.00	67.63	57.01	59.05	4.61
105	25.10	27.29	26.24	27.61	29.57	27.00	27.14	1.49
110	72.59	78.17	79.20	81.48	91.58	81.48	80.75	6.23
118	60.65	59.91	60.66	59.66	63.22	60.67	60.80	1.27
138+163+164	70.52	74.06	76.02	74.42	77.08	71.24	73.89	2.59
149	50.02	51.96	54.03	55.56	59.09	56.65	54.55	3.27
151	20.52	21.61	22.14	22.76	23.30	22.15	22.08	0.96
153	62.70	64.90	66.58	66.40	64.76	66.67	65.34	1.54
156	9.49	7.77	10.13	8.07	8.88	9.32	8.94	0.89
164	6.51	6.25	6.35	6.21	7.19	6.46	6.49	0.36
170	19.42	17.00	17.18	17.16	15.80	17.13	17.28	1.18
180	45.45	41.03	41.88	43.67	41.22	40.07	42.22	1.98
183	12.31	10.64	9.80	12.72	12.03	11.17	11.44	1.11
187	26.31	24.89	25.24	28.39	27.29	25.83	26.32	1.32
190	4.91	3.80	3.90	4.14	3.45	3.97	4.03	0.49
194	11.58	9.42	10.07	11.29	9.67	11.39	10.57	0.96
195	6.73	3.63	5.32	4.11	3.99	3.96	4.62	1.19
206	9.97	8.85	8.44	10.55	8.74	9.02	9.26	0.82
209	7.43	7.48	7.19	7.14	6.65	6.83	7.12	0.33

Figure A-2

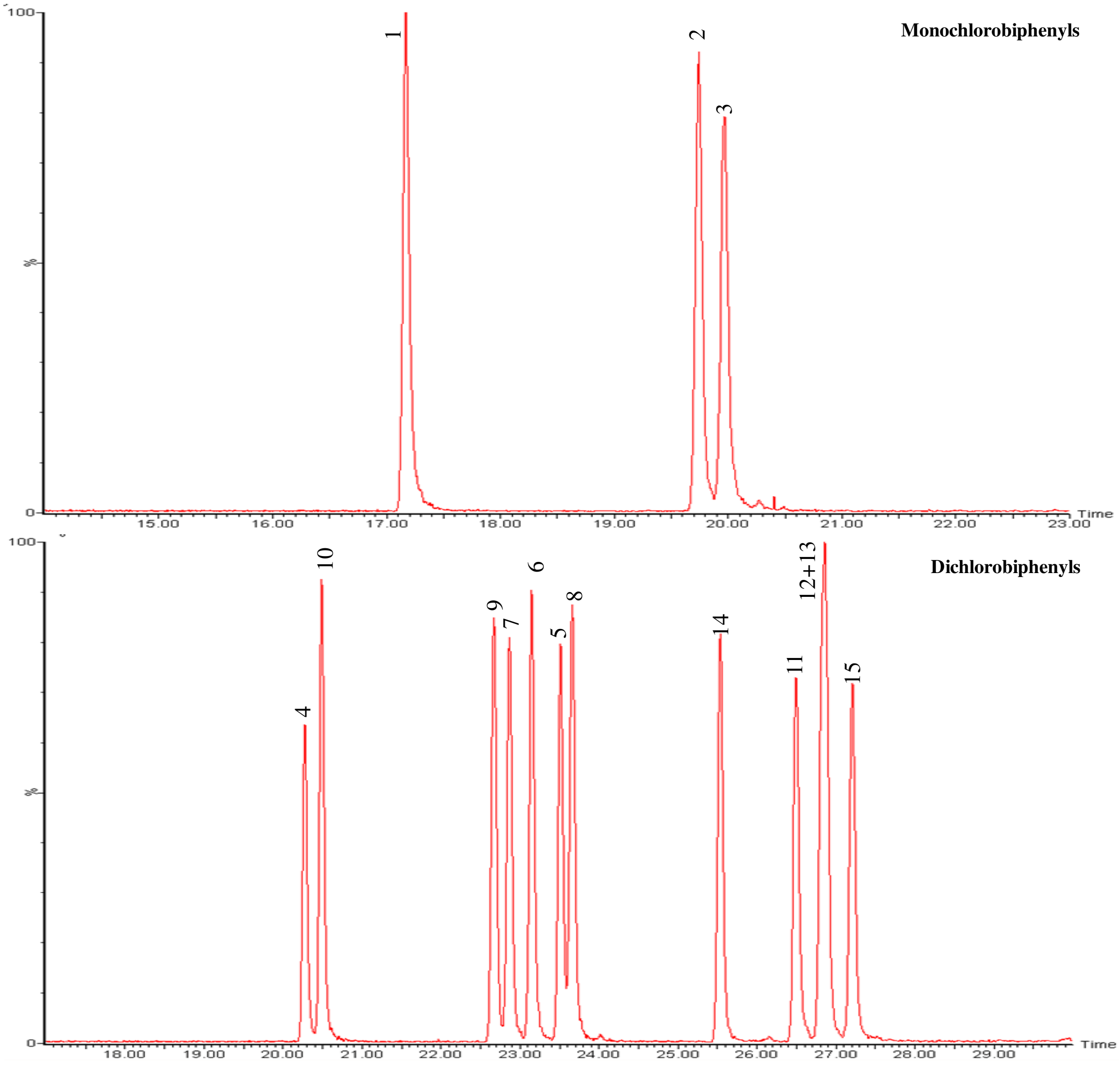


Figure A-2 Labeled chromatograms for 209 PCB congeners using GC/MS/MS (32). Chromatograms are divided into homolog groups (129)

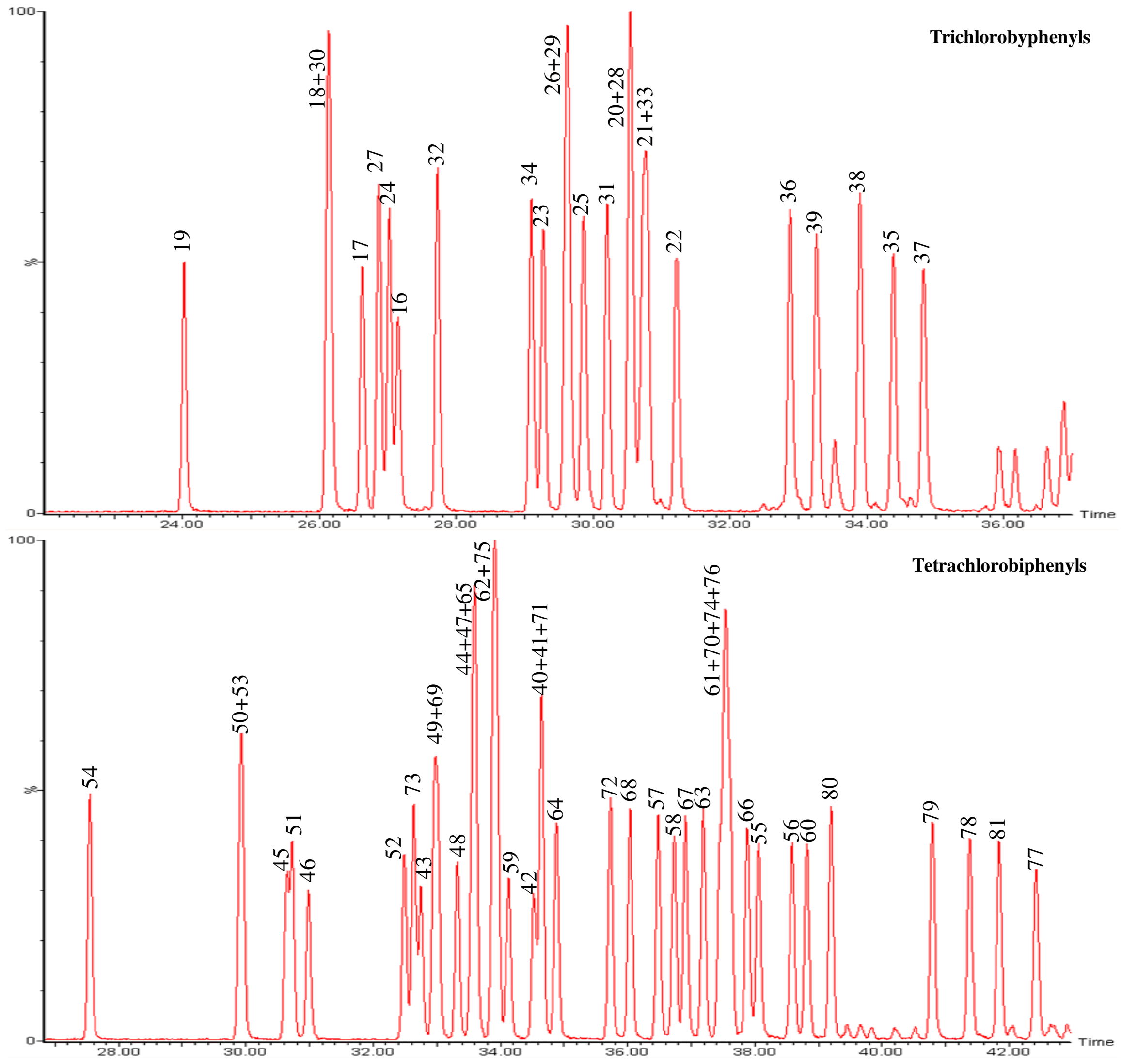


Figure A-2 continued

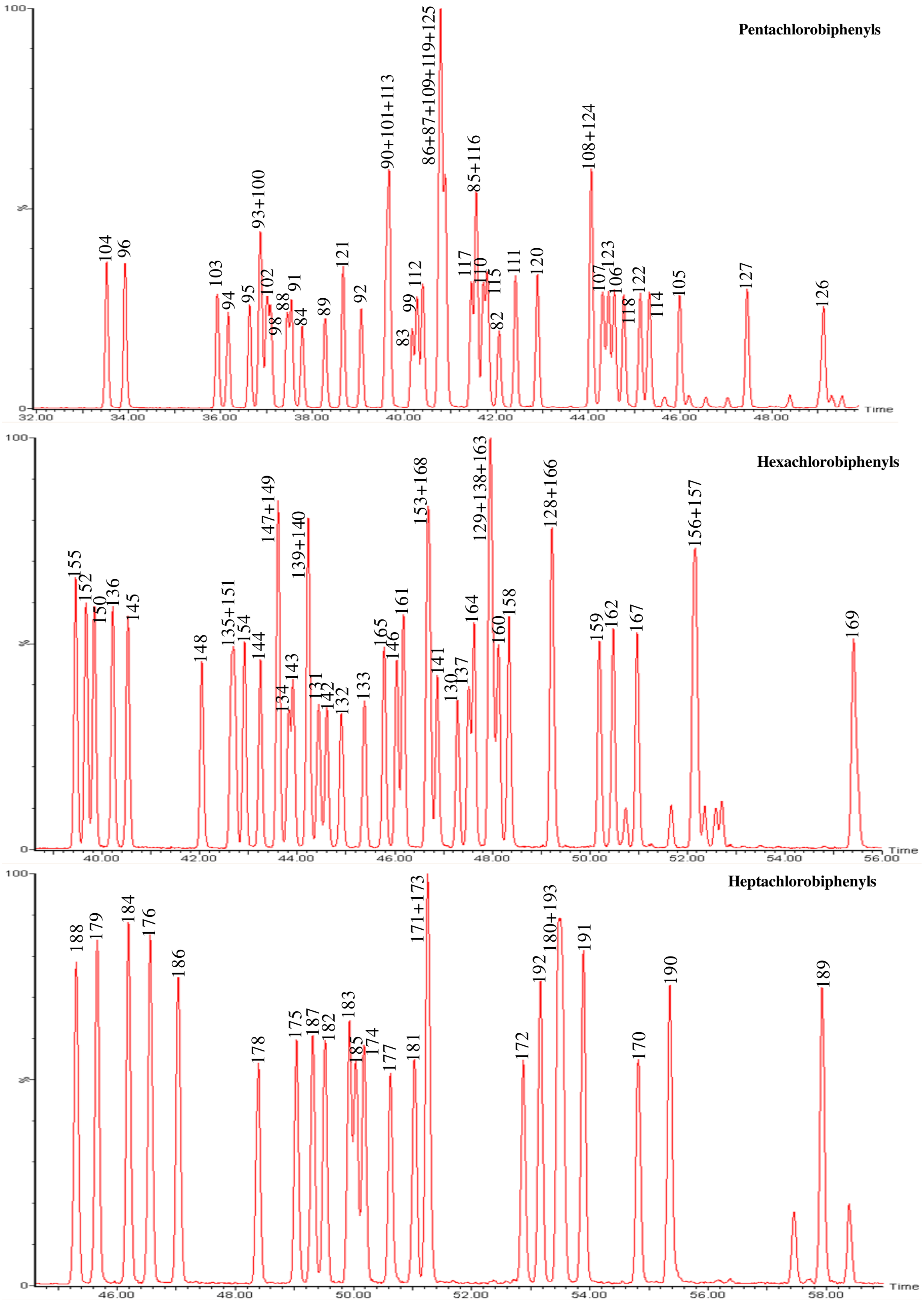


Figure A-2 continued

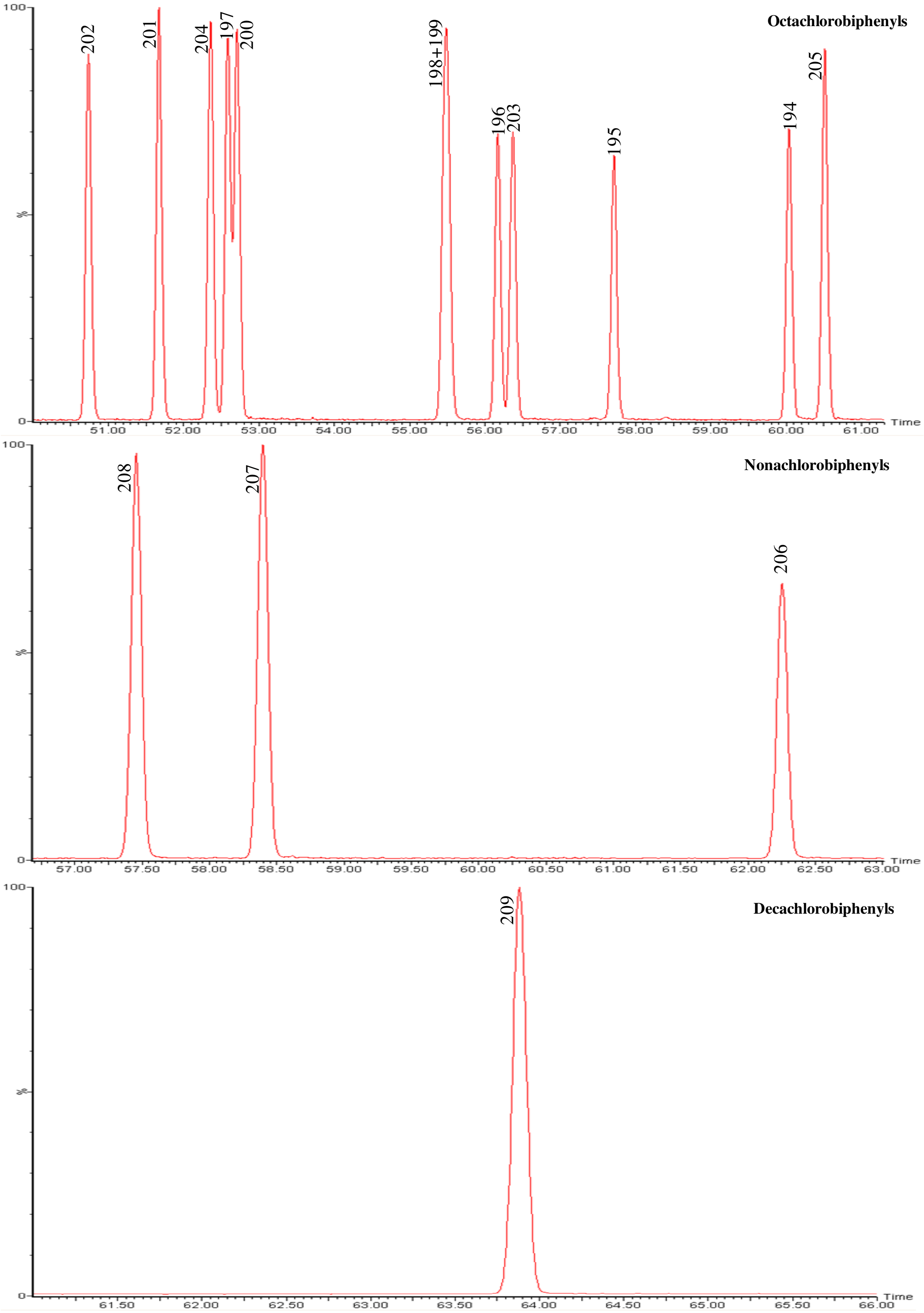


Figure A-2 continued

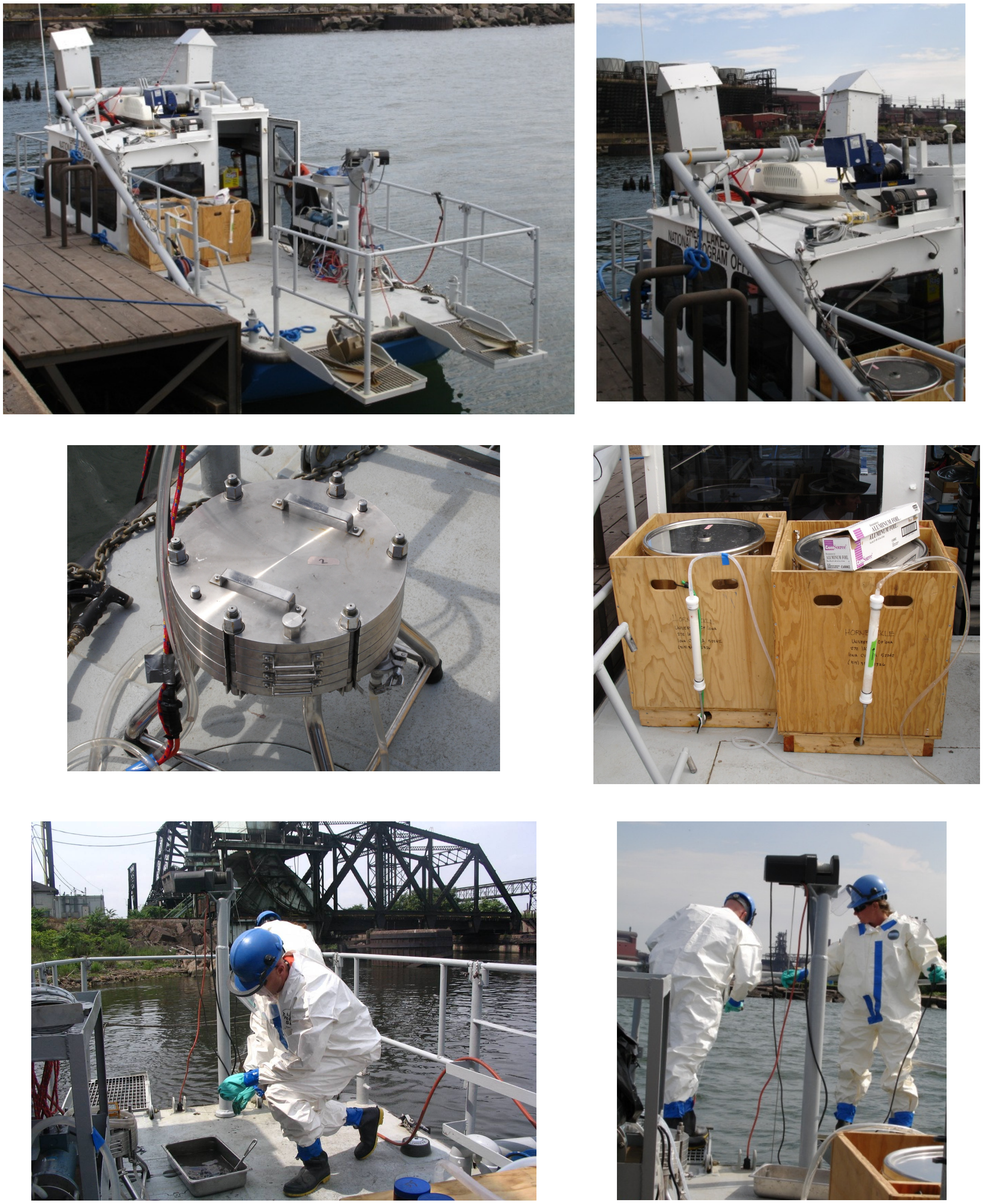


Figure A-3 Photographs of IHSC 2006 field campaign. Top photographs show U.S. Environmental Protection Agency's R/V Mudpuppy, and two high volumetric air samplers. Center left photograph shows the stainless steel pentaplate used to collect the suspended particulates in water. Center right photograph shows the glass columns packed with a water slurry of XAD-2 resin used to collect the dissolved phase in water. Bottom photographs show the surficial sediment collection

APPENDIX B: SUPPLEMENTAL INFORMATION CHAPTER III

Information Referenced in Chapter III: Sampling and Analytical Methods, QA/QC, Monte Carlo Parameters, Estimations and Assumptions, Mathematical Approach, Tables and Figures

Sampling Methods

Analytical Methods

Quality Assurance and Control

Monte Carlo parameters

Parameters estimation and Assumptions

Sediment-water

Air-water

Mathematical Approach

Definition of Terms

Table B-1 Sediment, dissolved-phase and gas phase concentrations of individual congeners measured in IHSC. These values were applied to the flux calculation and Monte Carlo simulation of the five day period in August 2006. Congeners are ordered by “IUPAC” nomenclature (2)

Table B-2 Summary of air gas phase and water dissolved and particulate for this study and other

Table B-3 Examples of arithmetic average of air-water and sediment-water parameters for PCB homolog groups calculated for the sampling period. Parameters were calculated using equations and constants described in Figure B-1, and the following environmental and hydraulic conditions. Homolog groups are ordered by “IUPAC” nomenclature (2)

Figure B-1 Equations developed for the fluxes calculations

Figure B-2 Total PCB concentrations measured in IHSC. Air n=16, dissolved-phase water n=10, suspended particulates water n=7 and sediment n=60. Asterisk (*) in the surficial sediment samples means that those samples are above the 95th percentile

Figure B-3 Congener profile distributions in the IHSC.The congeners in each sample was normalized to its total concentration, and the error bars represents one standard deviation about mean (sediment n=60, air gas phase n=16, suspended particulates water n=7 and dissolved-phase water n=10). Congeners are ordered by “IUPAC” nomenclature (2)

Sampling Methods

During the second week of August 2006, surficial sediment, water, and air were collected in IHSC from aboard the U.S. Environmental Protection Agency's R/V Mudpuppy. Surficial sediment samples were collected using a standard ponar dredge sampler (top 10 cm layer) as described previously (57). Water samples were collected using a submersible pump that pushed water from approximately 1 meter below the surface. The water was pushed at a rate of approximately 150 mL min-1 through a stainless steel pentaplate that held five 0.293 cm glass fiber filters (GFF) in parallel. The filtered water was collected in stainless steel tanks that were covered at the water surface by precleaned aluminum foil. The filtered water was then pulled at a rate of approximately 150 mL min-1 through 3 cm I.D. x 30 cm long glass columns packed with a water slurry of XAD-2 resin. An average volume of 30 L of water was collected in this manner at each of 10 sites. Air samples were collected using two high volumetric air samplers (Hi-Vol) mounted to the roof of the vessel. The Hi-Vols pulled air through a 20.3 cm x 25.4 cm GFF and then through 40 g XAD-2 resin at a rate of ~0.4 m^3 min^{-1}. QFF samples were archived and not used for this study. The samplers were operated continuously while water and sediment was being collected. The average sampling time for the air samples collected during the week was 7 hrs. In summary, this study collected 60 bulk sediment samples, 10 XAD water samples (operationally defined as dissolved-phase), 7 GFF water samples (operationally defined as suspended particles), and 17 XAD air samples (operationally defined as gas-phase), throughout the harbor and canal. In relation to the water samples, 4 samples were paired and 3 of suspended particles came from composite of 2 dissolved-phase samples.

Analytical Methods

Surficial sediment analysis is described in (57) and is briefly summarized here. Samples were dehydrated using combusted diatomaceous earth, then extracted with hexane in an accelerated solvent extraction (ASE 300, Dionex, Sunnyvale, CA). Prior to extraction, PCB14 (3,5-dichlorobiphenyl), PCB65 (2,3,5,6-tetrachlorabiphenyl) and PCB166 (2,3,4,4′,5,6-hexachlorobiphenyl) were injected and employed as surrogate standards. The resulting solution was again shaken with potassium hydroxide and sulfuric acid. The solution was then passed through Pasteur pipettes filled with combusted and acidified silica gel and eluted with hexane. The solution was reduced to approximately 0.5 mL and PCB204 (2,2′,3,4,4′,5,6,6′- octachlorobiphenyl) was spiked as internal standard.

XAD resin or fiber glass filters were extracted individually in a Soxhlet apparatus for 16 hrs using 500 mL of acetone/hexane (1:1 v/v) solution (58). Surrogate standards – PCB14, PCB65 and PCB166 – were spiked before extraction. Excess water and acetone was removed by liquid - liquid extraction. After concentration, the sample extract in hexane was eluted through Pasteur pipettes filled with combusted and acidified silica gel. The final 10 mL solution was again concentrated and PCB204 was spiked as internal standard.

Air samples were analyzed as described in Hu et al. (74). Briefly, samples were extracted in ASE 300 with acetone/hexane (1:1, v/v). Prior to extraction air samples were injected with surrogate standards PCB14, PCB65 and PCB166. The resulting extracts were further reduced to about 500 μL by a Turbovap concentration workstation, and the final solutions were injected with the internal standard PCB204.

Sediment, water, suspended water particles, and air samples were all analyzed for all 209 PCB congeners in 158 individual or coeluting congener using Tandem Mass Spectrometry GC/MS/MS (Quattro MicroTM GC, Micromass MS Technologies). The instrument was operated in multiple reaction monitoring mode (MRM) and we used the following pairs of parent/daughter ions to identify the PCBs: mono- to deca- homologs were 188/152, 117 222/152.10, 255.96/186, 291.92/222, 325.88/255.90, 359.84/289.90, 393.80/323.90, 118 427.76/357.80, 461.72/391.83, 497.68/427.70, respectively.

Quality Assurance and Control

Percentage recovery of PCB14 and PCB166 for gas phase samples were 60 ± 20% and 78 ±19%, respectively (n=16). Dissolved water samples yielded a percentage recovery of PCB14 and PCB166 of 59 ±12% and 76 ±12%, respectively (n=10). In the case of particulate in water, percentage recovery of PCB14 and PCB166 were 66 ±11% and 97 ±11%, respectively (n=7). Percentage recovery for sediment was 93 ±36% and 85 ±16% for PCB14 and PCB166, respectively (n=80). PCB65 acquired high values due to coelution issues and was not used for correction. Percentage recovery of PCB14 was used to correct mass congeners of PCB1 to PCB39 and PCB166 percentage recovery for PCB40 till PCB209. Field and lab blanks were analyzed. No mass correction was made from blanks, which were insignificant. In addition, Standard Reference Material 1944 was analyzed, showing acceptable results (57). Total organic carbon (TOC) was analyzed by Minnesota Valley Testing Laboratories. Inc (SW-846 Method SW 9060).

Monte Carlo parameters

The input parameters were wind speed (u_{10}), air (T_a) and water (T_w) temperatures, atmospheric pressure (P), water flow (Q), water depth of the canal (h), total organic carbon fraction (f_{oc}), air ($C_{PCBi\ a}$), water ($C_{PCBi\ w}$) and sediment ($C_{PCBi\ s}$) concentrations, Henry's law constant (HLC_{PCBi}) (3), octanol-water equilibrium coefficient ($K_{PCBi\ ow}$) (4), the parameters obtained from linear regressions use to calculate the internal energy for the transfer of water to air and octanol to air (5), and the parameters from the one-parameter linear free energy relationship (op-LFER) used to obtain the octanol-water equilibrium coefficients and the ($K_{PCBi\ oc}$) (66).

The frequency distribution for each parameter was determined as follows: histograms were plotted and the distribution was obtained for wind speed, air and water temperatures, atmospheric pressure, water flow and water depth of the canal. Total organic carbon fraction, air, water and sediment concentrations were considered as normal distribution. If the parameters were obtained from linear regressions such as the parameters obtained from linear regressions use to calculate the internal energy for the transfer of water to air and octanol to air, and the parameters from the one-parameter linear free energy relationship (op-LFER) used to obtain the octanol-water equilibrium coefficients and the ($K_{PCBi\ oc}$), the distribution was determined as normal and if the regression was logarithmic such as octanol-water equilibrium coefficient ($K_{PCBi\ ow}$) and Henry's law constant (HLC_{PCBi}), the distribution was considered lognormal. In summary, for this simulation, wind speed, HLC_{PCBi} and $K_{PCBi\ ow}$ were described as lognormal distribution and the rest of the parameters as normal distributions.

Parameters estimation and Assumptions

Sediment-water

We used the congener-specific $K_{PCBi\ ow}$ reported by Hawker and Connell (4) with water temperature correction from Goss (65) and Li et al. (5). The relationship between octanol-water equilibrium coefficients and the $K_{PCBi\ oc}$ controls the solid-water distribution coefficient which may vary with the quantity of the organic matter and the chemical nature of the organic matter (61). We used a one-parameter linear free energy relationship (op-LFER) developed by Nguyen et al. (66) to calculate $K_{PCBi\ oc}$ ($R^2 = 0.97$ and an absolute average value of the difference between measured and fitted values of 0.21). In addition, we estimated $K_{PCBi\ oc}$ (= C_{PCBi} particulate $\bullet foc^{-1} \bullet C_{PCBi\ \mathrm{dissolved}}^{-1}$) for each congener and compared with $K_{PCBi\ ow}$. We evaluated and found a weak relationship between both coefficients, suggesting that not all the organic carbon is acting as sorbent, i.e. presence of other types of carbons, kinetic problems (e.g. not at equilibrium), and presence of colloids in the dissolved measured phase (61, 63, 67). These findings do not significantly reduce the value of the model or our findings.

The mean flow velocity and mean hydraulic radius were calculated from the field conditions, i.e. flow, wide and water depth of the canal. The bioturbation component of the solubilization mass transfer coefficient was computed using values from literature, i.e.

bioturbated depth and biodiffusion coefficient from Erickson et al. (64) and the solids concentration of sediment from Birdwell and Thibodeaux (130).

Air-water

Diffusivity of PCBs in air was computed using water vapor as reference substance. Water vapor diffusivity was calculated as a function of air temperature and atmospheric pressure (61). Air exchange velocity for each congener was obtained from the ratio of PCB and water vapor diffusivity in air and the velocity of water in air, which is function of wind speed measured at 10 m above the water surface (61). One of the key parameters involved in the water exchange velocity calculation is the gas transfer velocity of CO_2 or k_{600} (k at 20°C in freshwater, i.e. k at a Schmidt number of 600). This parameter is not easy to measure or to estimate because it depends on the system (e.g. lakes, oceans, streams and estuaries), wind speed, rain fall, formation of thin layers and the roughness of the water surface (during sampling days the wind speed was narrow, ranging from 0 to 5.7 m s^{-1}). In the case of shallow stream and rivers, the k_{600} is influences by the stream depth and flow velocity, and not the wind speed (131, 132). Therefore, we employed that relationship to estimate the k_{600} for the different scenarios, as function of the stream depth and the flow velocity. The kinematic viscosity (i.e. viscosity to density ratio) was computed for each air and water temperature scenarios.

Table B-1 Sediment, dissolved-phase and gas phase concentrations of individual congeners measured in IHSC. These values were applied to the flux calculation and Monte Carlo simulation of the five day period in August 2006. Congeners are ordered by "IUPAC" nomenclature (2)

Congener	**Sediment Concentration (ng g^{-1} d.w.)**	**Dissolved-phase concentration (ng m^{-3})**	**Gas phase concentration (ng m^{-3})**
1	1.200	38.000	0.014
2	1.100	4.200	0.008
3	4.500	23.000	0.012
4	17.000	850.000	0.120
5	0.390	0.000	0.002
6	16.000	140.000	0.043
7	1.500	0.000	0.034
8	46.000	310.000	0.180
9	2.300	0.000	0.011
10	0.860	15.000	0.006
11	5.700	29.000	0.045
12+13	9.200	42.000	0.005
15	43.000	450.000	0.055
16	71.000	1200.000	0.140
17	85.000	1200.000	0.130
18/30	180.000	3400.000	0.310
19	19.000	710.000	0.052
20+28	340.000	2300.000	0.240
21+33	110.000	460.000	0.110
22	90.000	660.000	0.075
23	1.100	3.600	0.000
24	6.200	6.700	0.011
25	43.000	260.000	0.022
26+29	63.000	570.000	0.045
27	15.000	270.000	0.023
31	270.000	1800.000	0.220
32	80.000	1300.000	0.086
34	1.400	0.000	0.000
35	3.100	9.900	0.001
36	0.970	6.800	0.001
37	79.000	390.000	0.027
38	0.380	19.000	0.002
39	0.920	0.000	0.001
40+41+71	190.000	1400.000	0.079
42	120.000	630.000	0.040
43	14.000	87.000	0.004
45+51	110.000	950.000	0.050
46	29.000	320.000	0.012
48	72.000	380.000	0.032
49+69	240.000	1300.000	0.100
50+53	63.000	690.000	0.036
52	420.000	2700.000	0.220
54	0.580	0.000	0.000
55	29.000	0.000	0.002
56	140.000	580.000	0.028

Table B-1 continued

Congener	Sediment Concentration (ng g^{-1} d.w.)	Dissolved-phase concentration (ng m^{-3})	Gas phase concentration (ng m^{-3})
57	1.800	0.000	0.000
58	0.190	0.000	0.000
59+62+75	30.000	170.000	0.012
60	78.000	250.000	0.013
61+70+74+76	480.000	1300.000	0.150
63	13.000	8.800	0.001
64	160.000	1000.000	0.064
66	290.000	640.000	0.058
67	9.200	0.000	0.001
68	7.400	39.000	0.004
72	1.400	0.000	0.000
73	21.000	0.000	0.000
77	30.000	5.500	0.000
78	0.014	0.000	0.000
79	0.110	0.000	0.000
80	1.100	0.000	0.000
81	0.490	0.000	0.000
82	36.000	68.000	0.011
83+99	98.000	200.000	0.047
84	62.000	310.000	0.050
85+86+87+97+109+116+117+119+125	150.000	420.000	0.080
88+91	39.000	76.000	0.026
89	8.000	36.000	0.001
90+101+113	140.000	440.000	0.140
92	27.000	87.000	0.022
93+100	8.900	19.000	0.002
94	1.600	28.000	0.002
95	130.000	590.000	0.150
96	3.300	23.000	0.003
98+102	12.000	18.000	0.003
103	1.100	20.000	0.002
104	0.018	15.000	0.000
105	70.000	81.000	0.031
106	0.170	0.000	0.001
107	11.000	28.000	0.003
108+124	4.500	7.000	0.002
110+115	190.000	520.000	0.110
111	0.002	0.000	0.000
112	7.100	0.000	0.000
114	4.700	32.000	0.001
118	140.000	210.000	0.077
120	0.037	0.000	0.000
121	0.090	0.000	0.001
122	2.200	0.000	0.000
123	2.600	0.000	0.002
126	11.000	0.000	0.000
127	0.260	0.000	0.000
129+138+160+163	79.000	55.000	0.098
130	3.500	25.000	0.004
131	1.100	3.400	0.001

Table B-1 continued

Congener	**Sediment Concentration (ng g^{-1} d.w.)**	**Dissolved-phase concentration (ng m^{-3})**	**Gas phase concentration (ng m^{-3})**
132	25.000	65.000	0.039
133	0.890	0.000	0.001
134+143	2.300	57.000	0.007
135+151	26.000	35.000	0.049
136	11.000	22.000	0.026
137+164	8.900	2.600	0.007
139+140	2.000	0.000	0.002
141	15.000	0.000	0.023
142	0.810	2.600	0.001
144	3.800	22.000	0.007
145	1.300	0.000	0.000
146	11.000	27.000	0.011
147+149	63.000	95.000	0.110
148	0.110	0.000	0.000
150	0.013	5.200	0.000
152	2.400	8.000	0.001
153+168	59.000	48.000	0.093
154	0.310	2.700	0.001
155	0.001	4.600	0.000
156+157	7.100	0.000	0.012
158	7.600	2.700	0.008
159	0.900	0.000	0.000
161	0.250	0.000	0.000
162	0.270	0.000	0.000
165	0.009	0.780	0.001
167	1.800	2.500	0.001
169	1.000	0.000	0.000
170	19.000	14.000	0.008
171+173	6.500	11.000	0.006
172	3.200	38.000	0.004
174	19.000	40.000	0.028
175	0.340	15.000	0.004
176	2.400	30.000	0.006
177	13.000	20.000	0.017
178	3.800	24.000	0.007
179	9.500	53.000	0.021
180+193	45.000	46.000	0.029
181	0.062	45.000	0.004
182	0.031	9.700	0.002
183	10.000	40.000	0.020
184	0.068	26.000	0.004
185	2.500	30.000	0.004
186	0.420	19.000	0.002
187	29.000	66.000	0.040
188	0.032	29.000	0.001
189	0.220	0.000	0.004
190	3.200	13.000	0.000
191	0.320	19.000	0.001
192	0.380	50.000	0.000
194	10.000	3.500	0.003
195	3.000	0.000	0.000

Table B-1 continued

Congener	Sediment Concentration (ng g^{-1} d.w.)	Dissolved-phase concentration (ng m^{-3})	Gas phase concentration (ng m^{-3})
196	4.800	0.000	0.003
197	0.150	32.000	0.000
198+199	12.000	0.000	0.012
200	0.830	0.000	0.002
201	1.000	13.000	0.004
202	1.700	0.000	0.006
203	6.500	0.000	0.006
205	0.140	18.000	0.001
206	4.100	20.000	0.005
207	0.390	18.000	0.002
208	0.960	0.000	0.003
209	1.100	24.000	0.001

Table B-2 Summary of air gas phase and water dissolved and particulate for this study and other

Location	Air – gas phase (pg m^{-3})	Water – dissolved (ng L^{-1})	Water – particulate (ng L^{-1})	Ref.
IHSC (August, 2006)	1900 – 9000	10 - 70	11 - 36	(81)
IHSC (summers, 2003 – 2004)	190 - 310			(16)
Southern Baltic Sea (March, May, June, 1999)	10	0.008 – 0.016		(133)
New York – New Jersey Harbor Estuary (July, 1998)	1000 – 3100	1.4 – 4.2	2.3 – 5.2	(67)
IHSC (August, 1998)	1.34 – 1.61			(77)
Chicago (1996 – 2003)	100 – 9500			(134)
Southern Lake Michigan (May and July, 1994 and January, 1995)	132 – 1120	0.039 – 0.23		(68)
Green Bay (June to October, 1989)	250 - 2300	0.46 – 8	0.13 – 33.5	(63)

Table B-3 Examples of arithmetic average of air-water and sediment-water parameters for PCB homolog groups calculated for the sampling period. Parameters were calculated using equations and constants described in Figure B-1, and the following environmental and hydraulic conditions. Homolog groups are ordered by "IUPAC" nomenclature (2)

$T_w = 291.97$ K

$T_a = 296.78$ K

$P = 1018.77$ mbar

$u_{10} = 103{,}680$ (m day^{-1})

$Q = 18.97$ (m^3 s^{-1})

$h = 5$ (m)

$D_{water\ a} = 0.271$ (cm^2 s^{-1})

$D_{CO2\ w} = 0.0000162$ (cm^2 s^{-1})

$\nu_{water} = 0.0104$ (cm^2 s^{-1})

PCB homolog group	**Air-water exchange velocity**	**Schmidt number in water**	**Solid-water distribution coefficient corrected by water temperature**	**Benthic boundary layer coefficient**	**Solubilization mass transfer coefficient**
	$V_{PCBi\ a/w}$ (m day^{-1})	$Sc_{PCBi\ w}$	$K_{PCBi\ d}$ (L kg^{-1})	β_{PCBi} (m day^{-1})	$k_{f\ PCBi}$ (m day^{-1})
Monochlorobiphenyls	0.247	1330.000	0.268	0.268	0.001
Dichlorobiphenyls	0.237	1450.000	0.254	0.254	0.003
Trichlorobiphenyls	0.227	1550.000	0.242	0.242	0.008
Tetrachlorobiphenyls	0.213	1650.000	0.232	0.232	0.021
Pentachlorobiphenyls	0.200	1750.000	0.223	0.223	0.044

Table B-3 continued

PCB homolog group	**Air-water exchange velocity** $V_{PCBi\ a/w}$ **(m day^{-1})**	**Schmidt number in water** $Sc_{PCBi\ w}$	**Solid-water distribution coefficient corrected by water temperature** $K_{PCBi\ d}$ **(L kg^{-1})**	**Benthic boundary layer coefficient** β_{PCBi} **(m day^{-1})**	**Solubilization mass transfer coefficient** $k_{f\ PCBi}$ **(m day^{-1})**
Hexachlorobiphenyls	0.194	1840.000	0.216	0.216	0.073
Heptachlorobiphenyls	0.185	1930.000	0.210	0.210	0.110
Octachlorobiphenyls	0.164	2010.000	0.204	0.204	0.148
Nonachlorobiphenyls	0.158	2090.000	0.199	0.199	0.166
Decachlorobiphenyls	0.145	2160.000	0.194	0.194	0.178

$$F_{PCBi\,a/w} = V_{PCBi\,a/w} \times \left(C_{PCBi\,w} - C^{eq}_{PCBi\,w}\right)$$

$$C^{eq}_{PCBi\,w} = \left(\frac{C_{PCBi\,a}}{K_{PCBi\,a/w}}\right)$$

$$K_{PCBi\,a/w} = K_{PCBi\,a(T_a)/w(T_w)} = K_{PCBi\,(a/w)(T_w)} \times \frac{T_w}{T_a}$$

$$K_{PCBi\,(a/w)(T_w)} = K_{PCBi\,(a/w)(T_{std})} \times e^{\left(-\frac{\Delta U_{PCBi\,a/w}}{R} \times \left(\frac{1}{T_w} - \frac{1}{T_{std}}\right)\right)}$$

$$K_{PCBi\,(a/w)(T_{std})} = HLC_{PCBi} \times \left(\frac{1}{R \times T_{std}}\right)$$

$$HLC_{PCBi} = f($$

$$\frac{1}{V_{PCBi\,a/w}} = \left(\frac{1}{V_{PCBi\,w}}\right) + \left(\frac{1}{V_{PCBi\,a} \times K_{PCBi\,a/w}}\right)$$

$$V_{PCBi\,w} = V_{CO_2} \times \left(\frac{Sc_{PCBi\,w}}{Sc_{CO_2 w}}\right)^{-0.5} \times \left(0.24 \frac{h\,m}{day\,cm}\right)$$

$$Sc_{PCBi\,w} = \left(\frac{\nu_{water}}{D_{PCBi\,w}}\right)$$

$$D_{PCBi\,w} = D_{CO_2\,w} \times \left(\frac{MW_{PCBi}}{MW_{CO_2}}\right)^{-0.5}$$

$$D_{CO_2\,w} = f($$

$$\nu_{water} = f(T_w)$$

$$V_{CO_2} = 1.72 \times \left(\frac{\nu_x}{h}\right)^{0.5}$$

$$\nu_x = \frac{Q}{A} \times \left(100 \frac{cm}{m}\right)$$

$$A = w \times h$$

$$Sc_{CO_2\,w} = \left(\frac{\nu_{water}}{D_{CO_2\,w}}\right)$$

$$V_{PCBi\,a} = V_{water\,a} \times \left(\frac{D_{PCBi\,a}}{D_{water\,a}}\right)^{0.67}$$

$$D_{PCBi\,a} = D_{water\,a} \times \left(\frac{MW_{PCBi}}{MW_{water}}\right)^{-0.5}$$

$$D_{water\,a} = f(T_a, P)$$

$$V_{water\,a} = 0.2 \times u_{10} + 0.3$$

Figure B-1 Mathematical Approach. Equations developed for the fluxes calculations

Air-water exchange equations.

$$F_{PCBi\;w/s} = k_{f\;PCBi} \times \left(C_{PCBi\;pw} - C_{PCBi\;w}\right)$$

$$C_{PCBi\;pw} = \left(\frac{C_{PCBi\;s}}{K_{PCBi\;d(T_w)}}\right) \times \left(10^6 \frac{g\;L}{kg\;m^3}\right)$$

$$K_{PCBi\;d(T_w)} = f_{oc} \times K_{PCBi\;oc\;(T_w)}$$

$$\log\left(K_{PCBi\;oc(T_w)}\right) = a \times \log\left(K_{PCBi\;ow(T_w)}\right) - b$$

$$K_{PCBi\;ow(T_w)} = K_{PCBi\;ow(T_{std})} \times e^{\left(-\frac{\Delta U_{PCBi\;ow}}{R} \times \left(\frac{1}{T_w} - \frac{1}{T_{std}}\right)\right)}$$

$$K_{PCBi\;ow(T_{std})} = f(PCB_i)$$

$$K_{f\;PCBi} = \left(\frac{1}{\frac{1}{\beta_{PCBi}} + \frac{z}{D_b \times K_{PCBi\;oc(T_w)} \times f_{oc} \times \rho}}\right)$$

$$\beta_{PCBi} = \left(\frac{0.114 \times \upsilon}{\left(Sc_{PCBi\;w}\right)^{2/3}}\right)$$

$$\upsilon = \frac{v_x \times n}{\left(r_H\right)^{2/3}} \times \sqrt{h \times g}$$

$$v_x = \frac{Q}{A}$$

$$A = w \times h$$

$$r_H = \frac{A}{P_w}$$

$$P_w = w + 2h$$

$$Sc_{PCBi\;w} = \left(\frac{\nu_{water}}{D_{PCBi\;w}}\right)$$

$$D_{PCBi\;w} = D_{CO_2\;w} \times \left(\frac{MW_{PCBi}}{MW_{CO_2}}\right)^{-0.5}$$

$$D_{CO_2\;w} = f(T_w)$$

$$\nu_{water} = f(T_w)$$

$$\log\left(K_{PCBi\;oc(T_w)}\right) = a \times \log\left(K_{PCBi\;ow(T_w)}\right) - b$$

$$K_{PCBi\;ow(T_w)} = K_{PCBi\;ow(T_{std})} \times e^{\left(-\frac{\Delta U_{PCBi\;ow}}{R} \times \left(\frac{1}{T_w} - \frac{1}{T_{std}}\right)\right)}$$

$$K_{PCBi\;ow(T_{std})} = f(PCB_i)$$

Figure B-1 continued

Sediment-water exchange equations

Definition of Terms

The equations in the top half of Figure B-1depict the equations used for the air-water PCB exchange model. The equations in the bottom half depict the equations used for the sediment-water exchange model. The definitions and sources of parameters are defined as follows:

$F_{PCBi\ a/w}$ is the flux between air and water for the ith PCB (ng m^{-2} day^{-1}) (61).
$C_{PCBi\ w}$ is the concentration in the water column for the ith PCB (ng m^{-3}).
$C^{eq}_{PCBi\ w}$ is concentration in water in equilibrium with the gas phase for the ith PCB (ng m^{-3}).
$V_{PCBi\ a/w}$ is the air –water exchange velocity of the ith PCB (m day^{-1}) (61).
$C_{PCBi\ a}$ is the concentration in the gas phase for the ith PCB (ng m^{-3}).
$K_{PCBi\ a/w}$ or $K_{PCBi\ a(Ta)/w(Tw)}$ is the temperature corrected nondimensional Henry's law constant of the ith PCB (3, 5, 65).
T_w is the water temperature (K).
T_a is the air temperature (K).
$K_{PCBi\ a/w(Tw)}$ is the nondimensional Henry's law constant of the ith PCB corrected by water temperature (65).
$K_{PCBi\ a/w(Tstd)}$ is the nondimensional Henry's law constant of the ith PCB at standard temperature (3).
$\Delta U_{PCBi\ a/w}$ is the internal energy for the transfer of water to air transfer for the ith PCB (J mol^{-1}) (5).
R is the ideal gas constant (8.3144 J mol^{-1} K^{-1} or 8.3144 Pa m^3 mol^{-1} K^{-1}).
T_{std} is the standard temperature (298.15 K).
HLC_{PCBi} is the Henry's law constant for the ith PCB (Pa m^3 mol^{-1}) (3).
$V_{PCBi\ a}$ is the air exchange velocity of the ith PCB (m day^{-1}) (61).
$V_{water\ a}$ is the water vapor exchange velocity in air (m day^{-1}) (61).
$D_{PCBi\ a}$ is the diffusivity in air for the ith PCB (cm^2 s^{-1}) (61).
$D_{water\ a}$ is the water diffusivity in air corrected by air temperature and atmospheric pressure (cm^2 s^{-1}) (61).
P is the atmospheric pressure (mbar).
MW_{PCBi} is the molecular weight for the ith PCB (g mol^{-1}).
MW_{CO2} is the molecular weight of CO_2 (44.0094 g mol^{-1}).
u_{10} is the wind speed measured at 10 above the water surface (m day^{-1}).
$V_{PCBi\ w}$ is the water exchange velocity of the ith PCB (m day^{-1}) (61).
V_{CO2} or k_{600} is the CO_2 gas transfer velocity in water (cm h^{-1}) (131, 135, 136).
$Sc_{PCBi\ w}$ is the Schmidt number in water for the ith PCB (61).
$Sc_{PCBi\ CO2\ w}$ is the Schmidt number in water for CO_2 (61).
ν_{water} is the kinematic viscosity of water corrected by water temperature (cm^2 s^{-1}).
$D_{PCBi\ w}$ is the diffusivity in the water for the ith PCB (cm^2 s^{-1}) (61).
$D_{CO2\ w}$ is the CO_2 diffusivity in water corrected by water temperature (cm^2 s^{-1}) (137).
ν_x is the flow velocity (cm s^{-1}).
h is the water depth (m).

Q is the water flow ($m^3\ s^{-1}$).
w is the wide of the canal (75 m).
A is the sectional canal area (m^2).

$F_{PCBi\ w/s}$ is the flux between water and sediment for the ith PCB (ng m^{-2} day^{-1}) (62).
$k_{f\ PCBi}$ is the sediment/water mass transfer coefficient for the ith PCB (m day^{-1}) (62).
$C_{PCBi\ pw}$ is the porewater concentration in the sediment for the ith PCB (ng m^{-3}).
$C_{PCBi\ w}$ is the concentration in the water column for the ith PCB (ng m^{-3}).
$C_{PCBi\ s}$ is the sediment concentration for the ith PCB (ng g^{-1} d.w.).
$K_{PCBi\ d}$ or $K_{PCBi\ d(Tw)}$ is the solid-water distribution coefficient corrected by water temperature for the ith PCB (L kg^{-1}) (61).
foc is the organic carbon fraction (kg oc kg^{-1}).
$K_{PCBi\ oc\ (Tw)}$ is the organic carbon base partition coefficient corrected by water temperature for the ith PCB (L kg^{-1} oc) (66).
a is 0.94 ± 0.02 (66).
b is -0.42 ± 0.12 (66).
$K_{PCBi\ ow\ (Tw)}$ is the octanol-water partition coefficient corrected by water temperature for the ith PCB (L kg^{-1}) (5, 65).
$K_{PCBi\ ow\ (Tstd)}$ is the octanol-water partition coefficient at standard temperature for the ith PCB (Lkg^{-1}) (4).
$\Delta U_{PCBi\ o/w}$ is the internal energy for the transfer of octanol-water for the ith PCB (J mol^{-1}) (5).
R is the ideal gas constant (8.3144 J mol^{-1} K^{-1} or 8.3144 Pa m^3 mol^{-1} K^{-1}).
T_w is the water temperature (K).
T_{std} is the standard temperature (298.15 K).
β_{PCBi} is the benthic boundary layer coefficient for the ith PCB (m day^{-1}) (64).
z is the bioturbated depth (0.1 m) (64).
D_b is the biodiffusion coefficient (3.36×10^{-7} m^2 day^{-1}) (64).
ρ is the solids concentration of sediment (0.6 kg L^{-1}) (130).
ν is the water-to-bed friction velocity (m day^{-1}) (62).
ν_x is the flow velocity (m s^{-1}).
n is the coefficient of roughness (0.025 s $m^{-0.33}$) (62).
r_H is the mean hydraulic radius (m).
h is the water depth (m).
g is the gravitational acceleration constant (847,324.8 m day^{-2}).
Q is the water flow ($m^3\ s^{-1}$).
A is the sectional canal area (m^2).
P_w is the wet perimeter (m).
w is the wide of the canal (75 m).
$Sc_{PCBi\ w}$ is the Schmidt number in water for the ith PCB (61).
v_{water} is the kinematic viscosity of water corrected by water temperature ($cm^2\ s^{-1}$).
$D_{PCBi\ w}$ is the diffusivity in the water for the ith PCB ($cm^2\ s^{-1}$) (61).
$D_{CO2\ w}$ is the CO_2 diffusivity in water corrected by water temperature ($cm^2\ s^{-1}$) (137).
MW_{PCBi} is the molecular weight for the ith PCB (g mol^{-1}).
MW_{CO2} is the molecular weight of CO_2 (44.0094 g mol^{-1}).

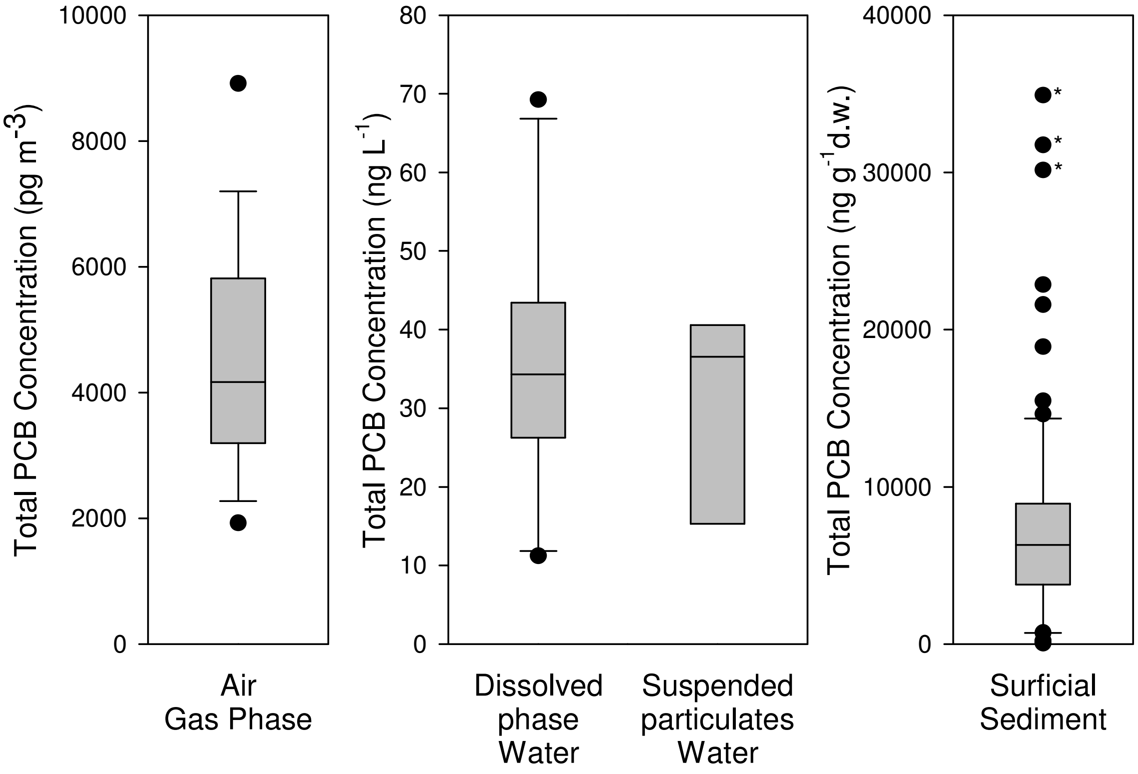


Figure B-2 Total PCB concentrations measured in IHSC. Air n=16, dissolved-phase water n=10, suspended particulates water n=7 and sediment n=60. Asterisk (*) in the surficial sediment samples means that those samples are above the 95th percentile

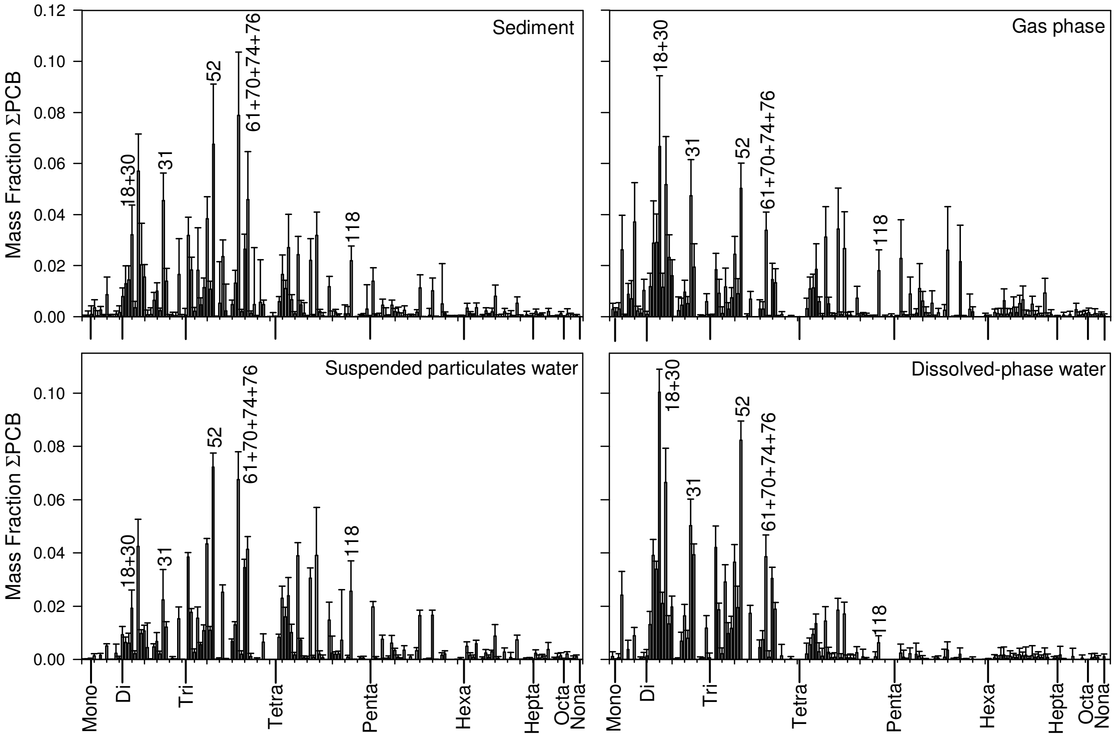


Figure B-3 Congener profile distributions in the IHSC.The congeners in each sample was normalized to its total concentration, and the error bars represents one standard deviation about mean (sediment n=60, air gas phase n=16, suspended particulates water n=7 and dissolved-phase water n=10). Congeners are ordered by “IUPAC” nomenclature (2)

Additional Information: PCB Release Model in Computer R Program and PCB Water Concentration Comparison, Sample Concentrations and Field Photographs

Release of PCB model in computer R program for sediment-water and air-water emissions.

Table B-4 Summary of dissolved phase and suspended particulates concentrations of PCBs in water in different studies

Table B-5 Concentration of PCB congeners in air gas phase, suspended particulates in water and dissolved-phase water IHSC

Figure B-4 Photographs of IHSC 2009 field campaign

Release of PCB model in computer R program for sediment-water emissions for 2006.

```
###### BEGIN OF FUNCTION DEFINITION ######

DeltaUaw = function(a1, MW.PCB, b1, nOrtho.Cl, c1)
{
(a1*MW.PCB-b1*nOrtho.Cl+c1)*1000
}
DeltaUoa = function(a2, MW.PCB, b2, nOrtho.Cl, c2)
{
(-a2*MW.PCB+b2*nOrtho.Cl-c2)*1000
}
Hoff = function(K, DeltaUow, R, T, T.water)
{
K*exp((-DeltaUow/R)*(1/(T.water+273.15)-1/T))
}
Isotherm = function(K, a, b)
{
10^(a*log10(K)+b)
}
Korgcorr = function(K, foc)
{
K*foc
}
dens.water = function(T.water)
{
(999.83952+16.945176*T.water-7.9870401*10^-3*T.water^2-46.170461*10^-6*3+105.56302*10^-9*T.water^4-280.54253*10^-12*T.water^5)/(1+16.87985*10^-3*T.water)
}
visc.water = function(T.water)
{
10^(-4.5318-220.57/(149.39-(273.15+T.water)))
}
diff.co2 = function(T.water, R)
{
0.05019*exp(-19.51*1000/(273.15+T.water)/R)
}
Area = function(w, h)
{
w*h
}
Pw = function(w, h)
{
w+2*h
}
Flow.veloc = function(Q, w, h)
{
Q/(w*h)
}
Rh = function(w, h)
{
w*h/(w+2*h)
}
###### END OF FUNCTION DEFINITION ######
```

```
final.result = function(MW.PCB, C.PCB.water.mean, C.PCB.water.error, Kow.mean, Kow.error,
C.PCB.sed.mean, C.PCB.sed.error, nOrtho.Cl, month)
{
# fixed parameters
R = 8.3144
T = 298.15
w = 75
Dens = 600
z = 10
Db = 0.00336

# random parameters

a1 = rnorm(1, 0.085, 0.007)
b1 = rnorm(1, 1, 0.5)
c1 = rnorm(1, 32.7, 1.6)
a2 = rnorm(1, 0.13, 0.02)
b2 = rnorm(1, 2.9, 1.2)
c2 = rnorm(1, 47.8, 4.3)
Kow = 10^(rnorm(1, Kow.mean, Kow.error))
a = rnorm(1, 0.94, 0.02)
b = rnorm(1, -0.42, 0.12)
foc = rnorm(1, 0.045626667, 0.04562667*0.0026)

#monthly average

C.PCB.water = rnorm(1, C.PCB.water.mean, C.PCB.water.error)

C.PCB.sed = rnorm(1, C.PCB.sed.mean, C.PCB.sed.error)

Q.mean = c(17.2243, 15.93786, 17.31477, 17.42189, 16.08166, 16.003259, 16.9457, 18.55552, 20.26576,
17.7212, 15.15944, 19.3873)
Q.std = c(1.78392, 1.707272, 2.364523, 2.2850749, 1.50133, 1.84128, 2.65936, 3.185998, 4.78462,
3.54723, 2.2289, 7.1914)
Q = rnorm(1, Q.mean[month], Q.std[month])

h.mean = c(4.8617, 4.8898, 4.922, 5.03, 5.084, 5.139, 5.0997, 5.1258, 5.0456, 4.92369, 4.9193, 4.958)
h.std = c(0.079303, 0.092714, 0.058335, 0.073527, 0.051346, 0.040321, 0.041799, 0.050175, 0.090437,
0.10298, 0.119287, 0.059161)
h = rnorm(1, h.mean[month], h.std[month])

T.water.mean = c(5.34, 5.42, 5.19, 8.69, 11.38, 15.09, 18.67, 19.45, 19.00, 15.81, 11.15, 7.43)
T.water.std = c(0.53, 0.98, 0.93, 1.17, 1.03, 1.30, 1.38, 1.06, 0.5, 1.58, 1.34, 0.97)
T.water = rnorm(1, T.water.mean[month], T.water.std[month])

# computed values

DeltaUow = DeltaUaw(a1, MW.PCB, b1, nOrtho.Cl, c1)+DeltaUoa(a2, MW.PCB, b2, nOrtho.Cl, c2)

K = Kow
K.sed.water = Hoff(K, DeltaUow, R, T, T.water)
K.Iso = Isotherm(K.sed.water, a, b)
Kd = Korgcorr(K.Iso, foc)

D.PCB.water = diff.co2(T.water, R)*(MW.PCB/44.0094)^(-0.5)
V = Flow.veloc(Q, w, h)*0.025*(Rh(w, h))^(-2/3)*(h*100*980.7)^0.5
```

```
v.water = visc.water(T.water)/dens.water(T.water)*10000
Sc.PCB.water = v.water/D.PCB.water

Beta = V*0.114*3600*24/(Sc.PCB.water)^(2/3)
Kf = 1/(1/Beta+z/(Db*Kd*Dens/1000))

F.PCB.sw = Kf*10*(C.PCB.sed*1000/Kd-C.PCB.water)

E.PCB.sw = F.PCB.sw*10^-9*30*1283836.2     #g/year

E.PCB.sw

}

single.month = function(pars, month)
{
Congener = pars$Congener
MW.PCB = pars$MW.PCB
C.PCB.water.mean = pars$C.PCB.water
C.PCB.water.error = pars$X.1
Kow.mean = pars$Kow
Kow.error = pars$X.3
C.PCB.sed.mean =pars$C.PCB.sed
C.PCB.sed.error = pars$X.4
nOrtho.Cl = pars$nOrtho.Cl

final.result(MW.PCB[i], C.PCB.water.mean[i], C.PCB.water.error[i], Kow.mean[i], Kow.error[i],
C.PCB.sed.mean[i], C.PCB.sed.error[i], nOrtho.Cl[i], month)
}

result.congener = NULL
for (i in 1:158)
{
result.E = NULL
for (replicate in 1:2500)
{
print(c(i, replicate))
        E = 0
        for (month in 1:12)
        {
        pars = read.csv(paste("H:/UIowa/Research/Model/Simulation/Annual variables per
        congener/Variables per congener ", month, ".csv", sep=""))
        E = E + single.month(pars, month)
        }
        result.E = c(result.E, E)
}
mmm = mean(result.E)
sss = sd(result.E)
result.congener = rbind(result.congener, c(i, mmm, sss, mmm-1.96*sss, mmm+1.96*sss))
}

end.result = data.frame(result.congener)
names(end.result) = c("Congener.ID", "Mean", "Std", "Lower Bound", "Upper Bound")
write.csv(end.result, row.names=FALSE, quote=FALSE,
file="H:/UIowa/Research/Model/Simulation/Sediment_water/All/Annual/result.csv")
```

Fate PCB model in computer R program for air-water emissions for 2006.

```
###### BEGIN OF FUNCTION DEFINITION ######

Delta = function(a, MW.PCB, b, nOrtho.Cl, c)
{
(a*MW.PCB-b*nOrtho.Cl+c)*1000
}
Hoff = function(K, DeltaUaw, R, T, T.water)
{
K*exp(-DeltaUaw/R*(1/(T.water+273.15)-1/T))
}
Hoff2 = function(K, T.air, T.water)
{
K*T.water/T.air
}
diff.water = function(T.air, P)
{
10^(-3)*1013.25*((273.15+T.air)^1.75*((1/28.97)+(1/18.0152))^(0.5))/P/(20.1^(1/3)+9.5^(1/3))^2
}
dens.water = function(T.water)
{
(999.83952+16.945176*T.water-7.9870401*10^-3*T.water^2-46.170461*10^-6*3+105.56302*10^-
9*T.water^4-280.54253*10^-12*T.water^5)/(1+16.87985*10^-3*T.water)
}
visc.water = function(T.water)
{
10^(-4.5318-220.57/(149.39-(273.15+T.water)))
}

diff.co2 = function(T.water, R)
{
0.05019*exp(-19.51*1000/(273.15+T.water)/R)
}
###### END OF FUNCTION DEFINITION ######

final.result = function(MW.PCB, H0.mean, H0.error, C.PCB.water.mean, C.PCB.water.error,
C.PCB.air.mean, C.PCB.air.error, nOrtho.Cl, month)
{
# fixed parameters
R = 8.3144
T = 298.15

# random parameters

a = rnorm(1, 0.085, 0.007)
b = rnorm(1, 1, 0.5)
c = rnorm(1, 32.7, 1.6)
H0 = 10^(rnorm(1, H0.mean, H0.error))

#monthly average

C.PCB.water = rnorm(1, C.PCB.water.mean, C.PCB.water.error)

C.PCB.air = rnorm(1, C.PCB.air.mean, C.PCB.air.error)
```

```
P.mean = c(1013.7, 1017.83, 1019.07, 1014.56, 1012.18, 1017.27, 1016.32, 1016.99, 1015.17, 1014.84,
1018.90, 1020.36)
P.std = c(9.47, 8.72, 9.32, 6.01, 6.60, 2.89, 3.85, 3.57, 5.34, 7.70, 7.23, 8.30)
P = rnorm(1, P.mean[month], P.std[month])

u.mean = c(3.95, 3.77, 4.41, 4.15, 3.16, 3.31, 2.99, 3.19, 3.03, 3.66, 3.78, 3.79)
u.std = c(2.05, 2.01, 2.71, 2.79, 1.95, 2.13, 1.87, 2.20, 1.86, 2.28, 2.68, 2.27)
u = 10^(rnorm(1, u.mean[month], u.std[month]))

T.water.mean = c(5.34, 5.42, 5.19, 8.69, 11.38, 15.09, 18.67, 19.45, 19.00, 15.81, 11.15, 7.43)
T.water.std = c(0.53, 0.98, 0.93, 1.17, 1.03, 1.30, 1.38, 1.06, 0.5, 1.58, 1.34, 0.97)
T.water = rnorm(1, T.water.mean[month], T.water.std[month])

T.air.mean = c(2.63, -1.28, 3.65, 11.45, 14.72, 19.28, 24.29, 23.05, 17.64, 10.51, 7.03, 1.93)
T.air.std = c(3.42, 4.96, 5.06, 5.42, 6.05, 4.40, 3.74, 3.11, 3.93, 5.70, 4.75, 5.81)
T.air = rnorm(1, T.air.mean[month], T.air.std[month])

# computed values

DeltaUaw = Delta(a, MW.PCB, b, nOrtho.Cl, c)

K = H0*101325/(R*T)
K.air.water = Hoff(K, DeltaUaw, R, T, T.water)
K.final = Hoff2(K.air.water, T.water, T.air)

D.PCB.air = diff.water(T.air, P)*(MW.PCB/18.0152)^(-0.5)
V.water.air = 0.2*u +0.3
V.PCB.air = V.water.air*(D.PCB.air/diff.water(T.air, P))^(2/3)

v.water = visc.water(T.water)/dens.water(T.water)*10000
D.PCB.water = diff.co2(T.water, R)*(MW.PCB/44.0094)^(-0.5)
Sc.PCB.water = v.water/D.PCB.water
V.PCB.water = 0.001389*(Sc.PCB.water/600)^(-0.5)

F.PCB.aw = 100^2*((1/V.PCB.water+1/(V.PCB.air*K.final))^(-1)*(C.PCB.water-
C.PCB.air/K.final/10^6))*3600*24/1000

E.PCB.aw = F.PCB.aw*10^-9*30*1283836.2  #g/year

E.PCB.aw
}

single.month = function(pars, month)
{
Congener = pars$Congener
MW.PCB = pars$MW.PCB
H0.mean = pars$H0
H0.error = pars$X
C.PCB.water.mean = pars$C.PCB.water
C.PCB.water.error = pars$X.1
C.PCB.air.mean = pars$C.PCB.air
C.PCB.air.error = pars$X.2
nOrtho.Cl = pars$nOrtho.Cl
```

```
final.result(MW.PCB[i], H0.mean[i], H0.error[i], C.PCB.water.mean[i], C.PCB.water.error[i],
C.PCB.air.mean[i], C.PCB.air.error[i], nOrtho.Cl[i], month)
}

result.congener = NULL
for (i in 1:158)
{
result.E = NULL
for (replicate in 1:1000)
{
print(c(i, replicate))
            E = 0
            for (month in 1:12)
            {
             pars = read.csv(paste("H:/UIowa/Research/Model/Simulation/Annual variables per
            congener/Variables per congener ", month, ".csv", sep=""))
            E = E + single.month(pars, month)
            }

            result.E = c(result.E, E)
}
mmm = mean(result.E)
sss = sd(result.E)

result.congener = rbind(result.congener, c(i, mmm, sss, mmm-1.96*sss, mmm+1.96*sss))
}

end.result = data.frame(result.congener)
names(end.result) = c("Congener.ID", "Mean", "Std", "Lower Bound", "Upper Bound")
write.csv(end.result, row.names=FALSE, quote=FALSE,
file="H:/UIowa/Research/Model/Simulation/Air_water/All/Annual/result.csv")
```

Table B-4 Summary of dissolved phase and suspended particulates concentrations of PCBs in water in different studies

Location	Station code	Dissolved phase (ng L^{-1})	Suspended particulate (ng L^{-1})	Total PCBs (ng L^{-1})	Dissolved phase (%)	Suspended particulates (%)	Ref.
France Etang de Thau (2005)[a]	T2			0.137			(138)
	C4			0.709			
	T11			0.402			
	T12			0.636			
	RV			0.390			
Italy Venice Lagoon (2001 to '03)[b]	1	0.529	0.239	0.768	69%	31%	(139)
	2	0.463	0.503	0.966	48%	52%	
Spain/France Mediterranean coast (2001-2002)[b]	Banyuls-sur-Mer (France)[c]	10.459	1.608	12.067	87%	13%	(140)
	[d]	5.200	1.243	6.443	81%	19%	
	Barcelona (Spain)[c]	3.791	4.555	8.346	45%	55%	
	[d]	3.910	1.795	5.705	69%	31%	
San Diego Bay (1999 – 2000)	1 (1999)[e]	0.024	<0.0095	0.024	100%	0%	(75)
	2 (1999)[e]	0.080	<0.0097	0.080	100%	0%	
	3 (1999)[e]	0.240	<0.016	0.240	100%	0%	
	4 (1999)[e]	0.204	<0.019	0.204	100%	0%	
	5 (1999)[e]	0.166	0.071	0.237	70%	30%	
	6 (1999)[e]	0.246	<0.0089	0.246	100%	0%	
	8 (1999)[e]	0.064	<0.0082	0.064	100%	0%	
	9 (1999)[e]	0.104	0.016	0.120	87%	2%	
	1 (2000)[e]	0.065	0.014	0.079	82%	2%	
	2 (2000)[e]	0.171	0.070	0.241	71%	10%	
	3 (2000)[e]	0.248	0.124	0.372	67%	19%	

Table B-4 Continued

Location	Station code	Dissolved phase (ng L^{-1})	Suspended particulate (ng L^{-1})	Total PCBs (ng L-1)	Dissolved phase (%)	Suspended particulates (%)	Ref.
	4 (2000)[e]	0.245	0.135	0.380	64%	21%	
	5 (2000)[e]	0.233	0.021	0.254	92%	2%	
	6 (2000)[e]	0.184	0.028	0.212	87%	3%	
	8 (2000)[e]	0.140	0.022	0.162	86%	3%	
	9 (2000)[e]	0.073	0.005	0.078	94%	1%	
	1 (1999)[f]	<0.011	<0.011	<0.011	0%	0%	
	3 (1999)[f]	0.127	<0.0072	0.127	100%	0%	
	4 (1999)[f]	g	g	g	g		
	5 (1999)[f]	0.174	0.031	0.205	85%	15%	
	5 (dup)[f]	0.244	0.029	0.273	89%	11%	
	7 (1999)[f]	0.152	<0.0082	0.152	100%	0%	
	8 (1999)[f]	0.217	<0.012	0.217	100%	0%	
	1 (2000)[f]	0.054	<0.037	0.054	100%	0%	
	3 (2000)[f]	0.331	0.088	0.419	79%	21%	
	4 (2000)[f]	0.220	<0.011	0.220	100%	0%	
	5 (2000)[f]	0.198	0.053	0.251	79%	21%	
	5 (dup)[f]	g	g	g	g		
	7 (2000)[f]	0.244	0.017	0.261	93%	7%	
	8 (2000)[f]	0.146	0.019	0.165	88%	12%	
Northwestern Black Sea (1995)[h]	Danube prodelta	0.087	0.016	0.103	84%	16%	(141)
	estuary and Odessa depression	0.087	0.016	0.103	84%	16%	
	Continental shelf and slope	0.060	0.004	0.064	94%	6%	
	Open sea	0.018	0.003	0.021	87%	13%	
Southern Lake Michigan (1994 – 1995)[i]							(73)
	LM5 (5/17/94)[j]	0.159	0.009	0.168	94%	6%	
	LM5 (dup)[j]	0.258	-	-	-	-	
	LM5 (5/18/94)[k]	0.134	0.101	0.235	57%	43%	
	LM5 (5/18/94)[j]	0.090	0.094	0.184	49%	51%	
	LM5 (7/19/94)[k]	0.130	0.076	0.206	63%	37%	
	LM5 (7/17/94)[j]	0.153	0.024	0.177	86%	14%	
	LM5 (7/18/94)[k]	0.080	0.007	0.087	92%	8%	
	LM5 (7/18/94)[j]	0.054	6.000	6.000	-	-	

Table B-4 Continued

Location	Station code	Dissolved phase (ng L^{-1})	Suspended particulate (ng L^{-1})	Total PCBs (ng L-1)	Dissolved phase (%)	Suspended particulates (%)	Ref.
	LM5 (7/19/94)[k]	0.097	0.014	0.111	88%	12%	
	LM5 (7/19/94)[j]	[m]	0.015	-	-	-	
	LM5 (7/20/94)[k]	0.148	0.021	0.169	87%	13%	
	LM5 (dup)[k]	0.168	0.000	0.000	-	-	
	LM1 (7/21/94)[k]	0.159	0.045	0.204	78%	22%	
	LM1 (7/21/94)[j]	0.078	0.005	0.083	94%	6%	
	LM1 (7/22/94)[k]	0.136	0.022	0.158	86%	14%	
	LM1 (7/22/94)[j]	0.167	0.020	0.187	89%	11%	
	LM5 (7/24/94)[j]	[m]	0.030	m	-	-	
	LM5 (7/25/94)[k]	0.100	0.027	0.127	79%	21%	
	LM5 (7/25/94)[j]	0.097	0.014	0.111	88%	12%	
	LM1 (7/26/94)[j]	0.063	0.012	0.075	84%	16%	
	LM1 (7/27/94)[k]	0.061	0.006	0.067	91%	9%	
	LM0 (7/27/94)[j]	0.048	0.029	0.077	62%	38%	
	LM0 (7/28/94)[j]	0.071	0.027	0.098	72%	28%	
	LM5 (1/17/95)[k]	0.173	0.109	0.282	61%	39%	
	LM5 (dup)[k]	0.228	-	-	-	-	
	LM5 (1/17/94)[k]	0.176	0.147	0.323	55%	45%	
	LM5 (1/18/95)[k]	0.162	0.126	0.288	56%	44%	
	LM5[l] (1/18/95)[j]	0.174	0.094	0.268	65%	35%	
	LM5 (1/18/95)[j]	0.159	0.009	0.168	85%	15%	
Laurentian							(142)
Great Lakes							
(spring 1993)[i]	LE1	0.130	0.068	0.200	66%	34%	
	LE1 (dup)	0.180	0.055	0.230	77%	23%	
	LE78	0.110	0.325	0.420	25%	75%	
	LE42	0.052	0.167	0.220	24%	76%	
	LE91	0.240	1.320	1.600	15%	85%	
	LE61	0.330	1.230	1.500	21%	79%	
	LH6	0.076	0.078	0.160	49%	51%	
	LH12	0.060	0.059	0.120	51%	49%	
	LH27	0.078	0.059	0.140	57%	43%	
	LH18	0.044	[n]	o	-	-	

Table B-4 Continued

Location	Station code	Dissolved phase (ng L^{-1})	Suspended particulate (ng L^{-1})	Total PCBs (ng L-1)	Dissolved phase (%)	Suspended particulates (%)	Ref.
	LH54	0.060	0.028	0.088	68%	32%	
	LH54 (dup)	0.092	0.036	0.130	72%	28%	
	LM47	0.140	0.052	0.190	73%	27%	
	LM27	0.130	0.082	0.220	61%	39%	
	LM18	0.140	0.059	0.210	70%	30%	
	LM18 (dup)	0.120	0.044	0.170	73%	27%	
	LM6	0.110	0.099	0.210	53%	47%	
	LM1	0.140	0.130	0.270	52%	48%	
	LO55	0.190	0.043	0.230	81%	19%	
	LO63	0.150	0.072	0.220	68%	32%	
	LO79	0.110	0.086	0.190	56%	44%	
	LO79 (dup)	[n]	0.074	3.000	-	-	
	LO41	0.140	0.054	0.190	72%	28%	
	LO25	0.160	0.088	0.250	65%	35%	
	LS1	0.064	0.014	0.078	82%	18%	
	LS8	0.063	0.007	0.070	90%	10%	
	LS17	0.056	[n]	o	-	-	
	LS1dd	0.160	[n]	o	-	-	
	LS1dd (dup)	0.085	0.017	0.100	84%	16%	
Lake Michigan (1991)[i]	11	1.170	0.195	1.370	86%	14%	(143)
	17	1.240	0.383	1.740	76%	24%	
	18	0.350	0.088	0.440	80%	20%	
	19	0.320	0.285	0.620	53%	47%	
	23	0.230	0.191	0.420	55%	45%	
	27	0.300	0.135	0.430	69%	31%	
	34	0.350	0.133	0.480	72%	28%	
	40	0.400	0.017	0.410	96%	4%	
	41b	0.320	0.014	0.340	96%	4%	
	47	0.420	0.147	0.560	74%	26%	
	47q	0.440	0.085	0.530	84%	16%	

[a] Total concentration (sum of suspended particulate and dissolved phase) was reported.

[b] Represents the average of the samples.

[c] Samples were collected in the SML (surface microlayer).

[d] Samples were collected in the ULW (underlying water column).

[e] Samples collected 1.5 m depth (distance from the sediment-water interface).

[f] Samples collected 5 m depth (distance from the sediment-water interface).

[g] No sample collected.

[h] Samples collected at similar locations.

[i] Suspended particulates concentration (ng L^{-1}) = suspended particulates (ng g^{-1}) x total suspended solids (mg L^{-1}) x (1/1000).

[j] Samples collected day.

[k] Samples collected night.

[l] Different depth sampling from the rest.

[m] Missing values.

[n] Data did not pass quality control.

[o] Not applicable due to quality control failure.

Table B-5 Concentration of PCB congeners in air gas phase, suspended particulates in water and dissolved phase water IHSC

Sample ID	**1**	**2**	**3**	**4**	**5**
Collection date	8/7/2006	8/7/2006	8/8/2006	8/8/2006	8/8/2006
Sample type	air gas phase	air gas phase	air gas phase	air gas phase	air gas phase
Lab batch #	1	1	1	2	3
PCB14 % recovery	64	50	54	78	35
PCB65 % recovery	111	88	81	153	51
PCB166 % recovery	73	65	53	100	58
PCB204	50 ng	50 ng	50 ng	50 ng	50 ng
Flow (m^3 min^{-1})	0.4	0.4	0.4	0.4	0.4
Minutes	513.6	507.6	420	526.8	429
Congener #	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**
1	0.00	3.81	0.00	0.00	8.83
2	6.68	3.27	0.00	25.13	3.26
3	8.46	7.26	22.48	15.88	4.12
4	42.36	37.40	42.39	0.00	79.75
5	0.00	0.00	0.00	0.00	1.04
6	19.38	11.27	16.72	22.69	22.60
7	47.10	10.25	7.14	0.00	15.55
8	60.81	60.11	50.75	75.34	95.85
9	6.06	6.47	0.00	0.00	7.58
10	0.00	0.00	5.44	22.89	4.88
11	45.13	37.33	27.90	0.00	32.68
12+13	0.00	0.00	0.00	0.00	0.00
15	25.50	26.30	31.52	21.33	31.80
16	43.57	60.00	0.00	88.83	69.28
17	65.80	55.64	70.63	24.29	82.45
18+30	94.76	92.92	121.65	149.78	209.92
19	21.19	19.97	27.59	0.00	35.88
20+28	77.66	92.21	108.14	90.55	149.53
21+33	50.65	37.36	53.26	35.54	51.02
22	24.71	23.59	30.41	63.55	45.51
23	0.00	0.00	0.00	0.00	0.00
24	0.00	0.00	23.28	0.00	0.00
25	9.93	0.00	7.47	0.00	13.99
26+29	18.65	15.88	21.49	21.93	31.12
27	9.51	10.53	13.38	0.00	15.72
31	100.14	97.18	91.62	141.40	114.94
32	39.52	33.49	39.77	70.01	68.03
34	0.00	0.00	0.00	0.00	0.00
35	6.60	2.88	0.00	0.00	0.00
36	1.63	1.41	0.00	0.00	0.00
37	15.85	19.78	13.73	5.25	18.52
38	1.53	2.29	0.00	6.88	0.00
39	0.00	0.00	0.00	0.00	0.00
40+41+71	52.47	59.83	53.80	55.84	44.41
42	23.05	30.53	20.21	68.86	19.49
43	0.00	0.00	0.00	0.00	2.89

Table B-5 continued

Sample ID **Congener #**	**1** **pg m^{-3}**	**2** **pg m^{-3}**	**3** **pg m^{-3}**	**4** **pg m^{-3}**	**5** **pg m^{-3}**
45+51	47.81	15.05	27.74	85.69	32.91
46	13.08	0.00	0.00	21.47	10.37
48	20.64	23.20	29.13	28.95	19.25
49+69	59.15	69.68	56.74	116.22	53.18
50+53	20.65	21.57	22.19	43.54	24.91
52	117.94	159.77	97.62	236.39	127.23
54	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	0.00	0.00	0.00
56	21.10	28.86	14.85	27.56	17.81
57	0.00	0.00	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	11.14	4.00	0.00	10.51	0.00
60	15.84	17.06	0.00	0.00	9.60
61+70+74+76	123.39	154.17	58.21	125.96	76.10
63	0.00	0.00	0.00	0.00	0.00
64	37.91	38.29	36.09	84.09	35.91
66	37.94	48.22	29.04	72.86	28.90
67	0.00	0.00	0.00	0.00	0.00
68	9.50	0.00	0.00	0.00	0.00
72	0.00	0.00	0.00	0.00	0.00
73	0.00	0.00	0.00	0.00	0.00
77	0.00	0.00	0.00	0.00	0.00
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	25.54	25.38	25.93	0.00	0.00
83+99	55.56	77.50	19.57	48.24	17.16
84	46.94	57.92	24.10	0.00	21.24
85+86+87+97+109+116+117+119+125	113.89	184.09	53.67	60.20	37.33
88+91	18.86	35.38	16.89	25.36	10.18
89	1.73	0.00	4.67	0.00	0.00
90+101+113	173.01	257.15	50.42	160.85	71.07
92	27.78	42.87	12.12	22.50	12.19
93+100	1.82	0.00	3.18	0.00	0.00
94	1.11	0.00	2.76	5.68	0.00
95	134.26	205.94	51.50	201.34	73.33
96	0.00	1.39	1.64	17.40	0.00
98+102	0.00	3.72	6.59	0.00	0.00
103	1.09	2.21	3.77	21.48	0.00
104	1.15	2.52	0.33	0.00	0.00
105	51.34	77.52	16.22	62.33	16.36
106	1.47	0.00	2.12	0.00	0.00
107	6.03	10.33	3.66	0.00	0.00
108+124	5.36	10.81	3.96	0.00	0.00
110+115	178.60	276.83	59.86	128.62	58.93
111	0.00	0.00	3.17	0.00	0.00
112	0.00	0.00	3.97	0.00	0.00
114	0.00	0.00	2.81	0.00	0.00
118	108.65	175.70	34.81	92.58	44.86
120	0.00	0.00	0.00	0.00	0.00
121	1.49	0.00	3.00	0.00	0.00

Table B-5 continued

Sample ID **Congener #**	**1** **pg m^{-3}**	**2** **pg m^{-3}**	**3** **pg m^{-3}**	**4** **pg m^{-3}**	**5** **pg m^{-3}**
122	0.00	0.00	0.00	0.00	0.00
123	0.00	5.02	0.00	0.00	0.00
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	3.18	0.00	0.00
129+138+160+163	169.66	277.25	41.17	119.63	63.42
130	0.00	19.98	0.00	0.00	4.28
131	3.41	5.77	0.00	0.00	0.00
132	63.51	92.67	14.32	62.24	18.71
133	0.00	7.15	0.00	0.00	0.00
134+143	10.52	18.90	0.00	0.00	0.00
135+151	95.97	146.21	0.00	76.71	29.84
136	35.25	48.07	8.89	37.05	11.91
137+164	11.57	38.31	0.00	0.00	3.48
139+140	3.38	5.74	0.00	0.00	0.00
141	48.46	60.64	0.00	57.21	12.87
142	0.00	0.00	0.00	0.00	0.00
144	16.95	26.19	0.00	0.00	0.00
145	0.00	0.00	0.00	0.00	0.00
146	24.56	33.21	0.00	0.00	6.51
147+149	209.67	312.66	38.67	149.97	56.82
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	173.41	263.21	33.66	129.80	50.54
154	4.20	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	10.63	14.78	0.00	0.00	0.00
158	16.37	26.96	0.00	0.00	6.04
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	5.33	0.00	0.00
167	4.99	0.00	0.00	0.00	2.25
169	0.00	0.00	0.00	0.00	0.00
170	0.00	14.39	2.63	0.00	0.00
171+173	0.00	16.40	0.00	28.32	0.00
172	0.00	0.00	0.00	14.06	0.00
174	52.93	77.84	0.00	43.69	13.94
175	0.00	0.00	0.00	31.52	0.00
176	10.97	11.91	1.45	25.79	2.01
177	16.80	22.97	7.96	64.91	0.00
178	0.00	21.77	2.24	0.00	0.00
179	34.95	53.16	10.33	43.17	8.47
180+193	49.78	79.18	12.78	59.45	0.00
181	0.00	0.00	0.00	8.71	0.00
182	0.00	0.00	0.00	27.34	0.00
183	28.20	45.36	9.05	48.51	7.85
184	0.00	0.00	0.62	20.18	0.00
185	0.00	0.00	17.74	0.00	0.00
186	0.00	0.00	0.00	15.94	0.00
187	69.01	102.62	19.23	46.37	ÿ5.16
188	0.00	0.00	0.00	18.00	0.00

Table B-5 continued

Sample ID **Congener #**	**1** **pg m^{-3}**	**2** **pg m^{-3}**	**3** **pg m^{-3}**	**4** **pg m^{-3}**	**5** **pg m^{-3}**
189	0.00	0.00	0.00	16.74	0.00
190	0.00	0.00	0.00	0.00	0.00
191	0.00	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	4.35	7.44	1.51	0.00	0.00
195	0.00	0.00	0.00	0.00	0.00
196	18.49	8.33	0.00	0.00	1.55
197	0.00	0.00	0.00	0.00	0.00
198+199	20.08	26.81	0.00	0.00	7.95
200	6.80	10.25	0.00	0.00	0.00
201	5.74	11.71	1.61	0.00	2.05
202	13.45	14.47	0.00	0.00	2.34
203	12.79	10.79	0.00	0.00	5.56
205	1.18	1.71	0.00	6.32	0.00
206	5.50	1.73	3.56	28.89	0.00
207	4.74	0.00	0.00	0.00	0.00
208	5.81	2.15	4.10	16.83	0.00
209	0.70	0.00	1.25	11.09	0.00
Total	**3675.22**	**4829.76**	**1924.39**	**3914.24**	**2423.01**

Table B-5 continued

Sample ID	**6**	**7**	**8**	**9**	**10**
Collection date	8/9/2006	8/9/2006	8/9/2006	8/9/2006	8/10/2006
Sample type	air gas phase	air gas phase	air gas phase	air gas phase	air gas phase
Lab batch #	2	3	3	2	2
PCB14 % recovery	96	44	38	57	76
PCB65 % recovery	114	88	94	86	159
PCB166 % recovery	90	74	67	72	94
PCB204	50 ng	50 ng	50 ng	50 ng	50 ng
Flow (m^3 min^{-1})	0.4	0.4	0.4	0.4	0.4
Minutes	373.8	373.2	903	504	517.2
Congener #	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**
1	12.02	11.90	12.81	35.51	26.69
2	12.12	3.68	7.07	12.33	17.80
3	0.00	4.87	9.17	19.95	23.00
4	135.74	115.18	86.59	115.24	233.16
5	0.00	3.77	2.24	0.00	0.00
6	0.00	42.06	31.15	46.73	76.66
7	0.00	110.37	10.15	0.00	0.00
8	129.84	171.60	137.64	150.83	274.76
9	0.00	12.84	10.18	0.00	21.09
10	0.00	7.80	5.09	0.00	0.00
11	39.48	72.29	30.64	81.37	39.69
12+13	0.00	9.66	6.14	0.00	0.00
15	24.81	58.09	40.68	0.00	86.86
16	106.26	117.87	95.03	63.59	429.69
17	108.44	144.53	99.87	75.15	183.53
18+30	268.01	346.72	240.87	145.29	540.56
19	40.74	54.81	35.48	18.57	117.61
20+28	191.97	265.20	211.78	147.44	342.27
21+33	61.94	107.51	97.53	80.44	140.59
22	30.09	85.62	67.87	31.72	131.11
23	0.00	0.00	0.00	0.00	0.00
24	0.00	1.35	2.62	0.00	114.92
25	0.00	26.94	15.50	15.54	51.99
26+29	0.00	54.90	36.58	23.54	75.83
27	24.50	23.82	15.50	0.00	39.00
31	195.72	222.92	187.29	124.44	393.07
32	68.02	103.14	70.75	39.89	0.00
34	0.00	0.00	0.00	0.00	0.00
35	0.00	0.00	1.46	0.00	0.00
36	0.00	0.00	0.00	0.00	0.00
37	0.00	32.16	27.37	0.00	46.64
38	0.00	0.00	0.00	0.00	0.00
39	8.22	0.00	0.00	0.00	0.00
40+41+71	60.32	76.24	64.77	39.36	160.41
42	0.00	35.59	29.81	0.00	117.02
43	22.39	0.00	0.00	0.00	0.00
45+51	0.00	89.61	37.99	0.00	75.90
46	12.00	0.00	12.40	0.00	13.63
48	0.00	30.96	28.79	0.00	58.16
49+69	117.39	96.91	81.69	93.03	166.20
50+53	71.33	33.18	26.24	0.00	0.00
52	188.08	225.55	195.69	275.40	317.07

Table B-5 continued

Sample ID **Congener #**	**6** **pg m^{-3}**	**7** **pg m^{-3}**	**8** **pg m^{-3}**	**9** **pg m^{-3}**	**10** **pg m^{-3}**
54	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	0.00	0.00	17.47
56	33.57	29.40	30.22	23.45	47.29
57	0.00	0.00	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	46.21	10.44	12.03	0.00	28.89
60	0.00	12.80	16.82	0.00	0.00
61+70+74+76	116.86	147.87	117.95	183.87	181.88
63	0.00	3.16	1.64	0.00	0.00
64	0.00	57.98	54.51	44.86	140.23
66	0.00	56.19	62.65	57.49	92.75
67	0.00	0.00	1.20	0.00	0.00
68	0.00	18.19	0.00	0.00	0.00
72	0.00	0.00	0.00	0.00	0.00
73	0.00	0.00	0.00	0.00	0.00
77	0.00	0.00	4.16	0.00	0.00
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	35.33	13.14	9.38	0.00	0.00
83+99	44.62	38.11	44.35	90.64	0.00
84	57.93	41.18	38.15	100.39	71.91
85+86+87+97+109+116+117+119+125	24.61	96.84	82.59	145.69	0.00
88+91	18.98	21.47	17.16	28.49	41.62
89	0.00	0.00	0.95	0.00	14.23
90+101+113	95.69	133.86	117.18	232.52	89.59
92	18.22	23.28	0.00	0.00	19.43
93+100	4.40	0.00	0.00	17.06	0.00
94	0.00	0.00	0.00	7.77	12.25
95	80.56	129.89	118.42	390.25	152.51
96	0.00	2.08	1.00	7.81	6.80
98+102	0.00	1.89	1.59	0.00	0.00
103	0.00	0.00	0.00	0.00	4.57
104	0.00	0.00	0.00	0.00	0.00
105	0.00	31.57	25.35	46.66	28.76
106	9.96	0.00	0.00	0.00	0.00
107	6.79	3.87	3.99	0.00	0.00
108+124	0.00	0.00	2.30	5.10	0.00
110+115	54.86	0.00	104.89	199.77	83.28
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	0.00	0.00	0.00	0.00	0.00
118	49.49	82.49	68.79	136.52	57.44
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	5.38
122	0.00	0.00	0.00	0.00	0.00
123	0.00	0.00	0.00	7.39	5.41
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	38.87	94.98	94.81	196.00	37.42
130	0.00	4.20	2.49	0.00	13.79

Table B-5 continued

Sample ID **Congener #**	**6** **pg m^{-3}**	**7** **pg m^{-3}**	**8** **pg m^{-3}**	**9** **pg m^{-3}**	**10** **pg m^{-3}**
131	0.00	0.00	0.00	0.00	0.00
132	0.00	32.12	33.87	112.96	27.20
133	0.00	0.00	0.00	4.90	9.08
134+143	0.00	3.38	4.32	0.00	14.00
135+151	0.00	33.51	34.38	127.27	0.00
136	27.35	19.80	20.60	72.88	5.84
137+164	13.19	7.02	10.31	0.00	4.84
139+140	11.65	0.00	0.00	0.00	0.00
141	0.00	18.28	21.39	44.38	0.00
142	0.00	0.00	0.00	0.00	9.13
144	0.00	6.85	6.90	13.02	0.00
145	0.00	0.00	0.00	0.00	0.00
146	0.00	13.26	12.11	25.23	15.42
147+149	43.95	92.91	93.42	220.21	62.13
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00
152	0.00	0.00	0.00	7.94	0.00
153+168	35.45	86.79	87.58	156.25	31.38
154	0.00	0.00	0.00	4.42	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	72.22	6.21	5.11	0.00	62.69
158	0.00	10.89	9.74	26.48	5.11
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	7.71	0.00
167	0.00	2.72	1.72	0.00	0.00
169	0.00	0.00	0.00	0.00	0.00
170	6.16	9.46	6.39	18.03	3.39
171+173	9.25	0.00	5.88	0.00	12.11
172	26.15	0.00	0.00	0.00	0.00
174	16.73	23.44	23.53	42.31	17.11
175	9.58	0.00	0.00	0.00	0.00
176	5.94	3.31	5.62	8.84	5.57
177	9.58	11.06	6.55	34.22	12.21
178	0.00	5.62	5.39	37.20	23.44
179	17.41	19.25	18.64	35.79	9.66
180+193	0.00	34.31	34.72	57.42	30.32
181	14.55	0.00	0.00	0.00	32.23
182	0.00	0.00	0.00	0.00	6.06
183	24.77	13.81	13.93	29.83	12.02
184	2.22	0.00	0.00	0.00	20.72
185	20.64	0.00	0.00	0.00	11.78
186	0.00	0.00	0.00	0.00	8.72
187	0.00	45.50	41.57	65.99	25.37
188	0.57	0.00	0.00	0.00	0.00
189	18.80	0.00	0.00	0.00	0.00
190	0.00	0.00	0.00	0.00	0.00
191	4.56	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	0.00	5.26	2.68	0.00	22.73
195	0.00	0.00	0.00	0.00	0.00

Table B-5 continued

Sample ID	**6**	**7**	**8**	**9**	**10**
Congener #	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**
196	0.00	5.24	4.23	0.00	0.00
197	0.00	0.00	0.00	0.00	0.00
198+199	8.72	18.48	14.92	41.83	0.00
200	14.51	1.57	0.00	0.00	0.00
201	0.00	2.30	4.75	22.01	0.00
202	0.00	10.70	6.27	0.00	0.00
203	0.00	12.53	8.67	30.48	0.00
205	0.00	0.00	0.00	0.00	0.00
206	5.97	3.72	0.00	8.12	12.33
207	0.00	0.00	0.00	9.68	0.00
208	0.00	3.94	0.00	0.00	0.00
209	0.75	0.00	0.00	0.00	2.24
Total	**3087.04**	**4417.76**	**3652.17**	**4822.50**	**5982.66**

Table B-5 continued

Sample ID	**11**	**12**	**13**	**14**	**15**
Collection date	8/10/2006	8/10/2006	8/11/2006	8/11/2006	8/11/2006
Sample type	air gas phase	air gas phase	air gas phase	air gas phase	air gas phase
Lab batch #	2	3	1	1	3
PCB14 % recovery	107	38	46	72	52
PCB65 % recovery	214	116	104	132	111
PCB166 % recovery	111	65	52	70	94
PCB204	50 ng	50 ng	50 ng	50 ng	50 ng
Flow (m^3 min^{-1})	0.4	0.4	0.4	0.4	0.4
Minutes	612.6	526.8	760.2	629.4	514.2
Congener #	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**	**pg m^{-3}**
1	11.05	56.96	0.00	2.03	19.77
2	8.37	16.14	0.00	0.00	5.85
3	13.37	28.58	11.82	4.14	8.53
4	163.78	439.74	115.04	43.36	150.75
5	0.00	13.84	4.77	0.00	2.89
6	53.60	151.91	47.44	17.01	47.61
7	49.82	92.75	31.87	17.86	33.82
8	220.09	644.28	201.01	69.46	195.63
9	0.00	46.79	21.83	10.22	15.48
10	0.00	22.38	8.61	0.00	7.61
11	65.79	69.24	36.10	18.19	33.60
12+13	0.00	30.81	0.00	0.00	10.71
15	92.16	170.12	72.91	36.07	61.77
16	140.94	379.96	188.73	97.14	151.23
17	178.03	398.87	178.52	75.54	162.89
18+30	415.56	943.40	312.38	159.78	402.17
19	74.64	149.08	78.26	39.44	62.08
20+28	289.22	691.43	284.87	146.10	284.52
21+33	123.06	307.65	195.11	56.25	117.01
22	92.71	216.53	91.91	39.23	88.52
23	0.00	0.00	0.00	0.97	0.00
24	0.00	14.90	3.83	0.00	6.35
25	29.35	66.14	32.24	11.51	27.75
26+29	49.75	144.36	59.51	28.60	58.94
27	48.98	62.09	31.06	15.16	29.20
31	302.48	558.77	251.93	112.48	229.01
32	170.40	265.46	108.98	58.03	118.06
34	0.00	0.00	0.00	0.00	0.00
35	0.00	2.77	0.00	0.00	0.00
36	5.50	0.00	0.00	2.60	0.00
37	38.68	77.49	34.80	21.75	34.40
38	8.45	0.00	5.93	0.00	0.00
39	7.02	0.00	0.00	2.62	0.00
40+41+71	105.80	157.87	120.31	80.69	71.64
42	56.44	79.45	56.82	46.13	34.91
43	0.00	14.81	0.00	21.09	1.87
45+51	0.00	142.45	77.47	49.17	66.43
46	0.00	38.32	19.71	25.38	15.12
48	62.47	66.75	50.00	33.79	30.18
49+69	171.95	188.01	130.42	95.82	86.35
50+53	75.86	82.54	50.35	43.70	40.25
52	346.72	366.78	257.66	176.10	162.56

Table B-5 continued

Sample ID **Congener #**	**11** **pg m^{-3}**	**12** **pg m^{-3}**	**13** **pg m^{-3}**	**14** **pg m^{-3}**	**15** **pg m^{-3}**
54	0.00	0.00	0.00	0.00	0.00
55	0.00	4.80	0.00	0.00	1.68
56	0.00	51.10	38.94	37.19	24.35
57	0.00	0.00	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	0.00	29.74	22.82	7.48	14.48
60	19.81	29.63	41.88	24.62	11.83
61+70+74+76	262.84	218.06	228.89	130.22	84.82
63	0.00	5.89	0.00	0.00	2.63
64	112.45	118.16	96.48	63.23	55.60
66	100.55	101.78	87.58	65.53	44.68
67	0.00	3.71	0.00	0.00	3.43
68	0.00	12.23	5.60	0.00	6.97
72	0.00	0.00	0.00	0.00	0.00
73	0.00	0.00	0.00	0.00	0.00
77	0.00	0.00	0.00	0.00	0.00
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	0.00	5.45	16.59	0.00	3.70
83+99	80.76	50.09	61.33	32.15	20.96
84	116.13	49.69	71.55	27.58	21.66
85+86+87+97+109+116+117+119+125	136.53	92.52	64.09	30.49	31.98
88+91	51.07	24.44	46.81	15.61	11.13
89	0.00	0.00	0.00	0.00	0.00
90+101+113	198.10	119.18	162.83	65.95	43.45
92	52.07	23.03	33.76	17.40	7.45
93+100	0.00	0.00	0.00	0.00	0.00
94	0.00	0.00	0.00	0.00	0.00
95	294.53	129.87	153.47	80.03	51.40
96	8.01	0.00	2.23	3.03	0.00
98+102	19.31	2.97	0.00	0.00	0.00
103	0.00	0.00	0.00	1.21	0.00
104	0.00	0.00	1.52	0.00	0.00
105	19.13	24.15	29.64	16.19	8.64
106	0.00	0.00	0.00	0.00	0.00
107	7.48	1.27	0.00	2.47	0.00
108+124	0.00	0.00	6.19	0.00	0.00
110+115	132.28	114.55	158.77	77.67	37.10
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	5.41	0.00	0.00	0.00	0.00
118	78.44	66.89	79.56	36.46	20.69
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.00	0.00	0.00	0.00	0.00
123	14.68	0.00	0.00	0.00	0.00
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+160+163	78.97	64.95	93.09	21.40	18.66
130	0.00	2.54	7.84	0.00	0.00

Table B-5 continued

Sample ID **Congener #**	**11** **pg m^{-3}**	**12** **pg m^{-3}**	**13** **pg m^{-3}**	**14** **pg m^{-3}**	**15** **pg m^{-3}**
131	8.49	0.00	0.00	0.00	0.00
132	40.51	24.77	30.96	8.12	9.01
133	0.00	0.00	0.00	0.00	0.00
134+143	36.12	5.16	13.66	0.00	0.00
135+151	48.07	32.60	56.47	20.63	9.34
136	42.88	16.92	25.30	10.84	4.57
137+164	0.00	2.93	0.00	0.00	1.27
139+140	4.53	0.00	2.51	0.00	0.00
141	26.95	6.72	22.85	7.84	3.95
142	0.00	0.00	0.00	2.53	0.00
144	15.65	0.00	9.51	3.62	0.00
145	0.00	0.00	0.00	0.00	0.00
146	0.00	7.44	13.36	3.18	0.00
147+149	134.28	72.33	114.18	34.96	24.01
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	1.66	1.11	0.00
152	0.00	0.00	0.00	0.00	0.00
153+168	84.83	59.91	90.29	36.48	16.14
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	2.49	0.00	0.00
156+157	0.00	3.59	0.00	0.00	0.00
158	0.00	3.28	10.64	0.00	1.91
159	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	5.67	0.00
167	0.00	0.00	0.00	0.00	0.00
169	0.00	0.00	0.00	0.00	0.00
170	27.35	4.21	11.22	5.27	0.00
171+173	0.00	0.00	6.58	0.00	0.00
172	4.39	0.00	9.10	0.00	0.00
174	41.48	14.67	29.83	2.81	4.25
175	4.67	0.00	0.00	10.09	0.00
176	0.00	2.46	3.88	2.68	0.00
177	38.09	7.04	11.62	2.05	0.00
178	0.00	0.00	8.87	2.41	0.00
179	13.41	12.73	22.50	9.45	3.56
180+193	37.13	22.62	32.24	8.01	8.34
181	0.00	0.00	0.00	4.04	0.00
182	0.00	0.00	1.14	0.00	0.00
183	36.80	8.50	10.49	5.39	4.34
184	5.92	0.00	0.00	7.20	0.00
185	0.00	0.00	0.00	6.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	34.37	28.92	43.48	13.86	10.86
188	3.07	0.00	0.00	0.00	0.00
189	10.12	0.00	7.32	2.98	0.00
190	0.00	0.00	0.00	0.00	0.00
191	3.87	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	0.00	0.00	0.00	0.00	0.00
195	0.00	0.00	0.00	0.00	0.00

Table B-5 continued

Sample ID **Congener #**	**11** **pg m^{-3}**	**12** **pg m^{-3}**	**13** **pg m^{-3}**	**14** **pg m^{-3}**	**15** **pg m^{-3}**
196	0.00	3.23	0.00	0.00	0.00
197	0.00	0.00	0.00	0.00	0.00
198+199	0.00	14.67	12.68	0.00	3.60
200	0.00	0.74	0.00	0.00	0.00
201	0.00	1.32	0.00	0.00	0.00
202	15.04	7.33	8.15	1.19	2.96
203	0.00	3.19	0.00	0.00	0.94
205	6.64	0.00	0.00	0.00	0.00
206	10.76	0.00	0.00	0.00	0.00
207	12.86	0.00	0.00	0.00	0.00
208	5.11	0.00	5.96	0.00	0.00
209	3.69	0.00	1.07	1.14	0.00
Total	**6017.67**	**8913.37**	**5303.68**	**2632.90**	**3511.84**

Table B-5 continued

Sample ID	**16**
Collection date	8/11/2006
Sample type	air gas phase
Lab batch #	3
PCB14 % recovery	48
PCB65 % recovery	132
PCB166 % recovery	113
PCB204	50 ng
Flow (m^3 min^{-1})	0.4
Minutes	516.6
Congener #	**pg m^{-3}**
1	28.72
2	9.61
3	16.30
4	195.81
5	8.92
6	80.54
7	120.20
8	348.43
9	21.33
10	14.39
11	85.70
12+13	18.57
15	100.65
16	200.29
17	220.53
18+30	473.29
19	61.87
20+28	404.65
21+33	223.42
22	132.42
23	0.00
24	8.30
25	39.83
26+29	78.15
27	30.45
31	350.82
32	128.06
34	0.00
35	4.05
36	0.00
37	48.53
38	0.00
39	0.00
40+41+71	52.48
42	27.63
43	5.27
45+51	56.53
46	11.13
48	26.72
49+69	84.07
50+53	27.34
52	255.15

Table B-5 continued

Sample ID **Congener #**	**16** **pg m^{-3}**
54	0.00
55	6.27
56	22.82
57	0.00
58	0.00
59+62+75	1.85
60	12.94
61+70+74+76	154.16
63	2.59
64	46.59
66	47.04
67	2.53
68	8.64
72	0.00
73	0.00
77	2.60
78	0.00
79	0.00
80	0.00
81	0.00
82	13.31
83+99	67.25
84	50.80
85+86+87+97+109+116+117+119+125	126.54
88+91	25.62
89	1.48
90+101+113	203.49
92	33.00
93+100	0.00
94	0.00
95	194.58
96	0.00
98+102	4.13
103	0.00
104	0.00
105	41.11
106	0.00
107	4.81
108+124	4.06
110+115	164.03
111	0.00
112	0.00
114	0.00
118	102.02
120	0.00
121	0.00
122	0.00
123	0.00
126	0.00
127	0.00
129+138+160+163	164.17
130	9.00

Table B-5 continued

Sample ID **Congener #**	**16** **pg m^{-3}**
131	0.00
132	53.18
133	0.00
134+143	10.21
135+151	78.67
136	35.69
137+164	17.03
139+140	1.56
141	37.51
142	0.00
144	11.47
145	0.00
146	23.60
147+149	163.60
148	0.00
150	0.00
152	0.00
153+168	148.32
154	0.00
155	0.00
156+157	12.95
158	15.88
159	0.00
161	0.00
162	0.00
165	0.00
167	0.00
169	0.00
170	15.36
171+173	8.94
172	3.27
174	40.67
175	0.00
176	7.89
177	21.06
178	12.18
179	30.25
180+193	0.00
181	0.00
182	0.00
183	26.76
184	0.00
185	0.00
186	0.00
187	72.65
188	0.00
189	0.00
190	4.78
191	0.00
192	0.00
194	5.94
195	5.14

Table B-5 continued

Sample ID **Congener #**	**16** **pg m^{-3}**
196	10.95
197	0.00
198+199	26.36
200	4.22
201	6.50
202	13.27
203	18.26
205	0.00
206	2.35
207	0.00
208	2.76
209	0.00
Total	**6466.79**

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Collection date	8/7/2006	8/8/2006	8/8/2006	8/9/2006
Sample type	Suspended particulates water	Suspended particulates water	Suspended particulates water	Suspended particulates water
Lab batch #	1	1	1	1
PCB14 % recovery	56	54	84	69
PCB65 % recovery	185	116	276	180
PCB166 % recovery	82	108	107	95
PCB204	100 ng	100 ng	100 ng	100 ng
Volume (mL)	70450	29690	54550	54550
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
1	0.000	0.000	0.009	0.004
2	0.003	0.000	0.006	0.004
3	0.009	0.000	0.003	0.002
4	0.023	0.027	0.000	0.024
5	0.000	0.000	0.000	0.000
6	0.028	0.000	0.052	0.025
7	0.000	0.000	0.000	0.000
8	0.094	0.078	0.139	0.068
9	0.000	0.000	0.010	0.000
10	0.000	0.000	0.006	0.000
11	0.015	0.043	0.021	0.000
12+13	0.000	0.000	0.049	0.000
15	0.165	0.181	0.242	0.147
16	0.198	0.068	0.149	0.066
17	0.242	0.000	0.136	0.087
18+30	0.616	0.252	0.361	0.196
19	0.064	0.000	0.067	0.030
20+28	1.148	0.586	0.952	0.554
21+33	0.198	0.133	0.268	0.155
22	0.284	0.134	0.273	0.145
23	0.000	0.000	0.000	0.000
24	0.008	0.000	0.000	0.000
25	0.102	0.067	0.081	0.073
26+29	0.194	0.091	0.155	0.095
27	0.058	0.000	0.064	0.034
31	0.711	0.287	0.592	0.338
32	0.297	0.147	0.294	0.170
34	0.003	0.000	0.000	0.000
35	0.027	0.000	0.037	0.000
36	0.000	0.000	0.000	0.000

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
37	0.308	0.279	0.382	0.210
38	0.000	0.000	0.007	0.000
39	0.000	0.000	0.000	0.000
40+41+71	0.776	0.430	1.150	0.574
42	0.370	0.174	0.462	0.270
43	0.068	0.026	0.079	0.000
45+51	0.335	0.090	0.512	0.292
46	0.114	0.045	0.173	0.100
48	0.248	0.162	0.247	0.152
49+69	0.816	0.465	1.249	0.725
50+53	0.222	0.110	0.293	0.189
52	1.467	0.745	2.117	1.061
54	0.000	0.000	0.000	0.000
55	0.022	0.000	0.000	0.000
56	0.495	0.220	0.758	0.389
57	0.000	0.000	0.000	0.000
58	0.000	0.000	0.000	0.000
59+62+75	0.129	0.082	0.203	0.126
60	0.266	0.152	0.318	0.189
61+70+74+76	1.096	0.739	1.870	0.901
63	0.036	0.029	0.000	0.000
64	0.692	0.401	1.040	0.521
66	0.891	0.443	1.069	0.562
67	0.036	0.000	0.078	0.000
68	0.000	0.000	0.000	0.000
72	0.012	0.000	0.000	0.000
73	0.000	0.000	0.000	0.000
77	0.137	0.000	0.247	0.145
78	0.000	0.000	0.000	0.000
79	0.000	0.000	0.000	0.000
80	0.000	0.000	0.000	0.000
81	0.000	0.000	0.000	0.000
82	0.158	0.069	0.267	0.127
83+99	0.344	0.182	0.805	0.414
84	0.245	0.266	0.493	0.225
85+86+87+97+109+116+117+119+125	0.390	0.227	0.974	0.456
88+91	0.139	0.171	0.382	0.167
89	0.027	0.032	0.073	0.000
90+101+113	0.619	0.468	1.265	0.677

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
92	0.119	0.095	0.205	0.110
93+100	0.026	0.000	0.000	0.000
94	0.007	0.023	0.000	0.000
95	0.507	0.368	0.961	0.526
96	0.014	0.000	0.030	0.031
98+102	0.065	0.021	0.076	0.011
103	0.000	0.000	0.000	0.011
104	0.000	0.000	0.000	0.000
105	0.272	0.217	0.512	0.295
106	0.000	0.000	0.000	0.000
107	0.025	0.030	0.071	0.031
108+124	0.017	0.050	0.045	0.032
110+115	0.717	0.431	1.543	0.846
111	0.000	0.000	0.000	0.000
112	0.000	0.000	0.000	0.000
114	0.019	0.000	0.000	0.030
118	0.000	0.322	0.830	0.482
120	0.007	0.000	0.000	0.000
121	0.000	0.000	0.000	0.000
122	0.011	0.000	0.000	0.000
123	0.000	0.000	0.026	0.000
126	0.000	0.000	0.000	0.000
127	0.000	0.000	0.000	0.000
129+138+160+163	0.345	0.245	0.492	0.330
130	0.000	0.000	0.000	0.000
131	0.000	0.000	0.000	0.000
132	0.114	0.110	0.222	0.142
133	0.000	0.000	0.000	0.000
134+143	0.000	0.000	0.000	0.000
135+151	0.113	0.088	0.231	0.000
136	0.042	0.054	0.099	0.061
137+164	0.023	0.000	0.000	0.015
139+140	0.000	0.000	0.018	0.000
141	0.053	0.000	0.122	0.078
142	0.000	0.000	0.000	0.000
144	0.023	0.000	0.053	0.000
145	0.000	0.000	0.000	0.000
146	0.050	0.050	0.112	0.072
147+149	0.273	0.196	0.537	0.288

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
148	0.000	0.000	0.000	0.000
150	0.000	0.000	0.016	0.000
152	0.000	0.010	0.008	0.000
153+168	0.258	0.197	0.456	0.280
154	0.003	0.000	0.000	0.000
155	0.000	0.000	0.000	0.000
156+157	0.035	0.000	0.061	0.000
158	0.033	0.042	0.075	0.000
159	0.000	0.000	0.000	0.000
161	0.000	0.000	0.000	0.000
162	0.000	0.000	0.000	0.000
165	0.000	0.000	0.000	0.000
167	0.000	0.000	0.000	0.000
169	0.000	0.000	0.000	0.000
170	0.082	0.099	0.114	0.062
171+173	0.029	0.000	0.023	0.028
172	0.021	0.000	0.000	0.022
174	0.098	0.101	0.155	0.087
175	0.000	0.000	0.000	0.000
176	0.010	0.000	0.045	0.000
177	0.042	0.000	0.059	0.053
178	0.019	0.000	0.000	0.025
179	0.039	0.031	0.104	0.058
180+193	0.186	0.160	0.205	0.159
181	0.000	0.000	0.019	0.028
182	0.000	0.000	0.000	0.000
183	0.039	0.052	0.069	0.060
184	0.000	0.000	0.000	0.000
185	0.000	0.000	0.000	0.000
186	0.000	0.000	0.000	0.000
187	0.102	0.123	0.212	0.108
188	0.000	0.000	0.000	0.005
189	0.000	0.000	0.000	0.000
190	0.000	0.000	0.000	0.000
191	0.000	0.000	0.000	0.022
192	0.000	0.000	0.000	0.006
194	0.046	0.026	0.044	0.000
195	0.000	0.000	0.000	0.000
196	0.026	0.000	0.000	0.000

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
197	0.000	0.031	0.000	0.000
198+199	0.055	0.000	0.075	0.128
200	0.000	0.000	0.000	0.000
201	0.016	0.000	0.000	0.000
202	0.009	0.041	0.000	0.000
203	0.032	0.000	0.000	0.000
205	0.000	0.007	0.000	0.007
206	0.028	0.037	0.048	0.026
207	0.008	0.005	0.000	0.000
208	0.007	0.025	0.000	0.017
209	0.012	0.022	0.024	0.013
Total	**19.023**	**11.412**	**28.476**	**15.275**

Table B-5 continued

Sample ID	**5**	**6**	**7**
Collection date	8/9/2006	8/10/2006	8/10/2006
Sample type	Suspended particulates water	Suspended particulates water	Suspended particulates water
Lab batch #	1	1	1
PCB14 % recovery	72	72	58
PCB65 % recovery	209	163	115
PCB166 % recovery	100	88	87
PCB204	100 ng	100 ng	100 ng
Volume (mL)	64250	24860	29690
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
1	0.003	0.008	0.005
2	0.003	0.000	0.003
3	0.001	0.000	0.013
4	0.024	0.080	0.017
5	0.000	0.000	0.000
6	0.037	0.060	0.043
7	0.000	0.000	0.000
8	0.097	0.186	0.077
9	0.000	0.000	0.000
10	0.000	0.000	0.000
11	0.024	0.000	0.186
12+13	0.026	0.000	0.000
15	0.155	0.240	0.143
16	0.127	0.260	0.092
17	0.121	0.292	0.098
18+30	0.365	0.741	0.296
19	0.043	0.080	0.060
20+28	0.744	1.587	0.638
21+33	0.151	0.397	0.148
22	0.184	0.405	0.155
23	0.466	0.000	0.121
24	0.000	0.000	0.000
25	0.093	0.208	0.064
26+29	0.156	0.320	0.000
27	0.049	0.060	0.055
31	0.000	1.065	0.426
32	0.215	0.383	0.265
34	0.000	0.000	0.000
35	0.000	0.000	0.000
36	0.008	0.000	0.000

Table B-5 continued

Sample ID **Congener #**	**5** **ng L^{-1}**	**6** **ng L^{-1}**	**7** **ng L^{-1}**
37	0.269	0.529	0.202
38	0.000	0.000	0.000
39	0.000	0.000	0.000
40+41+71	0.686	1.443	0.720
42	0.335	0.687	0.355
43	0.047	0.125	0.077
45+51	0.243	0.507	0.373
46	0.104	0.177	0.112
48	0.209	0.385	0.159
49+69	0.805	1.566	0.836
50+53	0.172	0.402	0.247
52	1.270	2.631	1.553
54	0.004	0.000	0.000
55	0.000	0.000	0.000
56	0.512	0.986	0.482
57	0.000	0.000	0.012
58	0.000	0.000	0.000
59+62+75	0.114	0.197	0.129
60	0.261	0.520	0.224
61+70+74+76	1.541	3.004	1.185
63	0.061	0.123	0.048
64	0.590	1.070	0.747
66	0.867	1.694	0.718
67	0.028	0.064	0.000
68	0.000	0.000	0.000
72	0.012	0.027	0.000
73	0.000	0.000	0.000
77	0.127	0.247	0.139
78	0.000	0.000	0.000
79	0.000	0.000	0.000
80	0.000	0.000	0.000
81	0.000	0.000	0.000
82	0.147	0.308	0.192
83+99	0.447	0.847	0.483
84	0.272	0.477	0.317
85+86+87+97+109+116+117+119+125	0.469	0.910	0.261
88+91	0.149	0.250	0.176
89	0.037	0.054	0.039
90+101+113	0.663	1.233	0.796

Table B-5 continued

Sample ID **Congener #**	**5** **ng L^{-1}**	**6** **ng L^{-1}**	**7** **ng L^{-1}**
92	0.117	0.276	0.151
93+100	0.016	0.025	0.028
94	0.000	0.022	0.000
95	0.486	0.975	0.654
96	0.020	0.021	0.014
98+102	0.056	0.078	0.000
103	0.011	0.000	0.056
104	0.000	0.000	0.000
105	0.323	0.572	0.000
106	0.000	0.000	0.329
107	0.051	0.076	0.000
108+124	0.028	0.065	0.037
110+115	0.843	1.536	0.030
111	0.000	0.000	0.978
112	0.000	0.000	0.000
114	0.030	0.039	0.000
118	0.599	1.039	0.589
120	0.000	0.000	0.000
121	0.000	0.000	0.000
122	0.023	0.034	0.020
123	0.029	0.038	0.000
126	0.000	0.000	0.000
127	0.000	0.000	0.000
129+138+160+163	0.379	0.636	0.426
130	0.020	0.046	0.024
131	0.003	0.000	0.008
132	0.107	0.246	0.160
133	0.000	0.032	0.000
134+143	0.022	0.066	0.024
135+151	0.123	0.248	0.162
136	0.054	0.092	0.071
137+164	0.031	0.082	0.000
139+140	0.000	0.000	0.021
141	0.071	0.168	0.076
142	0.000	0.000	0.000
144	0.020	0.039	0.030
145	0.000	0.000	0.000
146	0.051	0.060	0.063
147+149	0.271	0.532	0.329

Table B-5 continued

Sample ID **Congener #**	**5** **ng L^{-1}**	**6** **ng L^{-1}**	**7** **ng L^{-1}**
148	0.000	0.000	0.000
150	0.000	0.000	0.000
152	0.000	0.000	0.000
153+168	0.297	0.563	0.379
154	0.000	0.000	0.000
155	0.000	0.000	0.000
156+157	0.038	0.088	0.044
158	0.039	0.086	0.041
159	0.000	0.000	0.000
161	0.000	0.000	0.000
162	0.000	0.000	0.000
165	0.000	0.000	0.004
167	0.019	0.000	0.014
169	0.000	0.000	0.000
170	0.085	0.142	0.103
171+173	0.038	0.049	0.061
172	0.017	0.044	0.038
174	0.086	0.210	0.114
175	0.000	0.000	0.000
176	0.010	0.000	0.000
177	0.050	0.083	0.083
178	0.034	0.048	0.000
179	0.044	0.103	0.057
180+193	0.200	0.334	0.000
181	0.000	0.000	0.000
182	0.000	0.000	0.000
183	0.052	0.000	0.072
184	0.000	0.000	0.000
185	0.000	0.188	0.000
186	0.000	0.018	0.000
187	0.116	0.227	0.163
188	0.000	0.000	0.000
189	0.007	0.000	0.000
190	0.024	0.000	0.000
191	0.000	0.000	0.000
192	0.000	0.000	0.000
194	0.049	0.111	0.084
195	0.018	0.000	0.056
196	0.036	0.061	0.041

Table B-5 continued

Sample ID	**5**	**6**	**7**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
197	0.002	0.000	0.000
198+199	0.063	0.159	0.094
200	0.004	0.000	0.000
201	0.000	0.000	0.028
202	0.013	0.000	0.036
203	0.052	0.069	0.050
205	0.000	0.000	0.000
206	0.025	0.063	0.059
207	0.000	0.000	0.000
208	0.000	0.000	0.000
209	0.018	0.025	0.036
Total	**18.751**	**36.544**	**19.421**

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Collection date	8/7/2006	8/7/2006	8/8/2006	8/8/2006
Sample type	Dissolved phase water	Dissolved phase water	Dissolved phase water	Dissolved phase water
Lab batch #	2	3	1	4
PCB14 % recovery	55	64	16	57
PCB65 % recovery	95	98	30	169
PCB166 % recovery	67	69	14	67
PCB204	100 ng	100 ng	100 ng	100 ng
Volume (mL)	35890	34560	29690	24860
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
1	0.011	0.000	0.167	0.000
2	0.000	0.000	0.000	0.000
3	0.000	0.000	0.144	0.000
4	0.610	0.162	0.581	1.099
5	0.000	0.000	0.000	0.000
6	0.121	0.000	0.000	0.000
7	0.000	0.000	0.000	0.000
8	0.209	0.090	0.312	0.272
9	0.000	0.000	0.000	0.000
10	0.028	0.000	0.000	0.000
11	0.095	0.000	0.000	0.000
12+13	0.000	0.000	0.215	0.000
15	0.220	0.162	0.000	0.627
16	0.667	0.454	1.247	1.397
17	0.571	0.332	1.075	1.423
18+30	1.885	1.037	2.294	4.226
19	0.514	0.199	0.440	0.804
20+28	1.013	0.707	1.139	2.722
21+33	0.226	0.134	0.194	0.487
22	0.324	0.236	0.301	0.891
23	0.000	0.000	0.000	0.000
24	0.000	0.000	0.000	0.000
25	0.070	0.044	0.000	0.342
26+29	0.279	0.136	0.204	0.686
27	0.144	0.102	0.000	0.344
31	0.838	0.471	0.882	2.094
32	0.716	0.423	1.011	1.522
34	0.000	0.000	0.000	0.000
35	0.000	0.000	0.000	0.000
36	0.000	0.000	0.000	0.019
37	0.294	0.123	0.000	0.524

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
38	0.000	0.000	0.163	0.022
39	0.000	0.000	0.000	0.000
40+41+71	0.603	0.537	1.575	2.020
42	0.318	0.161	0.469	0.850
43	0.000	0.000	0.000	0.000
45+51	0.411	0.436	0.796	1.482
46	0.131	0.187	0.000	0.401
48	0.295	0.134	0.000	0.691
49+69	0.621	0.437	0.561	1.600
50+53	0.301	0.000	0.799	0.942
52	1.461	0.983	2.627	3.728
54	0.000	0.000	0.000	0.000
55	0.000	0.000	0.000	0.000
56	0.238	0.236	0.637	0.640
57	0.000	0.000	0.000	0.000
58	0.000	0.000	0.000	0.000
59+62+75	0.108	0.000	0.000	0.232
60	0.137	0.141	0.000	0.406
61+70+74+76	0.672	0.369	0.638	1.832
63	0.000	0.088	0.000	0.000
64	0.446	0.299	0.999	1.581
66	0.264	0.224	0.391	0.861
67	0.000	0.000	0.000	0.000
68	0.000	0.000	0.392	0.000
72	0.000	0.000	0.000	0.000
73	0.000	0.000	0.000	0.000
77	0.000	0.000	0.000	0.000
78	0.000	0.000	0.000	0.000
79	0.000	0.000	0.000	0.000
80	0.000	0.000	0.000	0.000
81	0.000	0.000	0.000	0.000
82	0.063	0.000	0.369	0.000
83+99	0.096	0.000	0.257	0.269
84	0.178	0.119	0.366	0.383
85+86+87+97+109+116+117+119+125	0.251	0.209	0.543	0.630
88+91	0.022	0.032	0.311	0.000
89	0.000	0.000	0.281	0.000
90+101+113	0.452	0.227	0.245	0.499
92	0.107	0.000	0.154	0.115

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
93+100	0.000	0.000	0.145	0.043
94	0.000	0.000	0.139	0.139
95	0.487	0.265	0.356	0.687
96	0.000	0.000	0.144	0.035
98+102	0.000	0.000	0.088	0.043
103	0.000	0.000	0.125	0.079
104	0.000	0.000	0.105	0.000
105	0.000	0.000	0.186	0.170
106	0.000	0.000	0.000	0.000
107	0.000	0.000	0.266	0.000
108+124	0.000	0.000	0.000	0.000
110+115	0.351	0.275	0.537	0.784
111	0.000	0.000	0.000	0.000
112	0.000	0.000	0.000	0.000
114	0.000	0.000	0.188	0.041
118	0.159	0.118	0.063	0.206
120	0.000	0.000	0.000	0.000
121	0.000	0.000	□.000	0.000
122	0.000	0.000	0.000	0.000
123	0.000	0.000	0.000	0.000
126	0.000	0.000	0.000	0.000
127	0.000	0.000	0.000	0.000
129+138+160+163	0.000	0.120	0.000	0.000
130	0.000	0.000	0.245	0.000
131	0.000	0.000	0.000	0.000
132	0.000	0.082	0.000	0.162
133	0.000	0.000	0.000	0.000
134+143	0.024	0.000	0.401	0.063
135+151	0.027	0.053	0.000	0.000
136	0.000	0.000	0.000	0.072
137+164	0.000	0.000	0.000	0.000
139+140	0.000	0.000	0.000	0.000
141	0.000	0.000	0.000	0.000
142	0.000	0.026	0.000	0.000
144	0.000	0.000	0.000	0.082
145	0.000	0.000	0.000	0.000
146	0.000	0.000	0.268	0.000
147+149	0.000	0.109	0.000	0.219
148	0.000	0.000	0.000	0.000

Table B-5 continued

Sample ID **Congener #**	**1** **ng L^{-1}**	**2** **ng L^{-1}**	**3** **ng L^{-1}**	**4** **ng L^{-1}**
150	0.000	0.000	0.000	0.036
152	0.000	0.000	0.000	0.067
153+168	0.000	0.075	0.000	0.000
154	0.000	0.000	0.000	0.000
155	0.000	0.000	0.000	0.026
156+157	0.000	0.000	0.000	0.000
158	0.000	0.027	0.000	0.000
159	0.000	0.000	0.000	0.000
161	0.000	0.000	0.000	0.000
162	0.000	0.000	0.000	0.000
165	0.000	0.000	0.000	0.000
167	0.000	0.000	0.000	0.000
169	0.000	0.000	0.000	0.000
170	0.000	0.045	0.000	0.000
171+173	0.023	0.026	0.000	0.000
172	0.152	0.000	0.130	0.000
174	0.000	0.067	0.241	0.000
175	0.029	0.000	0.000	0.000
176	0.054	0.027	0.170	0.000
177	0.000	0.044	0.000	0.000
178	0.000	0.000	0.000	0.000
179	0.065	0.017	0.229	0.000
180+193	0.000	0.000	0.054	0.168
181	0.038	0.000	0.290	0.000
182	0.000	0.026	0.000	0.000
183	0.028	0.000	0.349	0.000
184	0.030	0.000	0.000	0.168
185	0.000	0.029	0.165	0.034
186	0.000	0.020	0.067	0.000
187	0.000	0.053	0.207	0.000
188	0.000	0.000	0.121	0.049
189	0.000	0.000	0.000	0.000
190	0.000	0.024	0.000	0.000
191	0.021	0.000	0.051	0.030
192	0.000	0.023	0.313	0.080
194	0.000	0.000	0.000	0.000
195	0.000	0.000	0.000	0.000
196	0.000	0.000	0.000	0.000
197	0.000	0.000	0.291	0.000

Table B-5 continued

Sample ID	**1**	**2**	**3**	**4**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
198+199	0.000	0.000	0.000	0.000
200	0.000	0.000	0.000	0.000
201	0.000	0.013	0.111	0.000
202	0.000	0.000	0.000	0.000
203	0.000	0.000	0.000	0.000
205	0.000	0.004	0.149	0.018
206	0.079	0.000	0.059	0.000
207	0.032	0.000	0.000	0.000
208	0.000	0.000	0.000	0.000
209	0.062	0.012	0.066	0.023
Total	**17.671**	**11.210**	**29.097**	**42.187**

Table B-5 continued

Sample ID	**5**	**6**	**7**	**8**
Collection date	8/8/2006	8/9/2006	8/9/2006	8/9/2006
Sample type	Dissolved phase water	Dissolved phase water	Dissolved phase water	Dissolved phase water
Lab batch #	4	4	3	3
PCB14 % recovery	72	71	50	46
PCB65 % recovery	187	220	159	151
PCB166 % recovery	87	85	89	81
PCB204	100 ng	100 ng	100 ng	100 ng
Volume (mL)	29690	64250	29690	24860
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
1	0.000	0.022	0.000	0.079
2	0.000	0.004	0.000	0.013
3	0.000	0.005	0.000	0.000
4	0.792	0.573	0.467	0.508
5	0.000	0.000	0.000	0.000
6	0.126	0.139	0.078	0.075
7	0.000	0.000	0.000	0.000
8	0.239	0.241	0.155	0.319
9	0.000	0.000	0.000	0.000
10	0.000	0.000	0.000	0.000
11	0.000	0.031	0.000	0.000
12+13	0.000	0.060	0.053	0.061
15	0.473	0.299	0.569	0.619
16	1.276	0.983	1.146	1.936
17	0.991	0.708	0.995	1.501
18+30	3.226	2.244	3.279	4.581
19	0.638	0.435	0.539	0.933
20+28	2.145	1.517	2.518	3.718
21+33	0.448	0.336	0.471	0.736
22	0.674	0.449	0.770	1.022
23	0.010	0.000	0.000	0.026
24	0.000	0.000	0.000	0.020
25	0.227	0.206	0.303	0.380
26+29	0.601	0.378	0.608	0.963
27	0.249	0.193	0.286	0.501
31	1.590	1.147	1.968	2.462
32	1.176	0.771	1.512	1.920
34	0.000	0.000	0.000	0.000
35	0.000	0.000	0.000	0.099
36	0.000	0.000	0.000	0.000
37	0.355	0.244	0.540	0.618

Table B-5 continued

Sample ID	**5**	**6**	**7**	**8**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
38	0.000	0.000	0.000	0.000
39	0.000	0.000	0.000	0.000
40+41+71	1.527	0.631	1.338	1.915
42	0.654	0.481	0.530	0.796
43	0.078	0.073	0.055	0.171
45+51	0.722	0.545	0.847	1.152
46	0.310	0.204	0.317	0.468
48	0.424	0.285	0.301	0.512
49+69	1.165	0.757	1.184	1.579
50+53	0.804	0.436	0.480	0.916
52	2.639	1.635	2.270	2.988
54	0.000	0.000	0.000	0.000
55	0.000	0.000	0.000	0.000
56	0.601	0.357	0.509	0.752
57	0.000	0.000	0.000	0.000
58	0.000	0.000	0.000	0.000
59+62+75	0.186	0.123	0.161	0.106
60	0.161	0.142	0.199	0.423
61+70+74+76	1.555	0.735	1.086	2.009
63	0.000	0.000	0.000	0.000
64	1.160	0.642	0.893	1.178
66	0.626	0.421	0.665	0.852
67	0.000	0.000	0.000	0.000
68	0.000	0.000	0.000	0.000
72	0.000	0.000	0.000	0.000
73	0.000	0.000	0.000	0.000
77	0.000	0.055	0.000	0.000
78	0.000	0.000	0.000	0.000
79	0.000	0.000	0.000	0.000
80	0.000	0.000	0.000	0.000
81	0.000	0.000	0.000	0.000
82	0.000	0.044	0.000	0.000
83+99	0.148	0.140	0.197	0.360
84	0.204	0.166	0.299	0.289
85+86+87+97+109+116+117+119+125	0.343	0.273	0.499	0.412
88+91	0.185	0.071	0.141	0.000
89	0.076	0.000	0.000	0.000
90+101+113	0.401	0.229	0.595	0.431
92	0.069	0.051	0.079	0.000

Table B-5 continued

Sample ID	**5**	**6**	**7**	**8**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
93+100	0.000	0.000	0.000	0.000
94	0.000	0.000	0.000	0.000
95	0.651	0.338	0.573	0.651
96	0.000	0.000	0.000	0.000
98+102	0.000	0.045	0.000	0.000
103	0.000	0.000	0.000	0.000
104	0.029	0.000	0.000	0.021
105	0.125	0.059	0.148	0.125
106	0.000	0.000	0.000	0.000
107	0.000	0.013	0.000	0.000
108+124	0.052	0.000	0.000	0.000
110+115	0.435	0.353	0.588	0.480
111	0.000	0.000	0.000	0.000
112	0.000	0.000	0.000	0.000
114	0.000	0.014	0.000	0.030
118	0.202	0.071	0.202	0.182
120	0.000	0.000	0.000	0.000
121	0.000	0.000	0.000	0.000
122	0.000	0.000	0.000	0.000
123	0.000	0.000	0.000	0.000
126	0.000	0.000	0.000	0.000
127	0.000	0.000	0.000	0.000
129+138+160+163	0.000	0.065	0.159	0.101
130	0.000	0.000	0.000	0.000
131	0.034	0.000	0.000	0.000
132	0.053	0.042	0.085	0.076
133	0.000	0.000	0.000	0.000
134+143	0.082	0.000	0.000	0.000
135+151	0.000	0.000	0.131	0.000
136	0.000	0.000	0.074	0.070
137+164	0.026	0.000	0.000	0.000
139+140	0.000	0.000	0.000	0.000
141	0.000	0.000	0.000	0.000
142	0.000	0.000	0.000	0.000
144	0.039	0.000	0.000	0.056
145	0.000	0.000	0.000	0.000
146	0.000	0.000	0.000	0.000
147+149	0.184	0.081	0.170	0.076
148	0.000	0.000	0.000	0.000

Table B-5 continued

Sample ID	**5**	**6**	**7**	**8**
Congener #	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**	**ng L^{-1}**
150	0.016	0.000	0.000	0.000
152	0.000	0.000	0.000	0.013
153+168	0.121	0.044	0.134	0.106
154	0.015	0.000	0.012	0.000
155	0.020	0.000	0.000	0.000
156+157	0.000	0.000	0.000	0.000
158	0.000	0.000	0.000	0.000
159	0.000	0.000	0.000	0.000
161	0.000	0.000	0.000	0.000
162	0.000	0.000	0.000	0.000
165	0.000	0.000	0.008	0.000
167	0.000	0.000	0.025	0.000
169	0.000	0.000	0.000	0.000
170	0.000	0.022	0.000	0.000
171+173	0.000	0.017	0.000	0.000
172	0.047	0.000	0.000	0.053
174	0.029	0.036	0.000	0.025
175	0.050	0.000	0.000	0.071
176	0.000	0.000	0.000	0.047
177	0.000	0.007	0.032	0.000
178	0.089	0.000	0.066	0.050
179	0.000	0.009	0.076	0.048
180+193	0.092	0.049	0.000	0.023
181	0.043	0.000	0.000	0.000
182	0.000	0.000	0.000	0.053
183	0.000	0.009	0.000	0.000
184	0.000	0.000	0.000	0.011
185	0.000	0.009	0.060	0.000
186	0.068	0.009	0.000	0.000
187	0.082	0.000	0.022	0.085
188	0.000	0.000	0.000	0.031
189	0.000	0.000	0.000	0.000
190	0.008	0.000	0.000	0.000
191	0.010	0.019	0.000	0.007
192	0.000	0.000	0.038	0.000
194	0.000	0.000	0.021	0.014
195	0.000	0.000	0.000	0.000
196	0.000	0.000	0.000	0.000
197	0.000	0.010	0.000	0.000

Table B-5 continued

Sample ID **Congener #**	**5** **ng L^{-1}**	**6** **ng L^{-1}**	**7** **ng L^{-1}**	**8** **ng L^{-1}**
198+199	0.000	0.000	0.000	0.000
200	0.000	0.000	0.000	0.000
201	0.009	0.000	0.000	0.000
202	0.000	0.000	0.000	0.000
203	0.000	0.000	0.000	0.000
205	0.000	0.004	0.000	0.000
206	0.016	0.004	0.000	0.000
207	0.049	0.000	0.039	0.000
208	0.000	0.000	0.000	0.000
209	0.000	0.017	0.010	0.009
Total	**31.951**	**20.826**	**31.577**	**42.909**

Table B-5 continued

Sample ID	**9**	**10**
Collection date	8/10/2006	8/10/2006
Sample type	Dissolved phase water	Dissolved phase water
Lab batch #	2	4
PCB14 % recovery	44	75
PCB65 % recovery	136	194
PCB166 % recovery	54	81
PCB204	100 ng	100 ng
Volume (mL)	24860	29690
Congener #	**ng L^{-1}**	**ng L^{-1}**
1	0.103	0.000
2	0.025	0.000
3	0.082	0.000
4	2.641	1.098
5	0.000	0.000
6	0.706	0.185
7	0.000	0.000
8	1.000	0.253
9	0.000	0.000
10	0.105	0.018
11	0.160	0.000
12+13	0.000	0.028
15	1.035	0.486
16	1.850	1.524
17	2.748	1.303
18+30	7.202	3.729
19	1.688	0.918
20+28	4.920	2.302
21+33	1.161	0.413
22	1.278	0.614
23	0.000	0.000
24	0.000	0.047
25	0.731	0.265
26+29	1.279	0.578
27	0.537	0.302
31	4.399	1.658
32	2.743	1.389
34	0.000	0.000
35	0.000	0.000
36	0.000	0.049
37	0.799	0.418

Table B-5 continued

Sample ID	**9**	**10**
Congener #	**ng L^{-1}**	**ng L^{-1}**
38	0.000	0.000
39	0.000	0.000
40+41+71	2.853	1.135
42	1.267	0.762
43	0.270	0.224
45+51	1.672	1.471
46	0.738	0.450
48	0.726	0.447
49+69	3.012	1.585
50+53	1.221	1.012
52	5.688	3.293
54	0.000	0.000
55	0.000	0.000
56	1.330	0.488
57	0.000	0.000
58	0.000	0.000
59+62+75	0.504	0.266
60	0.563	0.314
61+70+74+76	2.521	1.743
63	0.000	0.000
64	1.869	1.106
66	1.384	0.698
67	0.000	0.000
68	0.000	0.000
72	0.000	0.000
73	0.000	0.000
77	0.000	0.000
78	0.000	0.000
79	0.000	0.000
80	0.000	0.000
81	0.000	0.000
82	0.204	0.000
83+99	0.347	0.153
84	0.708	0.418
85+86+87+97+109+116+117+119+125	0.643	0.366
88+91	0.000	0.000
89	0.000	0.000
90+101+113	0.852	0.484
92	0.230	0.065

Table B-5 continued

Sample ID **Congener #**	**9** **ng L^{-1}**	**10** **ng L^{-1}**
93+100	0.000	0.000
94	0.000	0.000
95	1.218	0.659
96	0.049	0.000
98+102	0.000	0.000
103	0.000	0.000
104	0.000	0.000
105	0.000	0.000
106	0.000	0.000
107	0.000	0.000
108+124	0.000	0.018
110+115	0.665	0.721
111	0.000	0.000
112	0.000	0.000
114	0.000	0.042
118	0.627	0.234
120	0.000	0.000
121	0.000	0.000
122	0.000	0.000
123	0.000	0.000
126	0.000	0.000
127	0.000	0.000
129+138+160+163	0.000	0.102
130	0.000	0.000
131	0.000	0.000
132	0.154	0.000
133	0.000	0.000
134+143	0.000	0.000
135+151	0.135	0.000
136	0.000	0.000
137+164	0.000	0.000
139+140	0.000	0.000
141	0.000	0.000
142	0.000	0.000
144	0.000	0.041
145	0.000	0.000
146	0.000	0.000
147+149	0.000	0.109
148	0.000	0.000

Table B-5 continued

Sample ID	**9**	**10**
Congener #	**ng L^{-1}**	**ng L^{-1}**
150	0.000	0.000
152	0.000	0.000
153+168	0.000	0.000
154	0.000	0.000
155	0.000	0.000
156+157	0.000	0.000
158	0.000	0.000
159	0.000	0.000
161	0.000	0.000
162	0.000	0.000
165	0.000	0.000
167	0.000	0.000
169	0.000	0.000
170	0.070	0.000
171+173	0.046	0.000
172	0.000	0.000
174	0.000	0.000
175	0.000	0.000
176	0.000	0.000
177	0.000	0.121
178	0.000	0.039
179	0.086	0.000
180+193	0.000	0.071
181	0.000	0.083
182	0.000	0.018
183	0.000	0.011
184	0.000	0.051
185	0.000	0.000
186	0.000	0.025
187	0.166	0.041
188	0.087	0.000
189	0.000	0.000
190	0.093	0.000
191	0.000	0.054
192	0.047	0.000
194	0.000	0.000
195	0.000	0.000
196	0.000	0.000
197	0.000	0.021

Table B-5 continued

Sample ID **Congener #**	**9** **ng L^{-1}**	**10** **ng L^{-1}**
198+199	0.000	0.000
200	0.000	0.000
201	0.000	0.000
202	0.000	0.000
203	0.000	0.000
205	0.000	0.000
206	0.000	0.040
207	0.000	0.063
208	0.000	0.000
209	0.000	0.037
Total	**69.239**	**36.657**

Figure B-4 Photographs of IHSC 2009 field campaign. Top photographs show the core collecting devise, a submersible vibro-coring system. Bottom photographs show how the cores were sliced and mixed

APPENDIX C: SUPPLEMENTAL INFORMATION CHAPTER IV

Information Referenced in Chapter IV: PCB Congener Concentrations used for Release Simulation

Table C-1 PCB sediment concentrations of individual congeners considered for the release simulation of PCBs. Congeners are ordered by “IUPAC” nomenclature (2)

Table C-1 PCB sediment concentrations of individual congeners considered for the release simulation of PCBs. Congeners are ordered by “IUPAC” nomenclature (2)

Congener #	**Scenario I Core 1 0.107 - 0.122 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario II Core 1 0.274 – 0.290 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario III Core 2 0.335 – 0.366 m section Sediment Concentration (ng g^{-1} d.w.)**
1	83.000	4.700	22.000
2	20.000	1.800	3.000
3	47.000	2.900	9.800
4	670.000	26.000	460.000
5	33.000	0.000	0.000
6	390.000	15.000	200.000
7	66.000	2.400	19.000
8	1900.000	64.000	1100.000
9	130.000	4.800	55.000
10	32.000	0.860	13.000
11	21.000	2.300	10.000
12+13	130.000	4.400	27.000
15	850.000	29.000	360.000
16	2200.000	80.000	910.000
17	2200.000	79.000	960.000
18+30	4800.000	190.000	2000.000
19	470.000	16.000	210.000
20+28	6100.000	200.000	2200.000
21+33	3400.000	120.000	1500.000
22	2100.000	72.000	680.000
23	6.400	0.000	3.000
24	0.000	0.000	0.000
25	410.000	13.000	170.000
26+29	1000.000	36.000	440.000
27	290.000	12.000	150.000
31	6000.000	210.000	2100.000
32	1500.000	51.000	540.000
34	22.000	1.000	8.500
35	73.000	3.600	27.000
36	37.000	0.000	6.200
37	1900.000	51.000	640.000
38	9.700	2.700	1.100
39	18.000	1.800	3.300
41+40+71	3000.000	110.000	660.000
42	1500.000	50.000	300.000
43	250.000	6.500	55.000
44+47+65	4600.000	190.000	970.000
45+51	1300.000	41.000	280.000
46	420.000	14.000	95.000
48	1100.000	47.000	290.000
49+69	2900.000	110.000	590.000
50+53	830.000	31.000	190.000
52	4800.000	210.000	980.000
54	12.000	0.000	3.200

Table C-1 continued

Congener #	**Scenario I Core 1 0.107 - 0.122 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario II Core 1 0.274 – 0.290 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario III Core 2 0.335 – 0.366 m section Sediment Concentration (ng g^{-1} d.w.)**
55	70.000	0.000	0.000
56	2300.000	76.000	410.000
57	24.000	0.000	8.200
58	10.000	0.000	0.000
59+62+75	450.000	12.000	110.000
60	1300.000	46.000	280.000
61+70+74+76	5700.000	270.000	1300.000
63	190.000	4.100	33.000
64	2200.000	78.000	410.000
66	4400.000	160.000	850.000
67	150.000	4.300	37.000
68	8.000	0.000	2.200
72	18.000	0.000	2.900
73	0.000	0.000	0.000
77	470.000	12.000	72.000
78	0.000	0.000	0.000
79	16.000	0.000	0.000
80	2.300	0.000	0.000
81	23.000	0.000	5.000
82	390.000	18.000	48.000
83+99	880.000	62.000	120.000
84	630.000	30.000	71.000
85+116+117	490.000	14.000	26.000
86+87+97+109+119+125	1300.000	67.000	160.000
88+91	440.000	19.000	33.000
89	71.000	2.700	8.400
90+101+113	1400.000	74.000	180.000
92	240.000	13.000	31.000
93+100	25.000	0.000	0.000
94	18.000	0.000	1.900
95	1200.000	68.000	170.000
96	37.000	1.600	4.400
98+102	95.000	7.500	15.000
103	11.000	0.000	1.300
104	0.900	0.000	0.000
105	880.000	35.000	72.000
106	1.400	0.000	0.000
107	110.000	7.300	11.000
108+124	58.000	2.700	5.900
110+115	1600.000	98.000	130.000
111	0.290	0.000	0.000
112	0.000	0.000	0.000
114	55.000	2.300	5.300
118	1400.000	71.000	130.000
120	0.000	0.000	0.000
121	0.000	0.000	0.000
122	31.000	0.000	2.900
123	40.000	1.400	3.200

Table C-1 continued

Congener #	**Scenario I Core 1 0.107 - 0.122 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario II Core 1 0.274 – 0.290 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario III Core 2 0.335 – 0.366 m section Sediment Concentration (ng g^{-1} d.w.)**
126	0.000	0.000	0.000
127	0.000	0.000	0.000
129+138+163	470.000	37.000	190.000
130	28.000	2.900	7.100
131	7.600	0.000	2.200
132	150.000	15.000	67.000
133	4.800	0.000	2.000
134+143	33.000	0.000	8.700
135+151	140.000	13.000	82.000
136	60.000	5.200	33.000
137+164	57.000	4.400	14.000
139+140	8.200	0.000	2.200
141	91.000	6.800	44.000
142	0.000	0.000	0.000
144	23.000	2.300	12.000
145	0.000	0.000	0.000
146	54.000	4.300	24.000
147+149	340.000	28.000	170.000
148	0.000	0.000	0.000
150	0.490	0.000	0.000
152	0.000	0.000	0.000
153+168	330.000	32.000	160.000
154	2.800	0.000	0.000
155	0.890	0.000	0.000
156+157	58.000	0.000	14.000
158	47.000	2.900	15.000
159	0.000	0.000	0.000
160	0.000	0.000	0.000
161	0.000	0.000	0.000
162	2.100	0.000	0.000
165	0.000	0.000	0.000
167	16.000	1.700	5.000
169	0.470	1.500	3.000
170	91.000	6.700	51.000
171+173	30.000	2.300	19.000
172	17.000	1.400	12.000
174	100.000	8.400	70.000
175	4.300	0.000	3.300
176	14.000	0.970	9.500
177	56.000	5.200	39.000
178	20.000	2.000	15.000
179	46.000	3.600	34.000
180+193	200.000	22.000	130.000
181	0.000	0.000	0.000
182	0.000	0.000	0.000
183	65.000	9.500	43.000
184	0.000	0.000	0.000
185	0.000	0.000	0.000

Table C-1 continued

Congener #	**Scenario I Core 1 0.107 - 0.122 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario II Core 1 0.274 – 0.290 m section Sediment Concentration (ng g^{-1} d.w.)**	**Scenario III Core 2 0.335 – 0.366 m section Sediment Concentration (ng g^{-1} d.w.)**
186	0.000	0.000	0.000
187	120.000	12.000	78.000
188	0.000	0.000	0.360
189	3.200	0.000	2.000
190	19.000	1.900	11.000
191	3.600	0.000	2.500
192	0.000	0.000	0.000
194	41.000	8.300	27.000
195	18.000	1.800	12.000
196	23.000	3.900	16.000
197	0.000	0.000	0.000
198+199	49.000	16.000	35.000
200	7.400	0.000	6.300
201	6.400	1.000	4.500
202	9.800	3.900	6.300
203	28.000	8.800	19.000
205	1.900	0.000	1.300
206	16.000	29.000	7.300
207	2.200	2.100	1.300
208	4.700	10.000	1.700
209	4.500	31.000	0.850
Total	**89000**	**3700**	**25400**

Additional Information: Results from the MCR-ALS Analysis and Sample Concentrations

Printout of the Matlab results from the MCR-ALS analysis.

Table C-2	Congener profile distribution (fraction) of Aroclors 1016, 1221, 1242, 1254 and 1248
Table C-3	Concentration of PCB congeners in cores 1 and 2 in IHSC sampled May 8th 2009

Printout of the Matlab results from the MCR-ALS analysis.

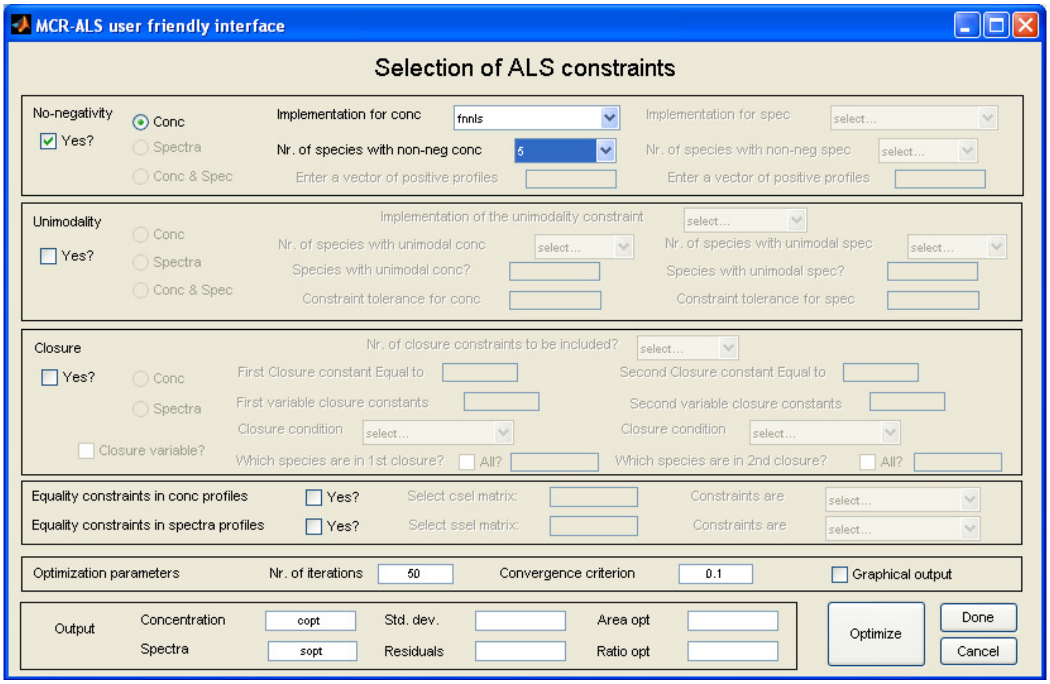

MCR-ALS user friendly interface

Selection of the data set

Data matrix: Core1

Initial estimate: Aroclor

Nr. of matrices: 1


MCR-ALS user friendly interface

Selection of ALS constraints

No-negativity ☑ Yes? ● Conc ○ Spectra ○ Conc & Spec

Implementation for conc: fnnls

Nr. of species with non-neg conc: 5

Implementation for spec: select...

Nr. of species with non-neg spec: select...

Enter a vector of positive profiles

Unimodality ☐ Yes? ○ Conc ○ Spectra ○ Conc & Spec

Implementation of the unimodality constraint: select...

Nr. of species with unimodal conc: select...

Nr. of species with unimodal spec: select...

Species with unimodal conc?

Species with unimodal spec?

Constraint tolerance for conc

Constraint tolerance for spec

Closure ☐ Yes? ○ Conc ○ Spectra ☐ Closure variable?

Nr. of closure constraints to be included?: select...

First Closure constant Equal to

Second Closure constant Equal to

First variable closure constants

Second variable closure constants

Closure condition: select...

Closure condition: select...

Which species are in 1st closure? ☐ All?

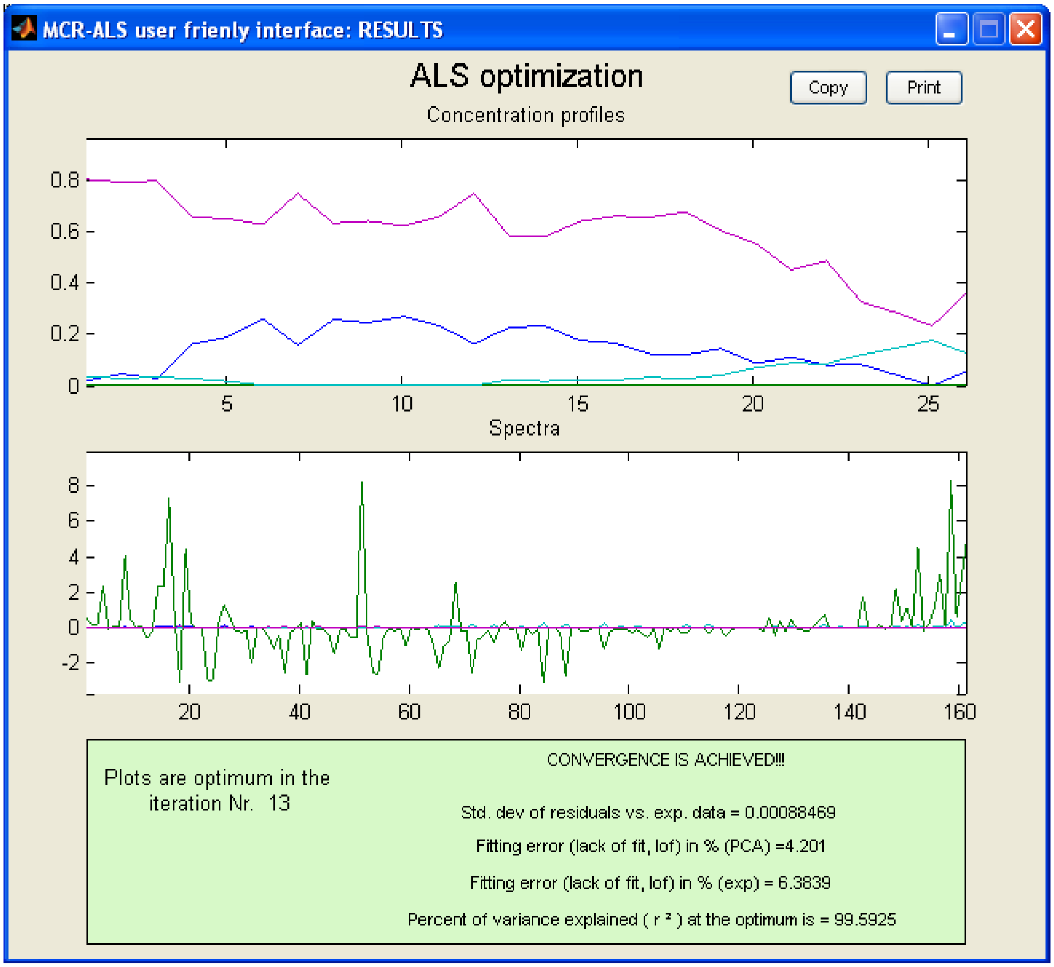
Which species are in 2nd closure? ☐ All?

Equality constraints in conc profiles ☐ Yes? Select csel matrix: Constraints are: select...

Equality constraints in spectra profiles ☐ Yes? Select ssel matrix: Constraints are: select...

Optimization parameters Nr. of iterations: 50 Convergence criterion: 0.1 ☐ Graphical output

Output Concentration: copt Spectra: sopt Std. dev. Residuals Area opt Ratio opt



```
Plots are optimum in the
    iteration Nr.  13

CONVERGENCE IS ACHIEVED!!!

Std. dev of residuals vs. exp. data = 0.00088469

Fitting error (lack of fit, lof) in % (PCA) =4.201

Fitting error (lack of fit, lof) in % (exp) = 6.3839

Percent of variance explained ( r ² ) at the optimum is = 99.5925
```

Table C-2 Congener profile distribution (fraction) of Aroclors 1016, 1221, 1242, 1254 and 1248

Congener #	**Aroclor 1016**	**Aroclor 1221**	**Aroclor 1242**	**Aroclor 1254**	**Aroclor 1248**
1	0.00685	0.45954	0.00798	0.00007	0.00021
2	0.00035	0.02942	0.00030	0.00000	0.00000
3	0.00207	0.19631	0.00199	0.00000	0.00000
4	0.01548	0.02369	0.01533	0.00000	0.00151
5	0.00000	0.08754	0.06455	0.00000	0.00000
6	0.01307	0.02288	0.01142	0.00000	0.00038
7	0.00276	0.01174	0.00249	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00004	0.00390
9	0.00427	0.00968	0.00383	0.00000	0.00000
10	0.00136	0.00409	0.00131	0.00000	0.00000
11	0.00000	0.00050	0.00028	0.00000	0.00000
12+13	0.00277	0.00830	0.00225	0.00000	0.00000
15	0.01789	0.01764	0.01475	0.00000	0.00043
16	0.04178	0.00516	0.03264	0.00000	0.00930
17	0.11082	0.01270	0.08950	0.00067	0.01335
18+30	0.03587	0.02048	0.01315	0.01223	0.03589
19	0.01083	0.00148	0.00879	0.00000	0.00187
20+28	0.15222	0.01592	0.11553	0.00076	0.04995
21+33	0.06301	0.00640	0.04781	0.00015	0.02570
22	0.03604	0.00378	0.02733	0.00012	0.01601
23	0.00099	0.00017	0.00073	0.00000	0.00000
24	0.00359	0.00052	0.00283	0.00000	0.00000
25	0.00761	0.00111	0.00584	0.00000	0.00009
26+29	0.03160	0.00384	0.02428	0.00000	0.00347
27	0.03887	0.00483	0.03124	0.00000	0.00226
31	0.07982	0.00813	0.06065	0.00133	0.04401
32	0.02240	0.00259	0.01756	0.00007	0.00942
34	0.00026	0.00000	0.00019	0.00000	0.00000
35	0.00099	0.00000	0.00077	0.00000	0.00000
36	0.00000	0.00000	0.00000	0.00010	0.00000
37	0.01729	0.00229	0.01601	0.00027	0.00836
38	0.00000	0.00000	0.00000	0.00006	0.00000
39	0.00000	0.00000	0.00000	0.00000	0.00000
40+41+71	0.02584	0.00233	0.01861	0.00224	0.03738
42	0.01266	0.00131	0.00928	0.00122	0.01499
43	0.02697	0.00255	0.01972	0.00481	0.00337
44+47+65	0.04372	0.00395	0.09939	0.00421	0.09449

Table C-2 continued

Congener #	Aroclor 1016	Aroclor 1221	Aroclor 1242	Aroclor 1254	Aroclor 1248
45+51	0.01472	0.00142	0.01061	0.00118	0.01341
46	0.00378	0.00031	0.00277	0.00023	0.00374
48	0.00000	0.00000	0.00831	0.00000	0.02089
49+69	0.03118	0.00310	0.02325	0.00204	0.04475
50+53	0.00000	0.00000	0.00024	0.00000	0.00928
52	0.02932	0.00280	0.02132	0.01087	0.07094
54	0.00017	0.00000	0.00012	0.00000	0.00000
55	0.00000	0.00000	0.00064	0.00014	0.00000
56	0.00117	0.00000	0.01036	0.01820	0.02371
57	0.00020	0.00000	0.00018	0.00000	0.00000
58	0.00065	0.00008	0.00069	0.00000	0.00000
59+62+75	0.02580	0.00251	0.00278	0.00572	0.00772
60	0.00027	0.00059	0.00293	0.00453	0.02165
61+70+74+76	0.03030	0.00741	0.06086	0.13732	0.10593
63	0.00000	0.00000	0.00000	0.00132	0.00226
64	0.01495	0.00133	0.01155	0.00308	0.03096
66	0.00781	0.00278	0.02286	0.03490	0.06601
67	0.00099	0.00019	0.00123	0.00013	0.00074
68	0.00000	0.00000	0.00000	0.00011	0.00000
72	0.00016	0.00000	0.00012	0.00000	0.00000
73	0.00136	0.00010	0.00102	0.00000	0.00000
77	0.00000	0.00024	0.00204	0.00196	0.00445
78	0.00000	0.00000	0.00000	0.00000	0.00000
79	0.00000	0.00000	0.00000	0.00000	0.00000
80	0.00000	0.00000	0.00000	0.00000	0.00000
81	0.00000	0.00000	0.00019	0.00052	0.00000
82	0.00000	0.00000	0.00158	0.01291	0.00527
83+99	0.00065	0.00114	0.00804	0.10679	0.02121
84	0.00107	0.00044	0.00244	0.01352	0.01016
85+116+117	0.00000	0.00027	0.00202	0.02287	0.00573
86+87+97+109+119+125	0.00000	0.00100	0.00706	0.07268	0.01957
88+91	0.00123	0.00019	0.00147	0.00446	0.00594
89	0.00000	0.00000	0.00000	0.00000	0.00072
90+101+113	0.00064	0.00081	0.00485	0.05445	0.02007
92	0.00024	0.00000	0.00082	0.00565	0.00355
93+100	0.00000	0.00000	0.00000	0.00000	0.00296
94	0.00000	0.00000	0.00011	0.00015	0.00000
95	0.00000	0.00000	0.00012	0.00000	0.01930
96	0.00028	0.00000	0.00018	0.00020	0.00081
98+102	0.00302	0.00044	0.00272	0.00947	0.00000

Table C-2 continued

Congener #	Aroclor 1016	Aroclor 1221	Aroclor 1242	Aroclor 1254	Aroclor 1248
103	0.00000	0.00000	0.00006	0.00000	0.00000
104	0.00000	0.00000	0.00000	0.00000	0.00000
105	0.00000	0.00000	0.00000	0.00040	0.01258
106	0.00000	0.00063	0.00447	0.12401	0.00000
107	0.00000	0.00000	0.00042	0.00000	0.00237
108+124	0.00000	0.00000	0.00047	0.01672	0.00087
110+115	0.00000	0.00079	0.00531	0.07479	0.02838
111	0.00000	0.00013	0.00000	0.00000	0.00000
112	0.00000	0.00000	0.00024	0.00135	0.00000
114	0.00000	0.00045	0.00332	0.07842	0.00000
118	0.00000	0.00000	0.00022	0.00365	0.01885
120	0.00000	0.00000	0.00000	0.00228	0.00000
121	0.00000	0.00000	0.00035	0.00068	0.00000
122	0.00000	0.00000	0.00000	0.00000	0.00000
123	0.00000	0.00000	0.00021	0.00317	0.00000
126	0.00000	0.00000	0.00000	0.00000	0.00000
127	0.00000	0.00000	0.00000	0.00000	0.00000
129+138+163	0.00000	0.00000	0.00000	0.00064	0.00439
130	0.00000	0.00000	0.00011	0.01420	0.00000
131	0.00000	0.00000	0.00000	0.00000	0.00000
132	0.00000	0.00000	0.00008	0.01333	0.00166
133	0.00000	0.00000	0.00007	0.00529	0.00000
134+143	0.00000	0.00000	0.00002	0.00113	0.00000
135+151	0.00000	0.00000	0.00000	0.00265	0.00068
136	0.00000	0.00000	0.00000	0.00000	0.00059
137+164	0.00000	0.00000	0.00000	0.00000	0.00000
139+140	0.00000	0.00000	0.00007	0.00610	0.00000
141	0.00000	0.00000	0.00000	0.00042	0.00114
142	0.00000	0.00000	0.00002	0.00149	0.00011
144	0.00000	0.00000	0.00000	0.00000	0.00000
145	0.00000	0.00000	0.00002	0.00080	0.00000
146	0.00000	0.00000	0.00002	0.00232	0.00064
147+149	0.00000	0.00000	0.00039	0.02688	0.00299
148	0.00000	0.00000	0.00004	0.00191	0.00000
150	0.00000	0.00000	0.00002	0.00089	0.00000
152	0.00000	0.00000	0.00000	0.00000	0.00000
153+168	0.00000	0.00000	0.00013	0.01157	0.00268
154	0.00000	0.00000	0.00000	0.00008	0.00011
155	0.00000	0.00000	0.00000	0.00000	0.00000
156+157	0.00000	0.00000	0.00000	0.00000	0.00037

Table C-2 continued

Congener #	Aroclor 1016	Aroclor 1221	Aroclor 1242	Aroclor 1254	Aroclor 1248
158	0.00000	0.00000	0.00000	0.00000	0.00000
159	0.00000	0.00000	0.00004	0.00784	0.00000
160	0.00000	0.00000	0.00000	0.00246	0.00000
161	0.00000	0.00000	0.00007	0.00921	0.00000
162	0.00000	0.00000	0.00001	0.00182	0.00000
165	0.00000	0.00000	0.00004	0.00353	0.00000
167	0.00000	0.00000	0.00000	0.00000	0.00000
169	0.00000	0.00000	0.00000	0.00000	0.00000
170	0.00000	0.00000	0.00000	0.00131	0.00000
171+173	0.00000	0.00000	0.00000	0.00084	0.00000
172	0.00000	0.00000	0.00000	0.00000	0.00000
174	0.00000	0.00000	0.00000	0.00160	0.00000
175	0.00000	0.00000	0.00000	0.00175	0.00000
176	0.00000	0.00000	0.00000	0.00000	0.00000
177	0.00000	0.00000	0.00000	0.00000	0.00000
178	0.00000	0.00000	0.00000	0.00000	0.00000
179	0.00000	0.00000	0.00000	0.00023	0.00033
180+193	0.00000	0.00000	0.00000	0.00460	0.00178
181	0.00000	0.00000	0.00000	0.00098	0.00000
182	0.00000	0.00000	0.00000	0.00204	0.00000
183	0.00000	0.00000	0.00000	0.00029	0.00000
184	0.00000	0.00000	0.00000	0.00035	0.00000
185	0.00000	0.00000	0.00000	0.00281	0.00000
186	0.00000	0.00000	0.00000	0.00023	0.00028
187	0.00000	0.00000	0.00000	0.00000	0.00000
188	0.00000	0.00000	0.00000	0.00000	0.00000
189	0.00000	0.00000	0.00000	0.00047	0.00000
190	0.00000	0.00000	0.00000	0.00000	0.00000
191	0.00000	0.00000	0.00000	0.00712	0.00000
192	0.00000	0.00000	0.00000	0.00000	0.00000
194	0.00000	0.00000	0.00000	0.00000	0.00040
195	0.00000	0.00000	0.00000	0.00000	0.00000
196	0.00000	0.00000	0.00000	0.00000	0.00000
197	0.00000	0.00000	0.00000	0.00000	0.00000
198+199	0.00000	0.00000	0.00000	0.00010	0.00000
200	0.00000	0.00000	0.00000	0.00000	0.00000
201	0.00000	0.00000	0.00000	0.00000	0.00000
202	0.00000	0.00000	0.00000	0.00000	0.00012
203	0.00000	0.00000	0.00000	0.00138	0.00000
205	0.00000	0.00000	0.00000	0.00000	0.00000

Table C-2 continued

Congener #	**Aroclor 1016**	**Aroclor 1221**	**Aroclor 1242**	**Aroclor 1254**	**Aroclor 1248**
206	0.00000	0.00000	0.00000	0.00012	0.00034
207	0.00000	0.00000	0.00000	0.00000	0.00000
208	0.00000	0.00000	0.00000	0.00000	0.00032
209	0.00000	0.00000	0.00000	0.00000	0.00000

Table C-3 Concentration of PCB congeners in cores 1 and 2 in IHSC sampled May 8th 2009

Sample ID (Core 1)	**1**	**2**	**3**	**4**	**5**
Core section (cm)	0-15	15-30	30-46	46-61	61-76
Lab batch #	4	4	4	5	5
PCB14 % recovery	58	59	63	54	61
d-PCB65 % recovery	59	59	66	74	68
PCB166 % recovery	60	66	72	73	69
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	68	50	50	63	62
Total organic carbon (%)	3.12	3.76	4.06	3.80	4.04
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	2.93	3.22	2.12	3.20	10.36
2	1.33	1.12	0.83	1.47	3.49
3	3.91	2.96	2.72	4.46	9.27
4	21.48	31.40	17.75	30.06	99.33
5	0.34	0.00	0.00	1.83	5.63
6	34.91	47.98	33.01	51.28	119.32
7	2.56	3.29	2.25	4.12	12.52
8	63.08	88.61	56.29	105.78	302.52
9	3.99	6.01	3.62	6.81	21.78
10	0.75	1.40	0.68	1.47	5.16
11	4.08	3.26	2.59	4.29	6.20
12+13	19.52	22.09	18.28	34.42	64.53
15	66.90	61.69	51.43	105.12	178.37
16	114.32	130.13	92.32	191.36	428.86
17	133.26	139.79	103.46	218.56	458.05
18+30	306.65	324.16	234.56	466.28	970.71
19	23.99	26.77	18.69	40.02	84.71
20+28	525.21	492.71	401.16	852.14	1412.71
21+33	160.45	174.78	128.67	264.86	554.69
22	145.50	145.81	115.27	241.72	441.35
23	0.00	0.00	0.00	1.13	2.06
24	0.00	0.00	0.00	0.00	0.00
25	87.25	84.22	70.39	146.25	234.12
26+29	126.42	117.60	93.25	201.93	304.36
27	25.23	24.65	19.05	34.06	65.29
31	456.86	450.76	352.23	746.97	1319.28
32	116.31	117.22	88.46	179.64	326.66
34	3.54	2.84	2.62	5.86	8.77
35	7.51	7.51	5.67	13.74	19.28

Table C-3 continued

Sample ID (Core 1) **Congener #**	**1** **ng g^{-1} d.w.**	**2** **ng g^{-1} d.w.**	**3** **ng g^{-1} d.w.**	**4** **ng g^{-1} d.w.**	**5** **ng g^{-1} d.w.**
36	4.95	4.08	4.07	7.69	0.68
37	127.16	112.81	94.47	254.16	322.04
38	1.18	0.74	0.56	2.27	3.31
39	1.35	1.22	1.26	4.36	6.13
40+41+71	405.29	361.01	296.95	398.30	773.73
42	204.02	184.11	151.89	238.62	398.70
43	25.84	21.11	22.97	36.55	65.51
44+47+65	707.24	618.04	526.62	788.38	1272.15
45+51	134.31	123.40	98.54	185.38	311.76
46	45.89	38.92	34.43	52.57	95.62
48	114.58	110.86	109.19	159.08	286.53
49+69	433.68	377.50	331.33	510.72	833.56
50+53	106.80	92.72	75.62	122.24	212.93
52	854.87	742.64	621.85	836.28	1343.54
54	1.62	1.36	1.23	2.36	4.03
55	0.00	0.00	0.00	12.16	23.37
56	274.57	243.79	207.04	331.78	556.74
57	3.23	3.73	3.76	5.22	8.74
58	0.00	0.00	0.00	2.68	5.12
59+62+75	48.45	44.67	34.35	72.43	126.42
60	151.42	135.24	111.65	183.48	313.62
61+70+74+76	926.11	839.58	698.25	804.12	1386.67
63	17.97	20.08	16.33	34.14	55.68
64	313.38	275.81	229.78	368.53	611.21
66	570.86	502.87	426.39	631.58	1026.84
67	12.50	15.56	12.81	27.60	48.62
68	3.40	2.18	2.31	4.24	5.67
72	5.01	3.58	3.41	5.19	7.97
73	0.00	0.00	0.00	0.00	0.00
77	54.88	45.24	40.50	83.16	114.27
78	0.00	0.00	1.07	0.00	2.35
79	3.01	3.20	2.46	4.00	4.87
80	0.00	0.00	0.00	0.00	2.31
81	0.00	2.59	2.78	2.94	7.29
82	81.05	67.81	59.33	80.91	123.57
83+99	264.53	220.76	193.42	209.74	299.79
84	128.27	108.58	95.23	133.22	196.89
85+116+117	74.45	62.56	52.42	116.15	162.68
86+87+97+109+119+125	279.23	234.89	204.39	142.53	204.74
88+91	81.43	70.12	60.31	67.07	97.12

Table C-3 continued

Sample ID (Core 1)	1	2	3	4	5
Congener #	ng g $^{-1}$ d.w.	ng g $^{-1}$ d.w.	ng g $^{-1}$ d.w.	ng g $^{-1}$ d.w.	ng g $^{-1}$ d.w.
89	14.54	12.65	10.28	15.46	23.65
90+101+113	303.56	255.16	224.21	322.08	470.10
92	59.93	49.98	45.20	62.23	86.80
93+100	31.27	25.30	22.24	7.43	11.14
94	4.42	3.69	3.47	4.83	7.79
95	286.22	237.38	207.85	272.11	395.53
96	7.57	6.20	5.67	8.06	13.41
98+102	0.00	0.00	0.00	22.71	34.17
103	3.39	2.78	2.67	3.80	5.96
104	0.00	0.00	0.00	0.71	1.35
105	139.09	120.34	104.08	178.43	248.78
106	0.00	0.00	0.00	2.06	1.39
107	28.66	22.47	21.04	24.14	35.99
108+124	10.52	9.73	8.13	13.87	21.54
110+115	410.56	342.87	302.31	398.15	568.86
111	0.00	0.00	0.00	0.75	1.84
112	0.00	0.00	0.00	0.00	0.00
114	10.79	9.09	8.08	11.94	18.19
118	276.16	234.45	203.96	311.14	440.61
120	0.00	0.00	0.00	1.41	2.26
121	0.00	0.00	0.00	0.00	1.43
122	6.83	5.55	5.53	7.44	11.53
123	5.99	3.81	3.43	10.31	13.26
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	1.57	2.11
129+138+163	147.68	105.43	102.73	181.14	235.27
130	9.17	5.20	5.79	11.35	15.19
131	2.91	1.62	1.65	2.89	5.15
132	54.22	41.13	38.86	57.10	76.53
133	1.94	1.55	1.56	3.12	4.51
134+143	0.00	0.00	0.00	13.68	20.01
135+151	50.69	40.93	36.92	58.50	74.79
136	22.51	17.04	15.09	22.96	31.55
137+164	15.48	9.22	10.07	23.53	28.67
139+140	2.95	1.76	1.82	3.84	7.04
141	26.19	20.07	16.56	30.99	43.38
142	0.00	0.00	0.00	0.00	1.55
144	7.79	5.29	5.19	9.17	12.34
145	0.00	0.00	0.00	0.57	1.71
146	21.67	15.84	14.86	23.05	29.49

Table C-3 continued

Sample ID (Core 1) **Congener #**	**1** **ng g^{-1} d.w.**	**2** **ng g^{-1} d.w.**	**3** **ng g^{-1} d.w.**	**4** **ng g^{-1} d.w.**	**5** **ng g^{-1} d.w.**
147+149	112.68	85.90	81.14	132.44	169.86
148	0.00	0.00	0.00	0.00	1.75
150	0.00	0.00	0.00	0.85	1.66
152	0.00	0.00	0.00	0.88	1.87
153+168	115.54	87.46	82.22	132.03	169.30
154	0.00	0.00	0.00	2.25	3.37
155	0.00	0.00	0.00	0.41	1.30
156+157	0.00	0.00	0.00	22.43	29.59
158	12.83	9.54	8.85	18.18	24.40
159	0.00	0.00	0.00	1.43	2.03
160	0.00	0.00	0.00	0.00	1.70
161	0.00	0.00	0.00	0.46	1.63
162	0.00	0.00	0.00	1.70	2.74
165	0.00	0.00	0.00	0.64	1.65
167	4.52	3.78	3.86	6.58	9.76
169	1.04	1.79	1.40	0.81	1.79
170	33.96	25.40	23.49	40.70	51.68
171+173	10.02	8.01	7.27	14.76	19.60
172	6.02	4.90	4.31	7.53	10.49
174	31.67	25.93	23.06	41.87	52.93
175	0.99	0.73	0.81	2.27	3.90
176	4.62	3.68	3.28	6.44	9.32
177	20.43	15.66	15.28	24.94	31.21
178	7.65	5.96	5.87	10.02	12.55
179	16.02	12.23	11.27	19.72	24.95
180+193	78.26	59.84	55.10	90.59	112.60
181	0.00	0.00	0.00	1.27	2.08
182	0.00	0.00	0.00	1.00	2.10
183	29.63	23.12	21.18	29.45	36.14
184	0.00	0.00	0.00	0.79	1.73
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.73	1.72
187	42.18	33.36	29.37	51.66	61.46
188	0.00	0.00	0.00	0.77	1.76
189	0.00	0.86	0.00	2.53	3.86
190	7.08	5.51	5.20	9.70	11.92
191	1.19	0.94	0.48	2.68	3.95
192	0.00	0.00	0.00	1.09	1.80
194	20.78	14.12	13.61	19.56	26.47
195	7.74	5.39	5.11	8.77	11.90

Table C-3 continued

Sample ID (Core 1) **Congener #**	**1** **ng g $^{-1}$ d.w.**	**2** **ng g $^{-1}$ d.w.**	**3** **ng g $^{-1}$ d.w.**	**4** **ng g $^{-1}$ d.w.**	**5** **ng g $^{-1}$ d.w.**
196	10.26	7.28	7.14	11.22	15.64
197	0.00	0.00	0.00	1.65	3.12
198+199	21.55	16.02	15.51	24.03	32.11
200	2.70	1.61	1.83	4.06	5.69
201	2.54	2.00	1.89	3.97	5.65
202	3.87	3.11	3.08	5.55	7.40
203	11.99	8.74	8.51	14.14	18.54
205	0.00	0.00	0.00	1.95	3.62
206	8.41	6.11	5.97	8.73	12.91
207	1.11	0.74	0.76	2.13	3.91
208	2.19	1.52	1.46	3.23	5.34
209	3.64	2.78	2.72	4.24	8.97
Total	**11516.63**	**10295.91**	**8626.64**	**13797.97**	**22840.47**

Table C-3 continued

Sample ID (Core 1)	**6**	**7**	**8**	**9**	**10**
Core section (cm)	76-91	91-107	107-122	122-137	152-168
Lab batch #	5	1	5	5	5
PCB14 % recovery	65	55	60	44	55
d-PCB65 % recovery	75	54	67	47	59
PCB166 % recovery	73	76	82	50	62
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	57	51	51	48	48
Total organic carbon (%)	5.78	6.74	6.96	6.73	6.74
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
1	36.13	96.05	83.40	66.92	108.19
2	8.62	21.69	19.72	17.67	23.81
3	24.42	55.27	47.20	43.07	74.91
4	378.63	727.00	672.30	496.17	676.57
5	20.61	19.80	33.37	25.21	41.07
6	280.15	414.08	385.44	278.54	406.01
7	43.47	65.00	65.58	48.89	78.17
8	1118.52	1713.25	1860.65	1377.14	1915.67
9	80.97	138.37	133.43	98.27	142.26
10	19.10	36.05	31.62	23.01	34.01
11	12.58	36.90	20.56	15.48	17.71
12+13	123.66	106.19	127.48	95.98	135.89
15	600.69	665.46	854.01	681.55	930.13
16	1452.18	1666.47	2219.60	1753.77	2126.39
17	1521.40	1877.47	2241.67	1730.00	2095.64
18+30	3166.80	4248.87	4815.02	3790.06	4535.69
19	313.24	469.60	474.96	393.05	403.46
20+28	4234.82	4663.37	6071.15	4537.48	5683.24
21+33	2129.01	2743.35	3433.71	2580.73	3145.19
22	1417.46	1519.67	2142.57	1625.23	1974.20
23	4.44	3.64	6.40	4.34	6.50
24	0.00	0.00	0.00	0.00	0.00
25	429.53	273.06	411.30	303.29	416.27
26+29	775.64	766.04	1034.67	785.67	1036.53
27	202.23	280.12	289.07	222.25	279.32
31	4072.10	4785.18	6048.87	4569.08	5604.48
32	1022.48	1432.81	1503.35	1160.62	1366.26
34	19.59	16.08	22.19	17.07	23.45
35	54.62	51.83	72.93	56.13	70.67
36	26.25	27.40	37.16	30.53	2.91
37	1287.71	1173.54	1918.37	1554.16	1888.47
38	6.87	4.85	9.74	7.46	8.31

Table C-3 continued

Sample ID (Core 1) Congener #	6 ng g^{-1} d.w.	7 ng g^{-1} d.w.	8 ng g^{-1} d.w.	9 ng g^{-1} d.w.	10 ng g^{-1} d.w.
39	14.37	9.12	18.44	15.10	17.48
40+41+71	2040.30	2836.02	2999.56	2381.20	2695.38
42	1018.09	1326.74	1473.14	1185.43	1360.69
43	171.47	129.17	249.53	160.86	221.78
44+47+65	3218.51	4363.69	4649.06	3918.68	4397.43
45+51	895.08	1090.53	1325.79	1081.27	1236.44
46	262.86	344.61	416.81	321.92	353.12
48	795.66	1008.54	1144.04	989.54	1186.20
49+69	2054.43	2642.79	2943.53	2386.91	2809.28
50+53	555.43	766.90	825.28	679.35	778.06
52	3350.22	5120.20	4778.68	3917.67	4570.68
54	8.25	12.18	11.87	10.29	11.74
55	53.56	0.00	70.49	39.98	57.22
56	1514.42	1930.70	2276.75	1806.71	2041.50
57	16.96	25.55	23.69	18.22	23.79
58	6.75	0.00	10.09	8.44	7.09
59+62+75	317.77	348.52	446.82	359.17	430.63
60	864.01	1089.37	1344.55	1062.63	1220.32
61+70+74+76	3796.94	7099.07	5717.23	4584.63	5192.10
63	134.33	145.71	191.54	147.90	176.05
64	1538.08	1882.83	2249.91	1763.30	2029.07
66	2875.81	3681.35	4438.79	3522.64	4050.74
67	111.87	104.23	148.63	118.30	150.45
68	6.50	7.16	7.97	6.73	7.99
72	14.59	16.19	17.91	15.28	17.49
73	0.00	0.00	0.00	0.00	0.00
77	303.39	301.43	473.82	405.32	462.86
78	0.00	0.00	0.00	0.00	0.00
79	5.34	15.88	15.74	6.63	6.70
80	0.00	0.00	2.29	0.00	3.75
81	13.79	16.15	23.03	10.19	10.18
82	261.11	368.29	387.22	328.32	345.84
83+99	627.84	936.01	880.49	737.12	852.65
84	428.18	624.79	630.27	520.68	547.59
85+116+117	332.09	365.39	486.75	433.63	407.35
86+87+97+109+119+125	429.97	1364.24	1335.13	535.82	580.03
88+91	207.03	417.68	435.60	242.20	270.13
89	48.82	69.21	71.09	61.42	64.43
90+101+113	992.34	1382.72	1403.02	1216.89	1193.52
92	173.54	243.95	238.64	209.20	231.65

Table C-3 continued

Sample ID (Core 1)	**6**	**7**	**8**	**9**	**10**
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
93+100	17.85	0.00	24.78	23.55	25.67
94	12.88	18.09	18.17	15.90	17.32
95	847.87	1312.56	1160.99	1010.53	1117.89
96	26.64	40.89	36.85	33.58	36.54
98+102	68.58	205.09	95.46	82.62	94.91
103	8.80	11.65	11.27	10.46	11.44
104	0.00	0.00	0.90	0.00	0.83
105	553.98	759.15	879.28	755.14	786.71
106	26.00	0.00	1.39	0.00	2.14
107	71.04	135.75	106.46	90.90	96.30
108+124	39.32	54.79	58.19	49.18	54.11
110+115	1155.03	1768.70	1644.58	1378.07	1495.51
111	0.00	0.00	0.29	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	35.62	49.68	55.44	47.63	51.74
118	934.71	1304.18	1404.27	1235.37	1308.66
120	0.00	0.00	0.00	0.00	2.00
121	0.00	0.00	0.00	0.00	0.00
122	20.38	26.93	31.46	25.84	28.26
123	25.43	27.50	40.43	35.14	35.43
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+163	421.89	395.58	468.67	446.12	467.84
130	25.64	22.78	28.46	26.64	29.10
131	6.64	6.02	7.60	6.23	7.13
132	142.51	149.84	154.37	141.53	154.41
133	4.68	4.13	4.84	4.99	5.11
134+143	31.42	19.07	33.39	30.69	23.55
135+151	131.45	135.19	142.06	134.30	139.85
136	56.79	55.02	59.61	53.90	59.81
137+164	47.39	35.09	57.28	49.52	51.95
139+140	7.54	7.69	8.21	7.44	8.24
141	79.11	72.15	91.48	86.90	87.70
142	0.00	0.00	0.00	0.00	0.00
144	21.66	18.59	23.06	22.66	23.62
145	0.00	0.00	0.00	0.00	0.00
146	50.09	50.85	54.46	51.05	53.27
147+149	308.51	274.97	336.21	309.94	331.29
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.49	0.00	0.00

Table C-3 continued

Sample ID (Core 1) **Congener #**	**6** **ng g^{-1} d.w.**	**7** **ng g^{-1} d.w.**	**8** **ng g^{-1} d.w.**	**9** **ng g^{-1} d.w.**	**10** **ng g^{-1} d.w.**
152	0.00	0.00	0.00	1.24	0.00
153+168	298.22	297.09	331.47	326.71	328.15
154	2.53	0.00	2.84	2.42	2.93
155	0.13	0.00	0.89	0.00	0.00
156+157	48.85	0.00	57.80	57.95	59.62
158	43.04	37.90	46.95	45.54	48.13
159	0.00	0.00	0.00	0.00	1.04
160	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	2.02	1.75	2.11	1.20	1.73
165	0.00	0.00	0.00	0.00	0.00
167	14.66	13.49	16.33	1.90	17.43
169	0.43	4.50	0.47	0.00	0.00
170	73.24	79.28	91.06	86.29	86.62
171+173	25.78	23.85	30.38	27.68	27.93
172	13.73	16.58	16.94	15.68	15.12
174	83.73	102.03	104.88	93.08	89.09
175	3.61	3.17	4.31	4.30	4.07
176	12.35	11.28	14.49	12.32	12.55
177	47.63	47.40	55.66	51.12	49.44
178	16.63	17.71	19.81	18.16	17.62
179	38.90	38.23	45.52	39.53	38.96
180+193	164.04	197.61	200.88	196.80	187.14
181	0.00	0.00	0.00	0.00	0.77
182	0.00	0.00	0.00	0.00	0.00
183	54.57	55.78	64.72	62.03	58.63
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	97.07	100.76	117.23	107.62	101.21
188	0.00	0.00	0.00	0.00	0.00
189	2.46	1.98	3.21	3.53	3.32
190	15.34	16.81	18.73	18.15	16.96
191	3.28	4.39	3.60	3.60	3.41
192	0.00	0.00	0.00	0.00	0.00
194	30.15	40.86	41.31	43.34	37.48
195	13.66	15.88	17.57	17.02	15.68
196	18.62	20.88	22.70	22.87	19.82
197	0.00	0.00	0.00	0.00	0.00
198+199	37.74	45.16	49.01	48.90	43.12

Table C-3 continued

Sample ID (Core 1) **Congener #**	**6** **ng g $^{-1}$ d.w.**	**7** **ng g $^{-1}$ d.w.**	**8** **ng g $^{-1}$ d.w.**	**9** **ng g $^{-1}$ d.w.**	**10** **ng g $^{-1}$ d.w.**
200	6.46	5.12	7.42	7.36	6.69
201	5.12	5.51	6.37	6.15	5.37
202	7.88	8.35	9.77	8.98	8.15
203	21.93	27.22	27.74	27.55	24.97
205	1.43	1.96	1.93	2.08	1.79
206	13.16	15.92	16.30	17.26	14.90
207	1.70	2.21	2.20	2.24	1.80
208	3.89	4.46	4.67	4.88	4.06
209	4.04	5.09	4.49	6.78	4.10
Total	**60751.12**	**80417.46**	**89752.85**	**71156.46**	**83238.94**

Table C-3 continued

Sample ID (Core 1)	**11**	**12**	**13**	**14**	**15**
Core section (cm)	168-183	183-198	229-244	244-259	259-274
Lab batch #	5	5	4	5	4
PCB14 % recovery	60	73	52	59	59
d-PCB65 % recovery	64	74	80	78	78
PCB166 % recovery	61	69	50	72	53
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	47	44	50	50	50
Total organic carbon (%)	7.34	7.64	7.74	7.54	7.20
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
1	60.96	30.67	4.60	4.14	3.98
2	18.40	11.26	1.63	1.18	1.41
3	39.22	19.07	3.17	2.61	2.60
4	492.11	443.01	23.00	26.19	20.13
5	22.07	8.71	0.00	0.00	0.00
6	273.60	143.76	12.76	15.01	11.24
7	44.11	19.88	1.82	2.29	0.78
8	1370.73	740.51	57.25	71.62	50.09
9	94.10	50.49	4.09	4.58	3.81
10	21.02	17.42	0.74	0.63	0.46
11	16.44	10.90	1.36	1.87	1.32
12+13	89.30	53.30	3.66	4.48	3.32
15	635.95	453.30	24.85	26.70	21.54
16	1789.13	1440.02	79.29	83.10	65.78
17	1785.56	1450.64	65.22	81.37	60.70
18+30	3959.26	3349.35	185.96	198.03	153.71
19	406.74	315.36	12.04	16.77	10.58
20+28	4769.41	3728.11	183.39	210.99	165.99
21+33	2752.83	1856.20	101.53	122.77	90.39
22	1694.33	1227.42	62.48	75.00	55.76
23	4.17	3.41	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	0.00
25	307.09	213.48	12.71	14.72	11.02
26+29	812.25	617.97	33.85	46.07	29.59
27	224.99	169.55	10.64	8.88	9.91
31	4916.93	3967.30	191.27	220.98	171.26
32	1198.95	986.55	31.82	54.97	28.97
34	17.15	13.12	0.00	1.90	0.00
35	54.88	38.37	0.00	3.41	2.71
36	32.60	2.23	1.13	0.32	2.08
37	1486.43	1082.54	45.23	60.40	41.16
38	7.76	6.20	0.00	0.00	0.89

Table C-3 continued

Sample ID (Core 1) **Congener #**	**11** **ng g $^{-1}$ d.w.**	**12** **ng g $^{-1}$ d.w.**	**13** **ng g $^{-1}$ d.w.**	**14** **ng g $^{-1}$ d.w.**	**15** **ng g $^{-1}$ d.w.**
39	15.37	26.54	1.20	1.73	1.93
40+41+71	2626.13	1921.98	83.07	89.22	91.53
42	1286.39	1074.43	45.04	46.11	44.79
43	212.28	175.98	0.00	6.24	5.35
44+47+65	4152.09	3567.05	153.87	148.29	154.19
45+51	1153.02	968.35	34.40	42.59	34.04
46	348.61	313.80	12.05	13.37	12.04
48	1017.25	875.05	34.38	36.05	37.25
49+69	2620.72	2174.09	84.52	91.82	87.52
50+53	739.95	635.50	26.52	26.87	25.17
52	4371.67	3603.57	184.77	159.22	179.68
54	10.69	8.65	0.39	0.00	0.00
55	56.95	37.59	0.00	0.00	0.00
56	1973.86	1556.89	57.46	67.18	63.11
57	20.63	15.16	0.00	0.00	1.24
58	7.12	8.48	0.00	0.00	0.00
59+62+75	380.48	298.97	9.28	11.59	10.43
60	1175.97	942.85	31.85	39.06	34.76
61+70+74+76	5045.25	5866.79	184.88	238.71	212.99
63	168.94	134.03	5.07	5.26	5.09
64	1958.74	1613.25	64.32	72.10	63.77
66	3868.43	3114.04	123.64	132.79	132.13
67	127.51	96.98	3.01	4.38	3.20
68	6.11	4.40	0.00	0.00	0.69
72	16.46	11.29	0.00	0.00	0.66
73	0.00	0.00	0.00	0.00	0.00
77	388.83	295.83	8.48	13.73	9.65
78	0.00	0.00	0.00	0.00	0.00
79	8.18	5.14	0.00	0.00	0.00
80	0.34	0.00	0.00	0.00	0.00
81	18.07	9.54	0.00	0.00	0.00
82	357.02	278.11	11.50	13.79	12.00
83+99	833.69	649.86	42.10	54.02	43.77
84	576.85	475.32	22.53	24.05	21.60
85+116+117	441.34	347.70	10.12	13.71	12.30
86+87+97+109+119+125	568.49	969.24	44.16	52.23	45.23
88+91	273.50	215.97	11.95	16.55	13.10
89	66.85	54.42	2.28	2.86	2.14
90+101+113	1292.91	1048.19	51.21	58.07	52.70
92	223.75	177.40	9.34	10.07	8.79

Table C-3 continued

Sample ID (Core 1) **Congener #**	**11** **ng g $^{-1}$ d.w.**	**12** **ng g $^{-1}$ d.w.**	**13** **ng g $^{-1}$ d.w.**	**14** **ng g $^{-1}$ d.w.**	**15** **ng g $^{-1}$ d.w.**
93+100	23.92	18.36	0.00	5.20	0.00
94	17.75	13.64	0.14	0.00	0.00
95	1108.31	899.53	52.34	48.68	49.46
96	35.64	28.48	1.23	1.39	1.51
98+102	92.67	74.42	5.47	0.00	4.78
103	11.00	8.19	0.27	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	771.90	991.30	18.49	32.52	20.53
106	0.00	0.00	0.00	0.44	0.00
107	94.30	74.47	3.31	4.74	4.26
108+124	51.61	39.97	1.75	2.82	1.61
110+115	1493.46	1203.40	62.33	78.23	63.54
111	0.00	0.47	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	49.75	36.50	1.04	2.10	1.51
118	1238.05	966.69	41.38	59.79	43.26
120	2.80	1.50	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	27.35	20.82	0.00	1.14	0.00
123	36.52	26.88	0.40	0.80	1.30
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+163	488.05	403.05	33.91	39.19	32.78
130	29.23	22.71	1.61	2.50	1.08
131	8.14	6.56	0.00	0.00	0.00
132	165.65	135.02	13.78	12.66	12.37
133	5.75	4.54	0.00	0.00	0.00
134+143	37.52	19.92	0.00	1.80	0.00
135+151	156.35	142.07	12.01	11.72	11.54
136	65.60	55.93	5.82	5.10	5.04
137+164	54.76	38.49	3.11	5.43	2.73
139+140	8.78	6.65	0.00	0.00	4.57
141	97.49	84.84	4.56	6.38	0.00
142	0.00	0.00	0.00	0.00	0.00
144	25.90	21.92	1.57	1.86	1.49
145	0.00	0.00	0.00	0.00	0.00
146	57.41	49.18	4.68	3.85	4.61
147+149	360.57	319.06	27.39	29.53	26.94
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 1) **Congener #**	**11** **ng g $^{-1}$ d.w.**	**12** **ng g $^{-1}$ d.w.**	**13** **ng g $^{-1}$ d.w.**	**14** **ng g $^{-1}$ d.w.**	**15** **ng g $^{-1}$ d.w.**
152	1.50	1.13	0.00	0.00	0.00
153+168	357.15	306.41	30.37	30.35	30.70
154	2.83	2.16	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	56.79	41.77	0.00	5.28	0.00
158	49.84	38.71	2.53	3.88	2.79
159	0.00	1.10	0.00	0.00	0.00
160	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	5.35	1.67	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	16.63	12.36	1.38	1.66	1.11
169	0.64	0.46	1.71	3.30	1.86
170	91.25	81.57	7.69	7.80	7.55
171+173	31.36	28.55	2.76	3.22	1.80
172	16.44	15.71	1.45	1.74	1.17
174	102.87	101.17	9.61	11.17	8.38
175	4.65	4.44	0.00	0.40	0.00
176	14.55	14.01	1.39	1.49	1.29
177	57.25	53.91	5.54	5.15	4.97
178	20.03	20.39	2.34	2.05	1.62
179	46.43	44.97	5.11	5.59	4.55
180+193	204.79	187.92	24.53	22.05	21.56
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	65.30	61.83	10.77	6.34	8.85
184	0.00	0.00	0.00	0.27	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.16	0.00
187	119.41	116.27	15.46	16.27	14.59
188	0.00	0.00	0.00	0.00	0.00
189	3.16	2.73	0.00	0.50	0.00
190	18.59	17.10	2.20	1.89	1.92
191	3.59	3.42	0.00	0.53	0.00
192	0.00	0.00	0.00	0.00	0.00
194	40.29	39.87	12.06	8.32	9.65
195	16.85	17.04	2.69	2.50	2.94
196	22.75	22.42	6.08	5.23	5.64
197	1.11	0.00	0.00	0.00	0.00
198+199	48.24	50.99	23.92	18.42	20.55

Table C-3 continued

Sample ID (Core 1) **Congener #**	**11** **ng g $^{-1}$ d.w.**	**12** **ng g $^{-1}$ d.w.**	**13** **ng g $^{-1}$ d.w.**	**14** **ng g $^{-1}$ d.w.**	**15** **ng g $^{-1}$ d.w.**
200	6.59	7.45	1.84	2.34	0.45
201	6.39	6.30	2.34	2.27	1.40
202	9.96	10.32	6.84	5.96	6.28
203	27.22	27.60	13.75	10.90	10.92
205	1.73	1.54	0.00	0.00	0.00
206	15.71	19.40	43.97	30.17	38.94
207	2.03	2.45	3.14	2.76	2.84
208	4.96	6.70	15.26	12.52	14.45
209	5.74	8.68	47.12	25.24	40.30
Total	**75925.16**	**63137.58**	**3109.28**	**3468.20**	**3008.03**

Table C-3 continued

Sample ID (Core 1)	**16**	**17**	**18**	**19**	**20**
Core section (cm)	274-290	290-305	305-320	320-335	335-351
Lab batch #	3	1	1	3	1
PCB14 % recovery	50	79	64	54	52
d-PCB65 % recovery	61	75	57	65	48
PCB166 % recovery	59	59	60	60	46
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	50	44	42	50	42
Total organic carbon (%)	7.19	7.34	7.52	7.70	8.17
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
1	4.70	2.27	2.79	2.35	1.39
2	1.78	1.07	0.92	0.86	0.44
3	2.94	1.66	1.82	1.51	0.46
4	25.52	16.44	16.59	12.14	7.43
5	0.00	0.00	0.00	0.00	0.00
6	15.48	8.50	9.53	6.70	3.95
7	2.40	1.27	1.44	0.83	0.33
8	64.20	38.49	38.44	30.58	16.21
9	4.79	3.44	3.28	1.97	1.24
10	0.86	0.55	0.00	0.39	0.48
11	2.29	1.31	1.04	1.88	0.76
12+13	4.36	1.78	2.10	2.02	1.48
15	28.96	14.30	14.65	12.76	6.57
16	79.77	35.31	36.81	33.80	16.20
17	79.24	45.72	46.04	34.59	19.38
18+30	185.69	99.51	97.46	86.29	40.89
19	16.03	9.26	10.00	7.81	4.26
20+28	199.98	97.63	100.06	91.87	43.75
21+33	118.35	57.87	59.64	55.13	24.46
22	72.27	32.46	34.65	33.97	15.43
23	0.00	0.00	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	0.00
25	13.19	5.86	6.04	6.97	3.95
26+29	36.21	17.10	17.09	17.06	0.00
27	12.37	5.93	6.16	4.42	2.62
31	207.93	101.86	106.20	97.49	46.11
32	51.30	28.44	31.27	23.55	13.75
34	1.04	0.00	0.00	0.00	0.00
35	3.62	0.00	0.00	1.97	0.00
36	0.00	0.00	0.00	0.00	0.00
37	50.61	23.24	24.00	23.96	13.25
38	2.71	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 1) **Congener #**	**16** **ng g $^{-1}$ d.w.**	**17** **ng g $^{-1}$ d.w.**	**18** **ng g $^{-1}$ d.w.**	**19** **ng g $^{-1}$ d.w.**	**20** **ng g $^{-1}$ d.w.**
39	1.77	0.00	0.00	0.00	0.00
40+41+71	108.84	67.58	69.72	51.99	27.53
42	49.91	29.88	32.36	23.85	14.09
43	6.48	3.27	4.64	3.18	2.01
44+47+65	190.72	106.36	107.89	90.00	50.87
45+51	40.83	26.26	26.16	19.23	11.00
46	13.68	8.00	8.26	6.15	2.54
48	46.91	22.98	25.20	19.74	11.04
49+69	112.81	63.99	65.71	51.33	29.25
50+53	30.84	18.53	20.04	14.04	8.96
52	213.95	124.08	127.59	107.18	60.66
54	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	0.00	0.00	0.00
56	76.11	43.15	46.99	35.90	19.44
57	0.00	0.00	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	12.16	7.54	8.14	5.69	3.83
60	46.19	22.21	24.41	20.77	10.51
61+70+74+76	272.03	160.77	166.11	128.83	75.98
63	4.09	3.46	3.08	1.99	1.15
64	78.44	41.40	43.70	35.31	21.14
66	158.20	79.28	86.40	75.49	38.94
67	4.33	2.44	2.66	1.84	0.68
68	0.00	0.00	0.00	0.00	0.00
72	0.00	0.00	0.00	0.00	0.00
73	0.00	0.00	0.00	0.00	0.00
77	12.39	6.49	7.71	6.95	3.88
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	18.11	8.58	10.86	12.33	5.72
83+99	62.05	26.81	27.05	31.35	20.86
84	30.41	16.81	19.41	17.38	10.55
85+116+117	14.41	10.92	13.64	12.57	9.38
86+87+97+109+119+125	66.81	35.87	41.83	38.81	25.39
88+91	19.11	10.71	11.27	9.49	5.96
89	2.67	2.02	1.61	1.03	1.14
90+101+113	74.00	42.37	42.54	41.52	31.84
92	13.37	7.58	7.47	7.81	6.45

Table C-3 continued

Sample ID (Core 1)	**16**	**17**	**18**	**19**	**20**
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
93+100	0.00	0.00	0.00	0.00	1.52
94	0.00	0.00	0.00	0.00	0.00
95	67.54	39.45	41.26	37.51	26.62
96	1.65	0.98	1.20	1.03	0.00
98+102	7.53	5.03	5.12	2.64	0.00
103	0.00	0.00	0.00	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	35.11	16.98	20.20	17.95	13.64
106	0.00	0.00	0.00	0.00	0.60
107	7.25	3.80	3.97	4.36	1.00
108+124	2.72	1.30	1.56	1.84	1.00
110+115	98.23	60.68	53.12	49.39	39.51
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	2.26	0.76	0.00	0.00	0.00
118	70.57	35.07	41.32	40.26	30.86
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.00	0.40	0.00	0.73	0.00
123	1.37	0.00	1.08	1.22	1.40
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+163	37.08	29.27	25.55	25.77	27.61
130	2.93	0.00	0.00	0.00	0.00
131	0.00	0.00	0.00	0.00	0.00
132	15.27	11.19	9.68	10.26	9.09
133	0.00	0.00	0.00	0.00	0.00
134+143	0.00	0.00	0.00	0.00	0.00
135+151	12.68	10.61	8.90	9.31	8.21
136	5.24	4.95	3.79	4.33	3.23
137+164	4.41	0.00	1.69	1.94	0.00
139+140	0.00	0.00	0.00	0.00	0.00
141	6.81	4.84	4.77	3.81	0.00
142	0.00	0.00	0.00	0.00	0.00
144	2.31	0.00	0.00	1.66	0.00
145	0.00	0.00	0.00	0.00	0.00
146	4.30	3.74	3.12	2.58	2.64
147+149	28.00	21.84	20.70	19.98	18.94
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 1) **Congener #**	**16** **ng g $^{-1}$ d.w.**	**17** **ng g $^{-1}$ d.w.**	**18** **ng g $^{-1}$ d.w.**	**19** **ng g $^{-1}$ d.w.**	**20** **ng g $^{-1}$ d.w.**
152	0.00	0.00	0.00	0.00	0.00
153+168	32.03	24.19	19.64	22.09	22.68
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	0.00	0.00	0.00	0.00	0.00
158	2.94	2.51	2.26	1.88	0.00
159	0.00	0.00	0.00	0.00	0.00
160	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	1.75	0.00	0.00	0.00	0.00
169	1.54	1.67	0.57	2.22	1.84
170	6.70	6.05	5.22	6.06	4.91
171+173	2.27	0.64	1.24	1.85	2.09
172	1.44	1.07	0.00	1.31	0.00
174	8.42	7.76	7.66	6.76	7.54
175	0.00	0.00	0.00	0.00	0.00
176	0.97	0.47	0.73	0.94	0.74
177	5.18	4.16	3.59	3.51	2.83
178	2.05	1.65	1.45	1.80	1.64
179	3.62	4.02	4.05	3.93	3.59
180+193	21.78	18.93	16.82	17.66	19.12
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	9.52	4.94	4.88	7.57	6.07
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	11.70	10.47	10.84	12.81	11.96
188	0.00	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	1.94	0.68	0.91	0.81	3.40
191	0.00	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	8.34	7.30	6.90	9.22	7.58
195	1.77	2.16	1.75	2.23	1.93
196	3.93	3.80	2.90	4.77	3.78
197	0.00	0.00	0.00	0.00	0.00
198+199	16.11	15.57	13.62	18.79	16.07

Table C-3 continued

Sample ID (Core 1) **Congener #**	**16** **ng g $^{-1}$ d.w.**	**17** **ng g $^{-1}$ d.w.**	**18** **ng g $^{-1}$ d.w.**	**19** **ng g $^{-1}$ d.w.**	**20** **ng g $^{-1}$ d.w.**
200	0.00	0.00	0.00	0.71	0.00
201	1.02	1.05	1.40	1.32	1.76
202	3.95	4.47	4.05	5.87	4.53
203	8.79	8.69	7.87	10.67	9.09
205	0.00	0.00	0.00	0.00	0.00
206	28.80	31.12	22.53	35.25	35.77
207	2.09	2.24	1.72	2.11	2.29
208	10.29	11.34	9.61	12.95	13.53
209	31.11	32.33	20.34	30.69	31.79
Total	**3713.53**	**2110.76**	**2140.03**	**1926.96**	**1197.98**

Table C-3 continued

Sample ID (Core 1)	**21**	**22**	**23**	**24**	**25**
Core section (cm)	351-366	366-381	381-396	396-411	411-427
Lab batch #	2	1	1	3	3
PCB14 % recovery	49	53	50	46	56
d-PCB65 % recovery	65	49	50	64	74
PCB166 % recovery	63	48	48	54	61
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	40	41	41	50	50
Total organic carbon (%)	7.35	7.79	7.45	8.14	7.72
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
1	0.34	0.71	0.55	0.38	0.00
2	0.00	0.57	0.00	0.39	0.00
3	0.31	0.47	0.00	0.37	0.15
4	3.43	3.98	1.35	1.30	0.88
5	0.00	0.00	0.00	0.00	0.00
6	1.97	2.20	1.08	0.59	0.00
7	0.00	0.39	0.00	0.00	0.00
8	7.92	9.26	3.57	2.82	0.00
9	0.50	0.79	0.54	0.27	0.00
10	0.00	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00
12+13	0.60	0.63	0.31	0.00	0.00
15	3.90	3.63	1.88	1.31	0.70
16	9.87	9.52	3.70	4.46	0.00
17	9.82	11.04	3.64	4.50	1.88
18+30	25.04	23.55	8.41	10.05	3.82
19	2.24	1.77	0.00	0.97	0.00
20+28	25.97	25.67	10.83	9.86	4.71
21+33	15.09	16.17	6.42	5.88	2.80
22	9.23	10.50	3.93	3.19	1.89
23	0.00	0.00	0.00	0.00	0.00
24	0.00	0.00	0.00	0.00	0.00
25	1.49	1.82	1.07	1.32	0.59
26+29	0.00	0.00	0.00	0.00	0.00
27	1.33	1.69	0.56	0.87	0.00
31	27.41	28.91	11.38	11.54	5.75
32	6.07	6.32	2.31	1.83	0.00
34	0.00	0.00	0.00	0.00	0.00
35	0.00	0.00	0.00	0.00	0.00
36	0.00	0.00	0.00	0.00	0.00
37	6.76	7.04	2.49	3.91	2.96
38	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 1)	**21**	**22**	**23**	**24**	**25**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
39	0.00	0.00	0.00	0.54	0.00
40+41+71	13.49	17.38	5.93	5.80	3.33
42	6.38	8.06	2.76	3.02	1.43
43	0.72	1.93	0.00	0.00	0.00
44+47+65	26.35	29.22	10.96	12.20	9.56
45+51	5.48	7.64	2.75	2.36	1.05
46	1.46	1.18	0.97	0.72	0.46
48	5.97	7.61	2.55	1.89	1.00
49+69	14.98	18.72	7.53	7.35	5.22
50+53	4.11	5.68	2.13	1.41	0.00
52	32.47	39.51	15.21	15.37	13.45
54	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	0.00	0.00	0.00
56	10.77	11.46	4.20	4.59	3.07
57	0.00	0.00	0.00	0.00	0.00
58	0.00	0.00	0.00	0.00	0.00
59+62+75	1.87	2.97	0.97	0.00	0.47
60	6.00	7.88	3.11	1.75	1.25
61+70+74+76	37.06	45.50	16.19	22.27	17.67
63	0.45	0.63	0.00	0.00	0.00
64	10.71	12.42	4.18	4.47	2.61
66	21.74	25.40	9.19	11.57	8.26
67	0.39	0.00	0.00	0.00	0.00
68	0.00	0.00	0.00	0.00	0.00
72	0.00	0.00	0.00	0.00	0.00
73	0.00	0.00	0.00	0.00	0.00
77	1.80	3.47	2.12	0.00	3.44
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.00	0.00	0.00	0.00
82	2.96	2.45	1.57	3.18	4.21
83+99	15.65	12.88	5.79	15.88	19.24
84	6.86	7.05	2.87	6.14	7.85
85+116+117	6.54	5.91	4.35	4.41	6.27
86+87+97+109+119+125	14.49	17.72	9.12	14.85	18.72
88+91	3.46	3.95	2.15	3.94	4.01
89	0.41	0.00	0.00	0.00	0.00
90+101+113	19.68	21.03	10.75	22.32	27.35
92	3.47	2.92	1.61	4.17	4.75

Table C-3 continued

Sample ID (Core 1) **Congener #**	**21** **ng g^{-1} d.w.**	**22** **ng g^{-1} d.w.**	**23** **ng g^{-1} d.w.**	**24** **ng g^{-1} d.w.**	**25** **ng g^{-1} d.w.**
93+100	0.00	0.00	0.00	0.00	0.00
94	0.00	0.00	0.00	0.00	0.00
95	16.94	17.80	9.92	17.55	18.94
96	0.39	0.00	0.00	0.00	0.00
98+102	0.75	0.00	0.00	0.80	0.00
103	0.00	0.00	0.00	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	7.72	7.81	4.38	7.48	9.02
106	0.00	0.00	0.00	0.00	0.00
107	1.31	1.46	0.00	2.15	1.87
108+124	0.75	0.91	0.62	0.56	1.15
110+115	23.01	24.87	11.52	27.00	31.46
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	0.62	0.00	0.00	0.00	0.00
118	19.19	22.01	11.18	23.00	27.83
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.00	0.00	0.00	0.00	0.00
123	0.57	0.00	0.00	0.21	0.81
126	0.00	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+163	16.83	17.78	11.15	22.52	31.51
130	0.00	0.00	0.00	0.00	0.00
131	0.00	0.00	0.00	0.00	0.00
132	5.75	6.98	4.45	7.76	11.08
133	0.00	0.00	0.00	0.00	0.00
134+143	0.00	0.00	0.00	0.00	0.00
135+151	5.53	6.26	3.80	7.51	9.37
136	2.22	2.77	0.00	3.27	4.50
137+164	2.32	0.00	0.00	1.97	1.30
139+140	0.00	0.00	0.00	0.68	0.00
141	0.00	0.00	0.00	2.83	4.80
142	0.00	0.00	0.00	0.00	0.00
144	0.00	0.00	0.00	0.98	0.00
145	0.00	0.00	0.00	0.00	0.00
146	2.31	1.96	1.24	2.46	4.26
147+149	12.97	13.17	10.43	17.61	23.12
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 1)	**21**	**22**	**23**	**24**	**25**
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
152	0.00	0.00	0.00	0.00	0.00
153+168	17.69	14.96	10.38	19.89	27.31
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	0.00	0.00	0.00	0.00	0.00
158	1.58	1.34	1.41	1.83	2.63
159	0.00	0.00	0.00	0.00	0.00
160	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	0.72	0.00	0.00	0.87	0.74
169	1.44	2.00	1.74	1.55	1.59
170	2.86	4.11	1.76	4.71	6.65
171+173	1.02	1.39	2.53	1.40	0.79
172	0.56	0.00	0.00	0.54	0.98
174	4.64	5.96	3.99	5.68	7.50
175	0.00	0.00	0.00	0.00	0.00
176	0.55	0.76	0.00	0.68	0.96
177	1.56	2.64	0.88	3.04	3.83
178	1.12	1.10	1.10	1.26	1.83
179	2.81	3.45	2.26	3.54	3.78
180+193	13.27	16.77	6.87	16.09	19.65
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	4.43	4.15	3.67	6.17	8.61
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	10.15	12.21	8.65	11.41	12.15
188	0.00	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00
190	1.04	0.88	1.64	1.30	1.67
191	0.00	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00
194	7.15	9.48	8.08	9.01	7.83
195	1.55	2.36	1.30	2.18	1.98
196	3.71	4.89	3.61	5.24	3.04
197	0.00	0.00	0.00	0.00	0.00
198+199	17.18	18.38	16.38	20.47	18.99

Table C-3 continued

Sample ID (Core 1) **Congener #**	**21** **ng g $^{-1}$ d.w.**	**22** **ng g $^{-1}$ d.w.**	**23** **ng g $^{-1}$ d.w.**	**24** **ng g $^{-1}$ d.w.**	**25** **ng g $^{-1}$ d.w.**
200	0.00	0.00	0.00	0.47	0.60
201	1.45	1.26	0.88	1.77	1.78
202	4.69	5.92	3.34	5.93	5.63
203	9.49	11.68	9.78	11.89	9.14
205	0.00	0.00	0.00	0.00	0.00
206	30.74	36.19	27.60	38.98	40.04
207	2.00	2.80	2.02	2.89	2.84
208	11.06	12.49	9.74	13.71	14.99
209	25.71	26.97	22.36	38.03	44.40
Total	**734.40**	**815.13**	**413.63**	**612.89**	**623.75**

Table C-3 continued

Sample ID (Core 1)	**26**
Core section (cm)	427-442
Lab batch #	3
PCB14 % recovery	50
d-PCB65 % recovery	67
PCB166 % recovery	55
PCB204	100 ng
Water content (%)	50
Total organic carbon (%)	7.32
Congener #	**ng g $^{-1}$ d.w.**
1	0.00
2	0.00
3	0.28
4	2.03
5	0.00
6	0.86
7	0.00
8	3.90
9	0.31
10	0.00
11	1.03
12+13	0.74
15	2.66
16	8.52
17	8.25
18+30	17.69
19	1.60
20+28	20.44
21+33	9.63
22	5.94
23	0.00
24	0.00
25	2.10
26+29	0.00
27	1.12
31	20.25
32	4.43
34	0.00
35	0.00
36	0.00
37	6.23
38	0.00

Table C-3 continued

Sample ID (Core 1) **Congener #**	**26** **ng g $^{-1}$ d.w.**
39	0.00
40+41+71	10.61
42	5.67
43	0.00
44+47+65	19.91
45+51	4.27
46	1.29
48	3.79
49+69	12.80
50+53	2.93
52	27.93
54	0.00
55	0.00
56	8.65
57	0.00
58	0.00
59+62+75	1.45
60	4.83
61+70+74+76	36.27
63	0.00
64	8.52
66	19.10
67	0.00
68	0.00
72	0.00
73	0.00
77	2.90
78	0.00
79	0.00
80	0.00
81	0.00
82	3.51
83+99	21.39
84	7.89
85+116+117	6.78
86+87+97+109+119+125	19.87
88+91	5.00
89	0.00
90+101+113	27.32
92	4.54

Table C-2 continued

Sample ID (Core 1) **Congener #**	**26** **ng g $^{-1}$ d.w.**
93+100	0.00
94	0.00
95	20.79
96	0.00
98+102	0.00
103	0.00
104	0.00
105	9.26
106	0.00
107	2.58
108+124	0.84
110+115	34.14
111	0.00
112	0.00
114	0.00
118	27.19
120	0.00
121	0.00
122	0.00
123	0.39
126	0.00
127	0.00
129+138+163	27.29
130	1.13
131	0.00
132	10.52
133	0.00
134+143	0.00
135+151	9.00
136	3.86
137+164	2.74
139+140	0.00
141	3.71
142	0.00
144	1.01
145	0.00
146	3.32
147+149	20.70
148	0.00
150	0.00

Table C-3 continued

Sample ID (Core 1) **Congener #**	**26** **ng g $^{-1}$ d.w.**
152	0.00
153+168	25.50
154	0.00
155	0.00
156+157	0.00
158	2.04
159	0.00
160	0.00
161	0.00
162	0.00
165	0.00
167	0.94
169	1.53
170	4.92
171+173	1.80
172	0.82
174	6.68
175	0.00
176	1.00
177	4.26
178	1.75
179	4.36
180+193	19.08
181	0.00
182	0.00
183	7.43
184	0.00
185	0.00
186	0.00
187	13.47
188	0.00
189	0.00
190	1.68
191	0.00
192	0.00
194	9.64
195	0.74
196	4.96
197	0.00
198+199	19.18

Table C-3 continued

Sample ID (Core 1) **Congener #**	**26** **ng g $^{-1}$ d.w.**
200	0.43
201	1.70
202	5.78
203	11.59
205	0.00
206	43.60
207	2.64
208	16.51
209	41.86
Total	**819.54**

Table C-3 continued

Sample ID (Core 2)	**1**	**2**	**3**	**4**	**5**
Core section (cm)	0-30	91-122	122-152	183-213	213-244
Lab batch #	3	1	1	3	1
PCB14 % recovery	94	41	65	75	53
d-PCB65 % recovery	106	54	85	55	65
PCB166 % recovery	75	56	69	44	65
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	49	55	50	56	55
Total organic carbon (%)	3.14	4.43	6.40	6.12	6.94
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
1	0.00	1.65	6.12	6.20	12.01
2	0.00	0.43	1.08	2.18	2.87
3	0.00	1.21	4.07	5.43	7.22
4	2.80	25.53	77.47	88.01	166.51
5	0.00	0.00	0.00	3.04	0.00
6	3.21	14.76	46.33	60.61	90.52
7	0.00	1.26	5.42	6.47	9.57
8	12.06	63.87	217.76	325.86	451.99
9	0.00	3.00	11.67	17.30	23.88
10	0.00	0.90	2.45	4.58	4.39
11	0.00	2.07	4.12	3.93	6.30
12+13	1.02	3.77	9.10	13.36	15.81
15	13.49	36.93	89.87	118.15	168.43
16	9.98	76.94	210.88	256.47	403.66
17	11.54	90.27	221.03	253.08	392.30
18+30	29.10	183.67	467.44	575.51	843.41
19	5.95	15.90	42.40	62.17	68.03
20+28	70.68	255.13	559.19	710.76	922.08
21+33	23.30	112.29	311.32	419.86	573.31
22	19.29	76.51	194.87	257.81	306.14
23	0.00	0.00	0.00	1.62	0.95
24	0.00	0.00	0.00	0.00	0.00
25	6.09	19.95	42.17	59.87	69.56
26+29	0.00	49.35	110.63	134.90	184.58
27	3.30	14.93	34.67	33.28	61.76
31	53.05	238.65	536.47	661.38	895.18
32	13.61	58.81	131.87	200.15	210.64
34	0.00	1.13	2.62	3.23	3.87
35	1.19	3.75	4.82	5.91	14.18
36	0.00	2.30	2.26	0.00	4.46
37	25.77	68.78	151.29	195.97	251.12
38	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 2) **Congener #**	**1** **ng g $^{-1}$ d.w.**	**2** **ng g $^{-1}$ d.w.**	**3** **ng g $^{-1}$ d.w.**	**4** **ng g $^{-1}$ d.w.**	**5** **ng g $^{-1}$ d.w.**
39	0.33	0.97	0.73	1.54	1.65
40+41+71	36.51	121.36	225.82	232.57	340.25
42	22.32	57.51	107.53	132.91	158.83
43	3.76	4.19	13.66	21.95	13.73
44+47+65	69.81	212.22	370.83	423.83	517.60
45+51	23.05	53.19	96.51	173.03	138.99
46	7.18	14.93	29.49	41.53	43.97
48	11.92	46.24	88.97	120.00	135.44
49+69	39.77	124.41	215.03	290.60	306.85
50+53	19.00	34.62	65.57	84.74	94.32
52	89.56	244.39	432.01	476.95	594.28
54	0.92	1.77	2.19	6.36	1.79
55	0.00	0.00	0.00	0.00	0.00
56	31.18	86.03	157.45	165.47	225.98
57	0.00	1.22	1.48	3.75	4.58
58	0.00	0.00	0.00	0.00	0.00
59+62+75	9.23	17.60	30.64	47.82	46.41
60	15.86	50.03	95.37	111.69	148.39
61+70+74+76	91.39	291.75	516.66	716.80	733.56
63	2.16	6.02	13.34	16.22	19.97
64	35.84	88.90	160.26	235.73	221.14
66	64.73	178.34	312.11	355.49	465.28
67	2.17	4.20	9.18	14.81	18.70
68	1.03	1.17	1.26	1.71	1.43
72	0.88	1.27	1.62	2.12	2.15
73	0.00	0.00	0.00	0.00	0.00
77	10.73	17.40	28.61	49.27	43.50
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	0.00	0.74	2.79	0.00	4.95
82	11.87	23.01	29.80	45.91	39.52
83+99	26.80	81.52	101.77	88.45	124.53
84	20.68	36.00	47.96	57.49	64.41
85+116+117	17.06	24.41	30.82	45.05	36.13
86+87+97+109+119+125	42.35	85.01	112.68	176.30	149.61
88+91	12.52	23.08	32.53	36.10	35.98
89	2.12	3.60	5.28	5.80	6.99
90+101+113	55.76	104.42	141.01	196.63	213.13
92	10.07	21.98	26.16	34.98	34.64

Table C-3 continued

Sample ID (Core 2) **Congener #**	**1** **ng g $^{-1}$ d.w.**	**2** **ng g $^{-1}$ d.w.**	**3** **ng g $^{-1}$ d.w.**	**4** **ng g $^{-1}$ d.w.**	**5** **ng g $^{-1}$ d.w.**
93+100	0.00	6.06	0.00	0.00	0.00
94	0.64	2.50	2.55	3.00	3.09
95	49.36	85.47	121.16	146.43	193.69
96	1.45	2.39	3.11	4.56	4.02
98+102	4.56	7.31	16.49	6.21	15.95
103	0.57	1.76	1.84	0.00	0.00
104	0.00	0.00	0.00	0.00	0.00
105	17.53	44.20	55.39	91.39	73.44
106	0.00	0.00	0.00	0.00	0.00
107	2.96	7.63	9.35	15.42	12.93
108+124	1.73	3.57	4.64	10.58	6.09
110+115	67.25	119.08	155.17	251.43	214.21
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	1.35	2.87	6.19	5.97	4.25
118	35.60	90.79	115.84	189.32	150.00
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	0.74	1.69	0.00	0.92	2.11
123	1.34	2.06	4.10	2.95	2.80
126	0.00	0.00	0.00	0.00	15.73
127	0.00	0.00	0.00	0.00	0.00
129+138+163	69.06	70.27	111.60	257.54	197.67
130	3.71	2.58	5.03	13.14	6.26
131	0.00	0.00	0.00	2.51	1.72
132	21.58	21.91	37.17	76.46	64.53
133	1.18	1.16	1.97	3.23	1.58
134+143	3.63	0.00	0.00	12.41	0.00
135+151	27.60	26.59	50.50	77.93	108.47
136	9.48	10.07	18.89	28.80	40.19
137+164	6.32	6.94	9.23	26.65	15.20
139+140	0.93	1.57	1.41	3.64	1.82
141	13.10	13.56	22.87	46.05	49.97
142	0.00	0.00	0.00	0.00	0.00
144	3.75	3.06	5.96	12.03	14.74
145	0.00	0.00	0.00	0.00	0.00
146	8.52	11.20	18.95	26.16	28.94
147+149	58.54	56.37	101.52	166.64	216.91
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 2) **Congener #**	**1** **ng g^{-1} d.w.**	**2** **ng g^{-1} d.w.**	**3** **ng g^{-1} d.w.**	**4** **ng g^{-1} d.w.**	**5** **ng g^{-1} d.w.**
152	0.00	0.00	0.00	0.00	0.00
153+168	57.86	60.52	106.35	170.69	211.56
154	0.00	0.52	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	3.72	0.00	0.00	33.48	0.00
158	6.72	5.43	10.07	23.51	16.30
159	0.00	0.00	0.00	0.00	0.00
160	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	1.65	1.98	3.69	9.24	5.01
169	1.10	0.81	1.50	2.59	4.09
170	16.10	16.16	27.53	50.20	64.82
171+173	6.79	5.10	9.07	14.83	22.09
172	3.41	2.65	4.92	8.51	12.13
174	20.17	18.01	32.01	58.72	89.69
175	0.99	0.33	0.79	2.95	3.65
176	3.52	2.62	4.74	7.82	12.48
177	12.01	10.44	18.89	27.05	48.19
178	4.08	4.35	8.42	11.14	18.16
179	9.22	8.59	15.86	24.05	41.57
180+193	39.25	37.78	66.83	112.86	168.18
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	12.01	13.42	25.46	27.97	57.70
184	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	22.72	22.92	41.37	54.61	98.25
188	0.00	0.00	0.00	0.00	0.00
189	0.71	0.00	0.00	2.69	0.00
190	3.05	2.89	5.27	10.03	13.17
191	0.73	0.00	0.36	1.70	2.20
192	0.00	0.00	0.00	0.00	0.00
194	6.35	9.10	12.81	18.91	34.44
195	2.66	1.29	5.38	7.31	16.75
196	4.29	4.62	8.29	12.18	20.83
197	0.00	0.00	0.00	0.00	0.00
198+199	8.09	10.87	17.30	22.86	43.29

Table C-3 continued

Sample ID (Core 2)	**1**	**2**	**3**	**4**	**5**
Congener #	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**	**ng g^{-1} d.w.**
200	0.65	0.25	1.76	2.16	4.94
201	1.41	1.42	2.20	3.34	6.03
202	2.02	2.31	3.35	4.33	7.72
203	5.08	5.97	9.51	11.37	23.89
205	0.00	0.00	0.00	1.51	1.62
206	2.81	3.14	3.93	4.96	8.05
207	0.00	0.48	0.66	1.32	1.17
208	0.88	0.70	0.91	1.30	1.63
209	0.00	1.01	0.89	1.28	0.64
Total	**1766.55**	**4345.53**	**8337.60**	**11129.51**	**13660.00**

Table C-3 continued

Sample ID (Core 2)	**6**	**7**	**8**	**9**	**10**
Core section (cm)	274-305	335-366	366-396	396-427	427-457
Lab batch #	1	2	2	2	2
PCB14 % recovery	45	91	124	56	120
d-PCB65 % recovery	54	101	135	68	120
PCB166 % recovery	55	62	76	50	63
PCB204	100 ng	100 ng	100 ng	100 ng	100 ng
Water content (%)	54	53	51	50	49
Total organic carbon (%)	7.06	6.56	8.10	7.38	6.98
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
1	15.26	21.50	7.01	4.40	9.53
2	3.18	2.99	1.23	0.88	1.29
3	8.61	9.82	3.00	1.89	3.65
4	460.34	458.67	185.29	127.28	407.38
5	0.00	0.00	0.00	0.00	0.00
6	237.37	203.79	77.35	53.46	166.81
7	17.50	19.25	5.67	3.33	10.39
8	1283.19	1050.62	403.05	286.89	883.21
9	54.86	55.04	19.29	12.64	40.73
10	9.32	13.41	1.70	3.74	7.96
11	15.30	10.01	3.61	2.85	8.10
12+13	29.65	26.87	8.36	5.19	17.55
15	433.54	362.60	138.25	107.42	305.37
16	1134.00	908.59	408.42	291.48	896.72
17	1047.59	955.17	417.04	289.21	917.78
18+30	2289.89	2012.89	896.11	634.25	2025.49
19	221.11	207.48	72.51	72.98	89.96
20+28	2415.02	2210.57	917.98	701.13	1910.65
21+33	1675.74	1450.61	552.36	490.17	1240.45
22	888.06	675.11	251.78	260.96	607.94
23	2.99	2.95	1.22	0.77	2.41
24	0.00	0.00	0.00	0.00	0.00
25	191.79	173.61	65.45	54.61	152.74
26+29	487.66	438.36	178.19	139.13	397.37
27	168.25	148.54	65.46	46.85	142.42
31	2363.25	2108.55	862.28	672.57	1837.18
32	618.80	538.10	197.06	201.54	484.84
34	9.09	8.53	3.65	2.75	7.59
35	33.68	27.49	8.58	6.18	18.25
36	9.17	6.19	2.33	1.88	5.09
37	658.65	635.83	203.08	204.37	449.09
38	1.71	1.10	0.53	1.06	2.13

Table C-3 continued

Sample ID (Core 2) Congener #	6 ng g $^{-1}$ d.w.	7 ng g $^{-1}$ d.w.	8 ng g $^{-1}$ d.w.	9 ng g $^{-1}$ d.w.	10 ng g $^{-1}$ d.w.
39	3.82	3.27	1.39	0.95	2.85
40+41+71	751.84	662.59	251.87	217.39	562.51
42	355.68	298.54	115.66	93.56	255.48
43	30.61	54.69	19.75	18.37	48.07
44+47+65	1111.07	971.13	383.02	314.15	878.95
45+51	304.45	275.17	119.98	86.52	264.01
46	105.42	94.85	42.17	30.63	89.89
48	296.29	□□5.75	111.24	89.77	247.07
49+69	649.58	589.96	229.90	179.32	515.75
50+53	205.75	188.22	82.86	59.16	182.94
52	1211.23	983.70	394.09	312.67	848.59
54	3.46	3.17	1.66	1.32	4.19
55	0.00	0.00	0.00	0.00	0.00
56	482.37	409.80	146.66	156.69	345.97
57	8.37	8.17	2.86	2.06	3.03
58	0.00	0.00	0.00	0.00	0.00
59+62+75	109.13	109.47	39.66	34.15	92.49
60	318.53	279.80	91.47	94.99	197.41
61+70+74+76	1516.02	1333.06	467.87	433.87	1051.25
63	38.14	32.78	11.52	10.37	15.08
64	468.29	407.44	155.99	136.09	349.17
66	986.51	849.18	294.34	272.71	613.97
67	41.98	37.23	13.42	12.57	26.07
68	2.65	2.24	1.22	1.14	2.09
72	3.85	2.90	1.53	1.13	3.23
73	0.00	0.00	0.00	0.00	0.00
77	89.03	72.39	25.85	32.49	46.77
78	0.00	0.00	0.00	0.00	0.00
79	0.00	0.00	0.00	0.00	0.00
80	0.00	0.00	0.00	0.00	0.00
81	3.80	4.96	1.36	2.57	4.41
82	63.03	47.63	16.14	16.59	32.35
83+99	180.85	119.40	41.88	38.12	75.03
84	99.01	70.57	26.41	25.84	49.30
85+116+117	51.79	25.56	14.82	15.68	22.37
86+87+97+109+119+125	228.85	156.03	57.77	59.77	103.78
88+91	56.91	32.57	12.42	10.20	24.10
89	10.61	8.40	2.50	2.50	4.94
90+101+113	281.64	181.28	91.88	120.02	121.71
92	47.65	30.88	12.87	15.88	19.45

Table C-3 continued

Sample ID (Core 2) **Congener #**	**6** **ng g $^{-1}$ d.w.**	**7** **ng g $^{-1}$ d.w.**	**8** **ng g $^{-1}$ d.w.**	**9** **ng g $^{-1}$ d.w.**	**10** **ng g $^{-1}$ d.w.**
93+100	0.00	0.00	0.00	0.00	0.00
94	2.96	1.88	1.05	0.76	1.51
95	256.86	169.73	88.45	113.87	122.04
96	6.12	4.43	1.70	1.41	3.53
98+102	24.90	15.20	4.38	4.15	10.29
103	1.53	1.25	0.52	0.51	1.27
104	0.00	0.00	0.00	0.00	0.00
105	108.96	72.12	25.06	28.97	46.21
106	0.00	0.00	0.00	0.00	0.00
107	17.13	11.47	3.25	3.85	7.09
108+124	8.87	5.86	1.57	2.56	3.78
110+115	296.57	126.93	79.01	95.96	127.83
111	0.00	0.00	0.00	0.00	0.00
112	0.00	0.00	0.00	0.00	0.00
114	7.80	5.32	3.25	5.59	1.82
118	210.64	128.18	45.70	53.10	77.76
120	0.00	0.00	0.00	0.00	0.00
121	0.00	0.00	0.00	0.00	0.00
122	5.09	2.92	0.00	0.00	0.00
123	6.36	3.24	1.49	1.40	2.23
126	22.16	0.00	0.00	0.00	0.00
127	0.00	0.00	0.00	0.00	0.00
129+138+163	242.93	190.31	205.29	311.73	184.37
130	10.31	7.10	4.88	7.71	6.55
131	1.08	2.18	0.00	1.32	1.20
132	0.00	67.18	66.35	97.21	60.84
133	2.39	1.98	2.22	2.60	1.75
134+143	81.61	8.67	0.00	0.00	0.00
135+151	123.26	81.97	114.95	166.60	84.73
136	45.67	33.04	40.86	60.29	31.38
137+164	23.89	13.56	12.96	18.61	12.85
139+140	1.90	2.17	0.00	0.00	1.14
141	0.00	44.44	62.30	88.66	52.89
142	0.00	0.00	0.00	0.00	0.00
144	16.81	12.11	17.13	22.67	12.63
145	0.00	0.00	0.00	0.00	0.00
146	34.65	23.55	27.39	37.81	22.86
147+149	248.07	172.20	216.83	333.78	176.32
148	0.00	0.00	0.00	0.00	0.00
150	0.00	0.00	0.00	0.00	0.00

Table C-3 continued

Sample ID (Core 2)	**6**	**7**	**8**	**9**	**10**
Congener #	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**	**ng g $^{-1}$ d.w.**
152	0.00	0.00	0.00	0.00	0.00
153+168	295.01	159.52	206.09	291.45	165.39
154	0.00	0.00	0.00	0.00	0.00
155	0.00	0.00	0.00	0.00	0.00
156+157	0.00	14.26	12.20	15.08	15.90
158	22.06	14.96	14.90	22.09	14.40
159	0.00	0.00	2.77	3.64	0.00
160	0.00	0.00	0.00	0.00	0.00
161	0.00	0.00	0.00	0.00	0.00
162	0.00	0.00	0.00	0.00	0.00
165	0.00	0.00	0.00	0.00	0.00
167	6.34	5.00	4.45	6.08	4.63
169	5.52	3.05	5.20	7.46	3.86
170	81.27	51.45	80.21	127.83	61.23
171+173	26.92	18.66	27.72	42.92	22.31
172	15.39	11.73	16.85	24.84	12.89
174	107.34	70.05	119.49	180.09	90.69
175	2.06	3.30	4.60	6.76	4.06
176	14.42	9.52	15.59	23.61	10.90
177	59.33	38.93	58.68	96.56	43.60
178	21.71	14.52	23.21	34.26	17.94
179	51.83	33.91	59.19	85.20	43.79
180+193	210.16	134.48	229.50	323.53	169.24
181	0.00	0.00	0.00	0.00	0.00
182	0.00	0.00	0.00	0.00	0.00
183	74.60	43.15	73.10	104.33	52.61
184	0.00	0.00	0.00	0.52	0.00
185	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00
187	123.22	78.15	130.35	191.70	96.85
188	0.00	0.36	0.00	0.43	0.00
189	2.44	1.96	2.03	3.95	2.23
190	14.79	11.09	19.00	28.64	14.24
191	1.18	2.50	4.02	5.76	2.80
192	0.00	0.00	0.00	0.00	0.00
194	43.94	27.24	48.60	64.65	35.84
195	20.16	11.86	21.86	30.95	16.55
196	26.35	16.49	29.45	39.78	22.08
197	0.00	0.00	1.25	0.00	0.00
198+199	53.19	35.34	63.58	85.63	45.61

Table C-3 continued

Sample ID (Core 2) **Congener #**	**6** **ng g^{-1} d.w.**	**7** **ng g^{-1} d.w.**	**8** **ng g^{-1} d.w.**	**9** **ng g^{-1} d.w.**	**10** **ng g^{-1} d.w.**
200	6.58	6.30	8.88	14.90	7.14
201	7.30	4.47	7.29	10.44	5.58
202	9.13	6.32	10.68	14.75	7.80
203	31.23	18.56	35.71	43.52	27.79
205	1.77	1.29	2.54	3.34	1.61
206	10.51	7.31	11.54	13.25	9.15
207	1.43	1.31	2.14	1.97	1.41
208	2.15	1.71	2.36	2.64	1.98
209	0.93	0.85	0.86	0.65	1.50
Total	**30061.59**	**25445.61**	**11624.32**	**10995.40**	**22242.80**

APPENDIX D: SUPPLEMENTAL INFORMATION CHAPTER V

Information Referenced in Chapter V: Table

Table D-1 Octanol–water partition coefficient, calculated sediment porewater concentrations, fiber–water equilibrium partitioning coefficient using linear regression and from previous studies, measured freely dissolved porewater concentration and ratio of measured:calculated porewater for each congener

Table D-1 Octanol–water partition coefficient, calculated sediment porewater concentrations, fiber–water equilibrium partitioning coefficient using linear regression and from previous studies, measured freely dissolved porewater concentration and ratio of measured:calculated porewater for each congener

Congener # (144)	**Log $K_{PCBi\ ow}$ (4) [a]**	**$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\ fiber/w}$**									**$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\ pw}$ measured: calculated**
			10 µm [a, c] this study	**15 µm (114) 42 days**	**7 µm (120) 24 days**	**7 µm (119) 96 hrs dynamic**	**7 µm (118) 3 days**	**7 µm (115) 37 days**	**30 µm (115) 37 days**	**7 µm (113)**	**30 µm (113)**		
1	4.50	5.40	3.70		4.44 ± 0.13	4.03						0.00 ± 0.00	0.00
2	4.70	2.30	3.90					4.09 ± 0.04	4.18 ± 0.06			0.00 ± 0.00	0.00
3	4.70	5.50	3.90									0.00 ± 0.00	0.00
4	4.70	51.00	3.90									8.90 ± 1.70	0.18

Table D-1 continued

Congener #	**Log $K_{PCBi\,ow}$**	**$C_{PCBi\,pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\,fiber/w}$**									**$C_{PCBi\,pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\,pw}$ measured: calculated**
			10 µm [a, c] this study	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**		
5	5.00	0.00	4.20									0.00 ± 0.00	-
6	5.10	15.00	4.30									1.50 ± 0.64	0.10
7	5.10	2.10	4.30									0.00 ± 0.00	0.00
8	5.10	64.00	4.30									5.20 ± 0.67	0.08
9	5.10	3.30	4.30									0.00 ± 0.00	0.00
10	4.80	0.00	4.00									0.00 ± 0.00	-

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$								$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	□ µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
11	5.30	0.00	4.50									0.00 ± 0.00	-
12/13	5.30	4.20	4.50									0.00 ± 0.00	0.00
15	5.30	36.00	4.50		5.11 ± 0.22	4.65						2.20 ± 0.59	0.06
16	5.30	49.00	4.50									4.70 ± 0.42	0.10
17	5.30	62.00	4.50									5.70 ± 0.83	0.09
18+30	5.30	140.00	4.50					5.05 ± 0.05 [e]	5.13 ± 0.07 [e]			10.00 ± 2.60	0.08

Table D-1 continued

Congener #	**Log $K_{PCBi\ ow}$**	**$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\ fiber/w}$** 10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	**$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\ pw}$ measured: calculated**
19	5.20	16.00	4.40									2.50 ± 0.15	0.16
20+28	5.70	110.00	4.90		5.47 ± 0.21 [c]	5.04 [e]	4.65 [e]	5.27 ± 0.06 [f]	5.34 ± 0.07 [f]			4.60 ± 1.10	0.04
21+33	5.60	50.00	4.80									2.30 ± 0.61	0.05
22	5.60	36.00	4.80									1.90 ± 0.44	0.05
23	5.60	0.00	4.80									0.00 ± 0.00	-
24	5.40	0.00	4.60									0.00 ± 0.00	-

Table D-1 continued

Congener #	**Log $K_{PCBi\,ow}$**	**$C_{PCBi\,pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\,fiber/w}$**									**$C_{PCBi\,pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\,pw}$ measured: calculated**
			10 µm [a, c] this study	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**		
25	5.70	8.50	4.90									0.51 ± 0.14	0.06
26+29	5.70	19.00	4.90									1.10 ± 0.29	0.05
27	5.40	6.40	4.70									0.00 ± 0.00	0.00
31	5.70	90.00	4.90									4.90 ± 0.69	0.05
32	5.40	37.00	4.70									3.30 ± 0.50	0.09
34	5.70	0.00	4.90									0.00 ± 0.00	-

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$ 10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
35	5.80	1.30	5.10					5.23 ± 0.05	5.30 ± 0.08			0.00 ± 0.00	0.00
36	5.90	0.00	5.10									0.00 ± 0.00	-
37	5.80	24.00	5.10									0.83 ± 0.14	0.03
38	5.80	0.00	5.00									0.00 ± 0.00	-
39	5.90	0.00	5.10									0.00 ± 0.00	-
40+41+71	6.00	28.00	5.20									2.30 ± 0.34	0.08

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$ 10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
42	5.80	23.00	5.00									2.10 ± 0.21	0.09
43	5.80	3.20	5.00									0.00 ± 0.00	0.00
44+47+65	5.80	61.00	5.00	5.35 ± 0.09 [g]								7.10 ± 0.38	0.12
45+51	5.80	20.00	5.00									2.80 ± 0.48	0.14
46	5.50	9.10	4.80									0.00 ± 0.00	0.00
48	5.80	16.00	5.00									1.60 ± 0.18	0.10

Table D-1 continued

Congener #	Log	$C_{PCBi\ pw}$				Log $K_{PCBi\ fiber/w}$						$C_{PCBi\ pw}$	Ratio [m]
	$K_{PCBi\ ow}$	Calculated	10 µm [a, c]	15 µm	7 µm	7 µm	7 µm	7 µm	30 µm	7 µm	30 µm	Measured	$C_{PCBi\ pw}$
		Porewater	this	42 days	24 days	96 hrs	3 days	37 days	37 days			Porewater	measured:
		ng L^{-1} [b]	study			dynamic						ng L^{-1} [d]	calculated
49+69	5.90	44.00	5.10									3.50 ± 0.34	0.08
50+53	5.60	18.00	4.90									3.30 ± 0.41	0.19
52	5.80	80.00	5.10	5.38 ± 0.11				5.58 ± 0.05	5.56 ± 0.07	5.66 ± 0.19	5.71 ± 0.03	5.90 ± 0.55	0.08
54	5.20	0.00	4.40									0.00 ± 0.00	-
55	6.10	0.00	5.40									0.00 ± 0.00	-
56	6.10	20.00	5.40									0.99 ± 0.09	0.05

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
57	6.20	0.00	5.40									0.00 ± 0.00	-
58	6.20	0.00	5.40									0.00 ± 0.00	-
59/62/75	6.00	5.90	5.20									0.58 ± 0.21	0.10
60	6.10	10.00	5.40									0.57 ± 0.07	0.06
61+70+76+74	6.20	49.00	5.40									2.70 ± 0.32	0.05
63	6.20	1.70	5.40									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
64	6.00	25.00	5.20									1.90 ± 0.20	0.08
66	6.20	31.00	5.40									1.60 ± 0.25	0.05
67	6.20	1.30	5.40									0.00 ± 0.00	0.00
68	6.30	0.00	5.50									0.44 ± 0.07	-
72	6.30	0.00	5.50					5.78 ± 0.06	5.86 ± 0.08			0.00 ± 0.00	-
73	6.00	0.00	5.30									0.00 ± 0.00	-

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
77	6.40	2.40	5.60					5.61 ± 0.05	5.67 ± 0.07			0.00 ± 0.00	0.00
78	6.40	0.00	5.60									0.00 ± 0.00	-
79	6.40	0.00	5.70									0.00 ± 0.00	-
80	6.50	0.00	5.70									0.00 ± 0.00	-
81	6.40	0.00	5.60									0.00 ± 0.00	-
82	6.20	3.10	5.40									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log $K_{PCBi\,ow}$	$C_{PCBi\,pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\,fiber/w}$									$C_{PCBi\,pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\,pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
83+99	6.40	5.50	5.60									0.35 ± 0.07	0.06
84	6.00	7.40	5.30									0.69 ± 0.06	0.09
85+116+117	6.30	3.70	5.60									2.50 ± 0.80	0.68
86+87+97+109+119+125	6.30	10.00	5.50									0.69 ± 0.07	0.07
88+91	6.10	3.90	5.40									0.46 ± 0.03	0.12
89	6.10	0.00	5.30									0.00 ± 0.00	-

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L$^{-1\ b}$	Log $K_{PCBi\ fiber/w}$ 10 µm $^{a,\ c}$ this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	$C_{PCBi\ pw}$ Measured Porewater ng L$^{-1\ d}$	Ratio ^{m} $C_{PCBi\ pw}$ measured: calculated
90+101+113	6.40	11.00	5.60	5.71 ± 0.06 ^{h}	6.21 ± 0.08 ^{h}		5.48 ^{h}	6.07 ± 0.06 ^{h}	6.14 ± 0.08 ^{h}			0.74 ± 0.11	0.06
92	6.40	2.50	5.60									0.00 ± 0.00	0.00
93+100	6.00	0.00	5.30									0.00 ± 0.00	-
94	6.10	0.00	5.40									0.00 ± 0.00	-
95	6.10	15.00	5.40									1.30 ± 0.15	0.09
96	5.70	0.00	4.90									0.00 ± 0.00	-

Table D-1 continued

Congener #	**Log**	**$C_{PCBi\ pw}$**	**Log $K_{PCBi\ fiber/w}$**									**$C_{PCBi\ pw}$**	**Ratio ^{m}**
	$K_{PCBi\ ow}$	**Calculated Porewater ng L^{-1} ^{b}**	**10 µm $^{a,\ c}$ this study**	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**	**Measured Porewater ng L^{-1} ^{d}**	**$C_{PCBi\ pw}$ measured: calculated**
98+102	6.20	1.70	5.40									0.00 ± 0.00	0.00
103	6.20	0.00	5.50									0.00 ± 0.00	-
104	5.80	0.00	5.00									0.00 ± 0.00	-
105	6.70	0.00	5.90	5.89 ± 0.03								0.13 ± 0.01	-
106	6.60	2.80	5.90									0.00 ± 0.00	0.00
107	6.70	0.51	6.00									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log	$C_{PCBi\ pw}$	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$	Ratio [m]
	$K_{PCBi\ ow}$	Calculated Porewater ng L^{-1} [b]	10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	Measured Porewater ng L^{-1} [d]	$C_{PCBi\ pw}$ measured: calculated
108+124	6.70	0.21	6.00									0.00 ± 0.00	0.00
110+115	6.50	9.50	5.70									0.87 ± 0.29	0.09
111	6.80	0.00	6.00									0.00 ± 0.00	-
112	6.50	0.00	5.70	5.71 ± 0.06								0.00 ± 0.00	-
114	6.70	0.00	5.90									0.17 ± 0.17	-
118	6.70	4.20	6.00	5.87 ± 0.03				6.10 ± 0.05	6.14 ± 0.08			0.18 ± 0.02	0.04

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
120	6.80	0.00	6.10									0.00 ± 0.00	-
121	6.60	0.00	5.90									0.00 ± 0.00	-
122	6.60	0.00	5.90									0.00 ± 0.00	-
123	6.70	0.00	6.00									0.00 ± 0.00	-
126	6.90	0.00	6.20					6.09 ± 0.08	6.14 ± 0.12			0.00 ± 0.00	-
127	7.00	0.00	6.20									0.00 ± 0.00	-

Table D-1 continued

Congener #	Log $K_{PCBi\,ow}$	$C_{PCBi\,pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\,fiber/w}$									$C_{PCBi\,pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\,pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
129+138+163	6.80	3.60	6.10	6.20 ± 0.07 [i]								0.21 ± 0.02	0.06
130	6.80	0.00	6.10									0.00 ± 0.00	-
131	6.60	0.00	5.80									0.00 ± 0.00	-
132	6.60	1.70	5.80									0.19 ± 0.02	0.11
133	6.90	0.00	6.10									0.00 ± 0.00	-
134+143	6.60	0.00	5.80									0.00 ± 0.00	-

Table D-1 continued

Congener #	**Log $K_{PCBi\ ow}$**	**$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\ fiber/w}$**									**$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\ pw}$ measured: calculated**
			10 µm [a, c] this study	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**		
135+151	6.60	2.10	5.90									0.20 ± 0.02	0.10
136	6.20	1.60	5.50									0.25 ± 0.04	0.16
137+164	6.80	0.38	6.10									0.00 ± 0.00	0.00
139+140	6.70	0.00	5.90									0.00 ± 0.00	-
141	6.80	0.80	6.10									0.06 ± 0.01	0.08
142	6.50	0.00	5.80									0.00 ± 0.00	-

Table D-1 continued

Congener #	**Log $K_{PCBi\ ow}$**	**$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\ fiber/w}$** 10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	**$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\ pw}$ measured: calculated**
144	6.70	0.00	5.90									0.00 ± 0.00	-
145	6.30	0.00	5.50									0.00 ± 0.00	-
146	6.90	0.60	6.20									0.03 ± 0.01	0.05
147+149	6.70	3.40	5.90									0.29 ± 0.02	0.08
148	6.70	0.00	6.00									0.00 ± 0.00	-
150	6.30	0.00	5.60									0.00 ± 0.00	-

Table D-1 continued

Congener #	**Log $K_{PCBi\ ow}$**	**$C_{PCBi\ pw}$ Calculated Porewater ng L$^{-1\ b}$**	**Log $K_{PCBi\ fiber/w}$**									**$C_{PCBi\ pw}$ Measured Porewater ng L$^{-1\ d}$**	**Ratio ^{m} $C_{PCBi\ pw}$ measured: calculated**
			10 µm $^{a, c}$ this study	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**		
152	6.20	0.00	5.50									0.00 ± 0.00	-
153+168	6.90	2.50	6.20	6.16 ± 0.09 ^{j}	6.68 ± 0.52 ^{j}	6.05 ^{j}	6.01 ^{j}	6.48 ± 0.07 ^{j}	6.53 ± 0.11 ^{j}	6.68 ± 0.20 ^{j}	6.59 ± 0.20 ^{j}	0.14 ± 0.02	0.06
154	6.80	0.00	6.00	6.17 ± 0.10								0.00 ± 0.00	-
155	6.40	0.00	5.70	6.03 ± 0.15								0.00 ± 0.00	-
156+157	7.20	0.11	6.50	6.28 ± 0.06 ^{k}								0.00 ± 0.00	0.00
158	7.00	0.20	6.30									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log	$C_{PCBi\ pw}$	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$	Ratio [m]
	$K_{PCBi\ ow}$	Calculated	10 µm [a, c]	15 µm	7 µm	7 µm	7 µm	7 µm	30 µm	7 µm	30 µm	Measured	$C_{PCBi\ pw}$
		Porewater	this	42 days	24 days	96 hrs	3 days	37 days	37 days			Porewater	measured:
		ng L^{-1} [b]	study			dynamic						ng L^{-1} [d]	calculated
159	7.20	0.00	6.50									0.00 ± 0.00	-
160	6.90	0.00	6.20									0.00 ± 0.00	-
161	7.10	0.00	6.40									0.00 ± 0.00	-
162	7.20	0.00	6.50									0.00 ± 0.00	-
165	7.10	0.00	6.30									0.00 ± 0.00	-
167	7.30	0.04	6.60									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log $K_{PCBi\,ow}$	$C_{PCBi\,pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\,fiber/w}$									$C_{PCBi\,pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\,pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
169	7.40	0.00	6.70									0.00 ± 0.00	-
170	7.30	0.46	6.60									0.02 ± 0.01	0.05
171+173	7.10	0.00	6.40									0.00 ± 0.00	-
172	7.30	0.07	6.60									0.00 ± 0.00	0.00
174	7.10	0.62	6.40									0.03 ± 0.01	0.05
175	7.20	0.00	6.40									0.00 ± 0.00	-

Table D-1 continued

Congener #	**Log $K_{PCBi\,ow}$**	**$C_{PCBi\,pw}$ Calculated Porewater ng L^{-1} [b]**	**Log $K_{PCBi\,fiber/w}$**									**$C_{PCBi\,pw}$ Measured Porewater ng L^{-1} [d]**	**Ratio [m] $C_{PCBi\,pw}$ measured: calculated**
			10 µm [a, c] this study	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**		
176	6.80	0.15	6.00									0.00 ± 0.00	0.00
177	7.10	0.46	6.40									0.00 ± 0.00	0.00
178	7.10	0.11	6.40									0.00 ± 0.00	0.00
179	6.70	0.62	6.00									0.06 ± 0.01	0.10
180+193	7.40	0.78	6.60	6.40 ± 0.10 [1]	6.76 ± 0.13 [1]	6.24 [1]	6.37 [1]	6.67 ± 0.10 [1]	6.78 ± 0.07 [1]	6.76 ± 0.22 [1]	6.37 ± 0.34 [1]	0.04 ± 0.01	0.05
181	7.10	0.00	6.40									0.00 ± 0.00	-

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$ 10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
182	7.20	0.00	6.50									0.00 ± 0.00	-
183	7.20	0.35	6.50									0.00 ± 0.00	0.00
184	6.90	0.00	6.10									0.00 ± 0.00	-
185	7.10	0.00	6.40									0.00 ± 0.00	-
186	6.70	0.00	6.00									0.00 ± 0.00	-
187	7.20	0.67	6.40									0.05 ± 0.01	0.07

Table D-1 continued

Congener #	**Log** $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ **Calculated Porewater ng L**$^{-1\ b}$	**Log** $K_{PCBi\ fiber/w}$ **10 µm**$^{a,\ c}$ **this study**	**15 µm 42 days**	**7 µm 24 days**	**7 µm 96 hrs dynamic**	**7 µm 3 days**	**7 µm 37 days**	**30 µm 37 days**	**7 µm**	**30 µm**	$C_{PCBi\ pw}$ **Measured Porewater ng L**$^{-1\ d}$	**Ratio**^{m} $C_{PCBi\ pw}$ **measured: calculated**
188	6.80	0.00	6.10									0.00 ± 0.00	-
189	7.70	0.00	7.00									0.00 ± 0.00	-
190	7.50	0.06	6.70									0.00 ± 0.00	0.00
191	7.60	0.00	6.80									0.00 ± 0.00	-
192	7.50	0.00	6.80									0.00 ± 0.00	-
194	7.80	0.08	7.10									0.01 ± 0.00	0.10

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$									$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
			10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm		
195	7.60	0.05	6.80									0.00 ± 0.00	0.00
196	7.70	0.05	6.90									0.00 ± 0.00	0.00
197	7.30	0.12	6.60									0.00 ± 0.00	0.00
198+199	7.60	0.00	6.90									0.01 ± 0.01	-
200	7.30	0.00	6.60									0.00 ± 0.00	-
201	7.60	0.01	6.90									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log $K_{PCBi\ ow}$	$C_{PCBi\ pw}$ Calculated Porewater ng L^{-1} [b]	Log $K_{PCBi\ fiber/w}$ 10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	$C_{PCBi\ pw}$ Measured Porewater ng L^{-1} [d]	Ratio [m] $C_{PCBi\ pw}$ measured: calculated
202	7.20	0.04	6.50		6.77 ± 0.17							0.02 ± 0.01	0.36
203	7.70	0.07	6.90					6.85 ± 0.17	7.05 ± 0.07			0.00 ± 0.00	0.00
205	8.00	0.00	7.30									0.00 ± 0.00	-
206	8.10	0.01	7.40		7.04 ± 0.11							0.00 ± 0.00	0.00
207	7.70	0.01	7.00									0.00 ± 0.00	0.00
208	7.70	0.01	7.00									0.00 ± 0.00	0.00

Table D-1 continued

Congener #	Log	$C_{PCBi\ pw}$	Log $K_{PCBi\ fiber/w}$								$C_{PCBi\ pw}$	Ratio [m]
	$K_{PCBi\ ow}$	Calculated Porewater ng L^{-1} [b]	10 µm [a, c] this study	15 µm 42 days	7 µm 24 days	7 µm 96 hrs dynamic	7 µm 3 days	7 µm 37 days	30 µm 37 days	7 µm	30 µm	Measured Porewater ng L^{-1} [d]	$C_{PCBi\ pw}$ measured: calculated
209	8.20	0.00	7.50		6.84 ± 0.08							0.00 ± 0.00	-
SumPCBs		1400.00										110.00 ± 7.30	

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[a] when more than one congener appears due to co-elution of two or more congeners, the data point was assigned the PCB congener in the coeluting group with the highest content in different Aroclor mixtures as reported by in Frame et al. (145).

[b] Calculated from bulk sediment concentration, $K_{PCBi\ ow}$ from (4) and op-LERF from (66).

[c] Calculated from linear regression provided by Dr. Reible (eq 5-5).

[d] Only congeners that comply with criterion establish in QA/QC (see text).

[e] Congener PCB18.

[f] Congener PCB28.

[g] Congener PCB65.

[h] Congener PCB101.

[i] Congener PCB138.

[j] Congener PCB153.

[k] Congener PCB156.

[l] Congener PCB180.

[m] “-“ means that the calculated porewater concentration or denominator is zero.

Additional Information: New op-LFER and Sample Mass from Isotherm Experiments

New one-parameter linear free energy relationship (op-LFER) developed from IHSC sediment porewater concentration measurements

New one-parameter linear free energy relationship (op-LFER) developed from IHSC sediment porewater concentration measurements

The measured sediment-porewater distribution coefficient ($K_{PCBi\ oc\ m}$, L kg^{-1} oc) is defined as (eq d-1)

$$K_{PCBi\ oc\ m} = \frac{C_{PCBi\ s}}{C_{PCBi\ pw\ m} f_{oc}} \left(10^6 \frac{g\ L}{kg\ m^3}\right) \qquad \text{(d-1)}$$

where $C_{PCBi\ s}$ and $C_{PCBi\ pw\ m}$ are the measured bulk sediment and porewater concentration in the sediment for the ith PCB (ng m^{-3}), respectively, and f_{oc} is the total organic carbon fraction (kg oc kg^{-1}). When log $K_{PCBi\ oc\ m}$ is plotted versus log $K_{PCBi\ ow}$, a new relationship is obtained ($R^2 = 0.90$) (Figure D-1)

$$logK_{PCBi\ oc\ m} = 0.97 logK_{PCBi\ ow} + 0.49 \qquad \text{(d-2)}$$

This new relationship (eq d-2) improves what we have used in the past to estimate the distribution coefficients (66). Although this relationship is only recommended for IHSC sediments.

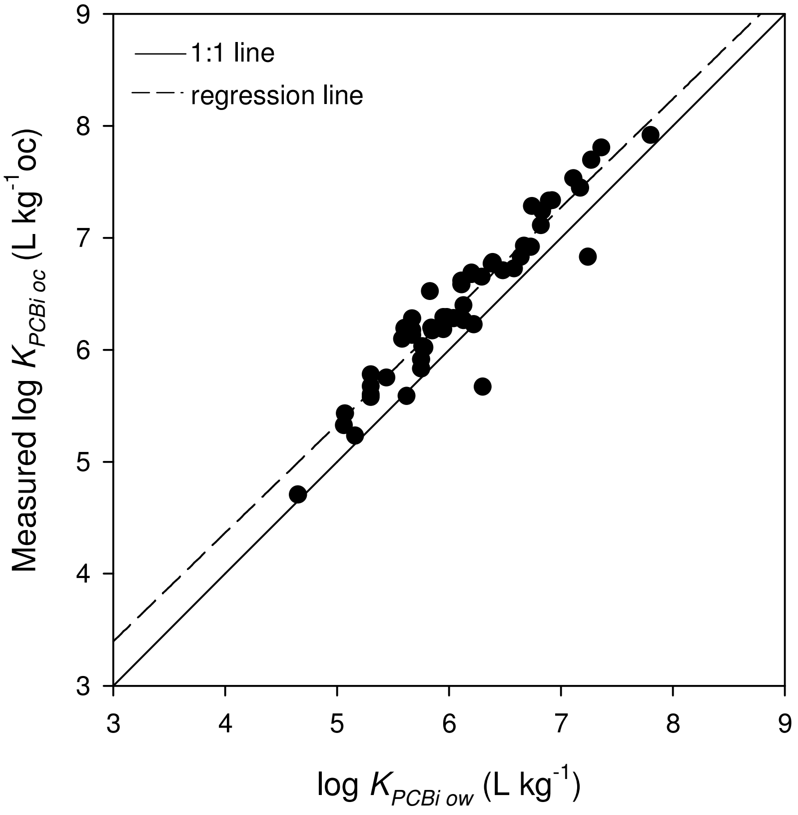

Figure D-1 Measured log $K_{PCBi\,oc}$ values versus log $K_{PCBi\,ow}$ (4). The regression line is described in eq d-2

Table D-2 Mass average of PCB congeners from isotherm experiments using SPME PDMS-fiber

Sample ID	**1**	**2**	**3**	**4**
Time (day)	15	30	45	60
Lab batch #	1	2	3	4
PCB14	50 ng	50 ng	50 ng	50 ng
d-PCB30	9.2 ng	9.2 ng	9.2 ng	9.2 ng
d-PCB65	50 ng	50 ng	50 ng	50 ng
PCB166	50 ng	50 ng	50 ng	50 ng
PCB204	9.32 ng	9.32 ng	9.32 ng	9.32 ng
Congener #	**ng**	**ng**	**ng**	**ng**
1	0.000	0.000	0.000	0.000
2	0.000	0.000	0.000	0.000
3	0.000	0.000	0.000	0.000
4	0.042	0.032	0.048	0.051
5	0.000	0.000	0.000	0.000
6	0.019	0.031	0.017	0.012
7	0.000	0.000	0.000	0.000
8	0.074	0.062	0.062	0.080
9	0.000	0.000	0.000	0.000
10	0.000	0.000	0.000	0.000
11	0.000	0.000	0.000	0.000
12+13	0.000	0.000	0.000	0.000
15	0.063	0.037	0.038	0.059
16	0.114	0.095	0.116	0.105
17	0.135	0.103	0.137	0.147
18+30	0.279	0.244	0.283	0.155
19	0.043	0.038	0.040	0.040
20+28	0.308	0.245	0.277	0.173
21+33	0.141	0.110	0.099	0.072
22	0.092	0.067	0.075	0.112
23	0.000	0.000	0.000	0.000
24	0.000	0.000	0.000	0.000
25	0.017	0.030	0.032	0.033
26+29	0.072	0.056	0.065	0.035
27	0.000	0.000	0.000	0.000
31	0.283	0.224	0.256	0.313
32	0.096	0.091	0.103	0.127
34	0.000	0.000	0.000	0.000
35	0.000	0.000	0.000	0.000
36	0.000	0.000	0.000	0.000

Table D-2 continued

Sample ID **Congener #**	**1** **ng**	**2** **ng**	**3** **ng**	**4** **ng**
37	0.082	0.054	0.066	0.065
38	0.000	0.000	0.000	0.000
39	0.000	0.000	0.000	0.000
40+41+71	0.280	0.208	0.294	0.282
42	0.146	0.127	0.149	0.162
43	0.000	0.000	0.000	0.000
44+47+65	0.505	0.443	0.479	0.473
45+51	0.160	0.199	0.230	0.167
46	0.000	0.000	0.000	0.000
48	0.121	0.095	0.123	0.107
49+69	0.280	0.273	0.337	0.299
50+53	0.142	0.185	0.173	0.149
52	0.495	0.426	0.532	0.508
54	0.000	0.000	0.000	0.000
55	0.000	0.000	0.000	0.000
56	0.165	0.135	0.164	0.155
57	0.000	0.000	0.000	0.000
58	0.000	0.000	0.000	0.000
59+62+75	0.089	0.061	0.063	0.034
60	0.098	0.074	0.089	0.094
61+70+74+76	0.573	0.429	0.539	0.512
63	0.000	0.000	0.000	0.000
64	0.215	0.191	0.227	0.180
66	0.309	0.249	0.311	0.369
67	0.000	0.000	0.000	0.000
68	0.100	0.082	0.096	0.118
72	0.000	0.000	0.000	0.000
73	0.000	0.000	0.000	0.000
77	0.000	0.000	0.000	0.000
78	0.000	0.000	0.000	0.000
79	0.000	0.000	0.000	0.000
80	0.000	0.000	0.000	0.000
81	0.000	0.000	0.000	0.000
82	0.000	0.000	0.000	0.000
83+99	0.127	0.082	0.100	0.118
84	0.082	0.090	0.100	0.097
85+116+117	0.508	0.510	0.560	0.917
86+87+97+109+119+125	0.165	0.183	0.173	0.143
88+91	0.075	0.068	0.080	0.078
89	0.000	0.000	0.000	0.000

Table D-2 continued

Sample ID **Congener #**	**1** **ng**	**2** **ng**	**3** **ng**	**4** **ng**
90+101+113	0.245	0.199	0.247	0.184
92	0.000	0.000	0.000	0.000
93+100	0.000	0.000	0.000	0.000
94	0.000	0.000	0.000	0.000
95	0.212	0.205	0.252	0.199
96	0.000	0.000	0.000	0.000
98+102	0.000	0.000	0.000	0.000
103	0.000	0.000	0.000	0.000
104	0.000	0.000	0.000	0.000
105	0.085	0.071	0.071	0.066
106	0.000	0.000	0.000	0.000
107	0.000	0.000	0.000	0.000
108+124	0.000	0.000	0.000	0.000
110+115	0.284	0.260	0.277	0.492
111	0.000	0.000	0.000	0.000
112	0.000	0.000	0.000	0.000
114	0.039	0.057	0.055	0.237
118	0.135	0.112	0.136	0.125
120	0.000	0.000	0.000	0.000
121	0.000	0.000	0.000	0.000
122	0.000	0.000	0.000	0.000
123	0.000	0.000	0.000	0.000
126	0.000	0.000	0.000	0.000
127	0.000	0.000	0.000	0.000
129+138+163	0.201	0.157	0.178	0.177
130	0.000	0.000	0.000	0.000
131	0.000	0.000	0.000	0.000
132	0.100	0.081	0.088	0.088
133	0.000	0.000	0.000	0.000
134+143	0.000	0.000	0.000	0.000
135+151	0.121	0.104	0.100	0.126
136	0.059	0.040	0.054	0.053
137+164	0.000	0.000	0.000	0.000
139+140	0.000	0.000	0.000	0.000
141	0.050	0.058	0.040	0.057
142	0.000	0.000	0.000	0.000
144	0.000	0.000	0.000	0.000
145	0.000	0.000	0.000	0.000
146	0.018	0.041	0.038	0.030
147+149	0.182	0.158	0.171	0.167

Table D-2 continued

Sample ID **Congener #**	**1** **ng**	**2** **ng**	**3** **ng**	**4** **ng**
148	0.000	0.000	0.000	0.000
150	0.000	0.000	0.000	0.000
152	0.000	0.000	0.000	0.000
153+168	0.187	0.136	0.143	0.138
154	0.000	0.000	0.000	0.000
155	0.000	0.000	0.000	0.000
156+157	0.000	0.000	0.000	0.000
158	0.000	0.000	0.000	0.000
159	0.000	0.000	0.000	0.000
160	0.000	0.000	0.000	0.000
161	0.000	0.000	0.000	0.000
162	0.000	0.000	0.000	0.000
165	0.000	0.000	0.000	0.000
167	0.000	0.000	0.000	0.000
169	0.000	0.000	0.000	0.000
170	0.054	0.043	0.081	0.057
171+173	0.000	0.000	0.000	0.000
172	0.000	0.000	0.000	0.000
174	0.065	0.033	0.077	0.052
175	0.000	0.000	0.000	0.000
176	0.000	0.000	0.000	0.000
177	0.000	0.000	0.000	0.000
178	0.000	0.000	0.000	0.000
179	0.033	0.038	0.054	0.038
180+193	0.142	0.092	0.136	0.097
181	0.000	0.000	0.000	0.000
182	0.000	0.000	0.000	0.000
183	0.000	0.000	0.000	0.000
184	0.000	0.000	0.000	0.000
185	0.000	0.000	0.000	0.000
186	0.000	0.000	0.000	0.000
187	0.118	0.071	0.102	0.096
188	0.000	0.000	0.000	0.000
189	0.000	0.000	0.000	0.000
190	0.000	0.000	0.000	0.000
191	0.000	0.000	0.000	0.000
192	0.000	0.000	0.000	0.000
194	0.099	0.042	0.073	0.046
195	0.000	0.000	0.000	0.000
196	0.000	0.000	0.000	0.000

Table D-2 continued

Sample ID **Congener #**	**1** **ng**	**2** **ng**	**3** **ng**	**4** **ng**
197	0.000	0.000	0.000	0.000
198+199	0.083	0.018	0.136	0.027
200	0.000	0.000	0.000	0.000
201	0.000	0.000	0.000	0.000
202	0.034	0.000	0.053	0.047
203	0.000	0.000	0.000	0.000
205	0.000	0.000	0.000	0.000
206	0.000	0.000	0.000	0.000
207	0.000	0.000	0.000	0.000
208	0.000	0.000	0.000	0.000
209	0.000	0.000	0.000	0.000
Total	**9.041**	**7.647**	**9.095**	**9.139**

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