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PCB Dose-Response Benthic Injury Models Using Equilibrium Partitioning

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PCB Dose-Response Benthic Injury Models Using Equilibrium Partitioning

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Contents

List of Tables

List of Figures

List of Appendices

ABSTRACT

The goal of this project was to develop a sediment PCB dose-response model based on benthic invertebrate effects to PCBs. We used an equilibrium partitioning (EqP) approach to generate predicted PCB sediment effect concentrations (largely Aroclor 1254) associated with a gradient of toxic effects in benthic organisms from effects observed in the aquatic toxicity studies. This report differs from all other EqP sediment investigations in that we examined a gradient of effects for multiple sites rather than a single, protective value.

We reviewed the chronic aquatic toxicity literature to identify measured aqueous PCB concentrations and the associated benthic invertebrate effects. We control- normalized the aquatic toxic effect data and expressed results from various studies as a common metric, % injury. Then we calculated organic carbon (oc) -normalized sediment PCB concentrations (mg/kg_{-oc}) from the aqueous PCB toxicity dataset using EqP theory based on EPA's (EPIWEB 4.1) derivation of Koc. Lastly, we constructed a non-linear dose-response numerical model for these synoptic sediment PCB concentrations and biological effects ($Y = 100/1 + 10^{(logEC50-logX) \cdot (Hill\ slope)}$). These models were used to generate easy to use "look-up" tables reporting % injury in benthic biota for a range of Aroclor-specific sediment concentrations. For example, the model using the EPIWEB 4.1 Koc estimate predicts the mean benthic injury of 23.3%, 46.0%, 70.6%, 87.1% and 95% for hypothetical sediment concentrations of 1, 2, 4, 8, 16 mg/kg dry wt. of Aroclor 1254, respectively (assuming 1% organic carbon).

Models for some Aroclors (1016, 1221, 1232, and 1268) could not be developed due to data gaps in the aquatic toxicity literature. Specific step-wise procedures are provided for predicting % benthic injury when sediment PCBs are reported as Aroclor, congeners, homolog groups or total PCBs. The report identifies and discusses the uncertainties associated with the numerical PCB dose-response models and the EqP approach and provides considerations for how other Koc values result in more or less conservative models. This paper provides recommendations for addressing outstanding issues, including the Koc calculation, the two-carbon model, and congener data. We recommend using the model presented for screening but suggest, when possible, to determine a site specific Koc; that along with the tables and equations herein allows users to create their own protective dose-response sediment concentration for a specific location.

INTRODUCTION

Polychlorinated biphenyls (PCBs) are mixtures of synthetic compounds (congeners) which vary in chlorine content and spatial configuration. PCB congeners can be grouped into isomeric homologs with the same chlorine content (i.e., monochloro-, dichloro- up to decachlorbiphenyls) but different spatial configurations (Ballschmiter and Zell 1980). PCBs were manufactured in the United States between 1929 and 1977 as various Aroclor mixtures (e.g., Aroclor 1016, A1242, A1248, A1254, A1260) with chlorine content ranging from 21% to 68% (Shiu and MacKay 1986, DeVoogt and Brinkman 1989). Aroclors were used primarily as dielectric fluids in transformers and capacitors but were also used as lubricants, in carbonless paper and heat- transfer systems. Production peaked in 1970 and subsequently ceased in 1977 as it became increasingly clear that PCBs had made their way into the environment and posed significant risks to human health and the environment (DeVoogt and Brinkman 1989, USEPA 1980, ATSDR 2000).

Like most environmental contaminants, early regulatory control of PCBs focused on "end of the pipe" discharges. In the U.S. as well as other countries, technical support for regulatory control for PCBs and other contaminants appeared in the form of chemical-specific ambient water quality documents (e.g., USEPA 1980) containing numerical criteria (Stephen et al. 1985). Many states adopted these water quality criteria as enforceable regulatory standards. As field investigations increased in number and scope, it became apparent that contaminants discharged into the aquatic environment were accumulating to high levels in bottom sediments. This was especially true for hydrophobic contaminants such as PCBs. Today PCBs are frequently identified as chemicals of concern at contaminated sediment sites in the U.S. and around the world (National Research Council 2001, 2007, USEPA 2005a, Holoubek 2000).

In response to the increasing concern regarding contaminated sediments, the USEPA embarked upon a regulatory research program to develop sediment quality criteria analogous to water quality criteria (USEPA 1988). Developing these sediment criteria eventually became part of the USEPA's strategy for managing contaminated sediments across its many regulatory programs (USEPA 1998). Two methods were generally advocated for developing sediment criteria. First is the Equilibrium Partitioning (EqP) approach that estimates a sediment concentration based on a pore water concentration protective of aquatic biota and EqP modeling to predict sediment concentration from pore water concentration. Applied research supporting the EqP approach has provided data that the chemical sensitivity of benthic/epibenthic organisms is not significantly different from pelagic organisms (USEPA 2008). The theoretical EqP approach helps answer the question, "Will this contaminant in this sediment matrix cause toxicity to benthic organisms?" The second approach for developing sediment criteria examines large datasets for numerical relationships between synoptic sediment chemistry and sediment toxicity data (largely 10-day amphipod bioassays). This empirical approach helps answer the question, "What's the likelihood this sediment will be toxic to benthic biota?" Both approaches have advantages and limitations as discussed in Burton (2002). However, as applied research continued, it became apparent that significant and substantial scientific uncertainties were associated with both approaches. This

prompted the USEPA to begin referring to the numerical sediment criteria as guidelines or benchmarks (USEPA 2008). Both approaches generate toxicity threshold sediment concentrations. The theoretical approach produces a sediment concentration believed to be protective of benthic organisms. The empirical approach produces values believed to represent threshold effects concentrations (e.g., ERL-Effects Range Low, TEL-Threshold Effects Level) as well as concentrations associated with a reasonable likelihood of effects (e.g., ERM-Effects Range Median, PEL- Probably Effects Level, AET-Apparent Effects Threshold). The empirical approach has subsequently incorporated the use of logistic regression modeling to estimate a continuum of probable benthic toxicity (e.g., 20%, 50%, 80%) (USEPA 2005b). No analogous effects continuum has been developed for the EqP approach.

At hazardous waste sites in the U.S., the ecological risks and potential injury of PCBs to biological resources are determined by conducting Ecological Risk Assessments (ERAs) and Natural Resource Damage Assessments (NRDAs), respectively (Barnthouse and Stahl 2002, Munns et al. 2009). Both programs have the goal of identifying chemicals responsible for the risk or injury. Sediment guidelines or benchmarks are often used in both ERAs and NRDAs to estimate adverse effects of PCB-contaminated sediments on benthic invertebrates. Based on the empirical approach discussed above, MacDonald et al. (2000) proposed the following three consensus Sediment Quality Guidelines (SQGs) for total PCBs: Threshold Effect Concentration (TEC) = 0.040 mg/kg dry wt., Midrange Effect Concentrations (MEC) = 0.40 mg/kg dry wt., Extreme Effect Concentrations (EEC) = 1.7 mg/kg dry wt. Using the theoretical EqP approach, Fuchsman et al. (2006) proposed protective oc-normalized chronic sediment quality benchmarks for the following Aroclor mixtures: A1242 = 210 µg/g-oc, A1248 = 490 µg/g-oc, A1254 = 1,500 µg/g-oc, A1260 = 3,800 µg/g-oc. Assuming 1% organic carbon, the benchmarks' dry-weight concentrations would be 2.1 mg/kg, 4.9 mg/kg, 15 mg/kg and 38 mg/kg, respectively. In this report, we use the theoretical EqP approach to generate a continuum of benthic injury dose-response for sediments contaminated with PCBs. We compare our approach to threshold values reported by Fuchsman et al. (2006). We discuss important uncertainties associated with the use and application of the benthic injury dose-response curve for PCB-contaminated sediments. Finally, we provide specific step-wise procedures for predicting % benthic injury when sediment PCBs are reported as Aroclors, congeners, homolog groups or total PCBs.

MATERIALS AND METHODS

Aqueous PCB Toxicity Literature

Multiple search strategies were used to compile literature reporting the results of laboratory toxicity tests where aquatic invertebrates were exposed to aqueous solutions of commercial PCB mixtures (Aroclors). These strategies included electronic literature searches (e.g., ISI Web of Knowledge, Aquatic Science & Fisheries Abstracts), review of published compilations of toxicity literature (e.g., USEPA 1980) and personal collections of papers. We excluded studies that had exposure concentrations greater than the Aroclor aqueous solubilities reported by Mackay et al. (2006). In addition, we only considered studies in which investigators reported measured aqueous Aroclor

exposure concentrations since actual concentrations can be one-half to an order-of-magnitude less than nominal concentration (Laughlin et al. 1977, Ho et al. 1997, Roesijadi et al. 1976). We also avoided acute lethality exposures (e.g., ≤ 96h LC50) in favor of longer chronic exposures measuring biologically important endpoints (survival, reproduction, growth). For each accepted investigation the following information was compiled: species tested, age/size of test organisms, exposure scenario (e.g., duration, flow-through, static-renewal), measured aqueous Aroclor exposure concentrations for each treatment and the corresponding biological effects.

Analysis of Aqueous PCB Toxicity Data

To combine laboratory toxicity results from different biological endpoints into a single dependent variable for use in the composite dose–response curve, Dillon et al. (2010) used a control-normalized common metric of % fish injury. A similar approach is used here for the aqueous PCB toxicity literature. For each experimental treatment in a toxicity test, a percent Control-Normalized Response (% CNR) was calculated using Equation 1.

$$\% \text{ CNR} = (\text{treatment response/control response}) \bullet (100) \quad (1)$$

To compare results from different test endpoints, % CNR results were expressed as a common metric, % benthic injury, according to Equation 2. In instances where a treatment response exceeded controls, % benthic injury was set to 0%.

$$\% \text{ Injury} = 100\% - \% \text{ CNR} \quad (2)$$

Aqueous PCB Dose-Response Curve

The paired observations of measured aqueous Aroclor concentrations and chronic biological effects obtained from the literature were used to construct a dose-response curve using GraphPad PRISM® software (Version 5.01; http//www.graphpad.com). The non-linear log (stimulation) versus normalized response module with a variable Hill slope was the model selected for this study. The numerical model for this curve is shown in Equation 3

$$Y = 100/1 + 10^{(\log EC50 - \log X) \bullet (\text{Hill slope})} \quad (3)$$

where Y = % benthic injury, X = aqueous Aroclor concentration (µg/L), EC50 = the effective Aroclor concentration that causes a response halfway between the baseline (0% benthic injury) and maximum response (100% benthic injury), and the Hill slope, which is the numerical value representing the steepness of the dose-response curve. Model outputs also include the Lower and Upper 95% Confidence Interval (CI) around the % benthic injury estimate. In constructing the numerical model, Aroclor concentrations must be $\log_{10}$-transformed. This is problematic for control treatments (0 µg/L) where measured detection limits were not reported. In those instances, a surrogate value of 0.05 µg/L was used. This value is one-half the 0.1 µg/L detection limit for water samples frequently reported in papers contemporary to the toxicity literature we used (Duke et al. 1970, Roesijadi et al. 1976, Borgman et al. 1990).

Equilibrium Partitioning (EqP) Modeling

As noted in the Introduction, Equilibrium Partitioning (EqP) modeling can be used to predict sediment concentrations from aqueous concentrations. Using EqP we model PCB concentrations in sediment from the aqueous concentrations used to construct the dose-response injury curve just described. In its simplest form, EqP modeling for PCBs can be expressed by the following equation

$$\text{Sediment Concentration} = \text{Interstitial Water Concentration} \bullet K_{oc} \bullet f_{\underline{oc}} \bullet 0.001 \quad (4)$$

where the oc-normalized PCB sediment concentration (mg/kg_{-oc}) is equal to the product of interstitial water PCB concentration (µg/L), the PCB-specific partition coefficient between water and organic carbon (K_{oc}) (L/kg), the mass fraction of organic carbon in sediment (f_{oc}) and 0.001 (for unit conversion). In practice, the more widely available and sometimes equivalent octanol-water partition coefficient (K_{ow}) is often substituted for K_{oc} (DiToro et al. 1991). However, equations to calculate the K_{oc} from the K_{ow} are available from the literature. For example, Hawthorne et al, 2011 (from Schwarzenbach et al. 2003) provides:

$$\log (K_{oc}) = 0.74 \log (K_{ow}) + 0.15 \quad (5)$$

and DiToro and McGrath (2000) use:

$$\log (K_{oc}) = 0.00028 + 0.983 \log (K_{ow}) \quad (6)$$

We note that Burgess et al. (2013) used this Kow-Koc transformation equation in their seminal paper on calculating EqP single sediment benchmarks for non-ionic organic chemicals other than PCBs. The Koc selection is likely the most variable and influential factor within the EqP equation and therefore deserves more attention.

Selecting an Appropriate Octanol-Water (Kow) and/or Organic Carbon (Koc) Partition Coefficient for EqP Modeling.

Uncertainties associated with the application of EqP theory to science and to regulatory implementation have been examined and discussed (e.g., DiToro et al. 1991, Burton 2002, USEPA 2008, Maruya et al. 2012). This report examines a major component of EqP modeling that significantly affects the development of a sediment PCB benthic injury curve; the selection of an appropriate Kow value to calculate oc-normalized sediment concentrations from aqueous PCB concentrations. Linkov et al. (2005) demonstrated that small changes in Kow can results in significant difference in EqP model predictions for hydrophobic chemicals such as PCBs and DDTs. Because our chronic toxicity PCB concentrations are based exclusively on Aroclor mixtures (Tables 1-4), selecting an Aroclor-specific Kow value is one approach for EqP modeling in this investigation. The homolog approach used by Fuchsman et al. (2006) is found later in the Discussion, , as is a congener approach. The handbook published by Mackay et al. (2006) may be one of the most widely cited and respected sources for physical-chemical properties of organic chemicals. Table 5 is a summary of individual Kow values for the seven Aroclor mixtures reported

by Mackay et al. (2006). Log Kow values generally range between 2 to 3 orders of magnitude for each Aroclor (n=8-13 studies per Aroclor). Descriptive statistics were calculated and reported in Table 5 for the non-logarithm expression of the Kow values because that is the number used in EqP model calculations. The percent coefficients of variation (standard deviation/mean) are high, exceeding 100% for all Aroclors except A1248 (Table 5). The mean and median Kow values are similar for some Aroclors (e.g., A1221 and A1232) but differ considerably for others (e.g., A1254). Large variation is perhaps not surprising because these Kow values were not sampled from a single population. Instead they were compiled from disparate sources published over a number of years by different investigators who used different analytical methods and partitioning techniques (e.g., shake-flask versus slow-stir methods). The median, which dampens the influence of very high and very low values, may be the most reasonable central tendency estimator for the highly variable Aroclor Kow values reported by Mackay et al. (2006). For example, using Equation 5 and the median log Kow of 6.11 (1,288,250 L/Kg) for Aroclor 1254, found in Table 5, the log (Koc) is 4.6714 (46,925 L/kg).

The EPA Estimation Program Interface (EPI) Suite Version 4.11, November 2012 (http://www.epa.gov/opptintr/exposure/pubs/episuite.htm) also provides a source of Koc values. The transformation equation provided in the KOCWIN Users Guide (Section 6.1.3 – Methodology) is:

$$\log (K_{oc}) = 0.55313 \log (K_{ow}) + 0.9251 + \text{correction factor} \quad (7)$$

The EPI Suite calculation of the Aroclor 1254 log (Koc) is 4.8252 (66,865 L/kg), consistent with, but slightly higher than the Koc calculated using the median Kow reported in Mackay et al. (2006) and Equation 5.

Predicted and measured Koc values reported in the literature likely under-predict Koc values calculated from measurements of the freely dissolved PCB fraction (Hawthorne et al. 2011). Therefore, we used a poly-parameter linear free energy relationship (PP-LFER) approach to predict an Aroclor 1254 Koc based on using the freely dissolved fraction (van Noort et al. 2010; Arp, personal communication 2014). Average homolog Koc was calculated from individual congener PP-LFER Koc, and the average homolog Kocs values were weighted by percent homolog composition (e.g., pentachlorobiphenyl is 59.12 % of A1254; ATSDR 2000) to calculate a log Koc of 7.5 (31,622,777 L/kg) for Aroclor 1254.

Koc selection is the biggest uncertainty in the EqP dose-response model and the Koc values from the three independent methods presented above cover a wide range. To build the dose-response relationship, we selected the log Koc value of 4.8252 from the EPA EPI Suite. This Koc is the best choice because it is consistent with the available aqueous toxicity dataset, i.e., Aroclor measurements of whole unfiltered water containing both colloids and dissolved organic matter. Although this results in the use of a Koc value well below the freely dissolved PCB Koc, it is consistent with the aqueous toxicity dataset and is supported by the Environmental Protection Agency.

RESULTS

Toxicity of Aqueous PCBs to Aquatic Invertebrates

Our literature search identified 17 individual Aroclor chronic toxicity tests (in six separate publications) with aquatic invertebrates in which investigators reported measured aqueous exposure concentrations (Table 1). Most experiments evaluated Aroclor 1254 (A1254). Two studies examined A1248 and one tested A1242. Both saltwater organisms (pink shrimp *Penaeus duorarum*, grass shrimp *Palaemonetes pugio*, Eastern oyster *Crassostrea virginica*) and freshwater organisms (water flea *Daphnia magna*, amphipod *Gammarus pseudolimnaeus*, midge *Tanytarsus dissimilis*) were evaluated in these chronic toxicity tests. All test organisms were crustaceans except two studies that tested Eastern oysters. Many exposures began with juvenile or early life stage organisms. With one exception, all exposure scenarios involved flowing water with Aroclor metered in by pump or syringe (Table 1). In the one exception (Roesijadi et al. 1976), static exposure water was renewed every 48 hours. Although all experiments used a carrier solvent for the hydrophobic Aroclors, measured PCB concentrations were below median aqueous solubilities reported in Mackay et al. (2006) (Table 2). In all but one of the 17 experiments survival was measured following chronic exposure to Aroclors (Table 1). In that one experiment investigators monitored the number of larval and pupal cases produced by the freshwater midge *Tanytarsus dissimilis* and stated these endpoints were a "measure of growth and survival". Various reproductive endpoints (e.g., Young per Initial Adult) were measured in five of the experiments involving freshwater *Daphnia magna* and *Gammarus pseudolimnaeus*. Growth was measured in three experiments as new shell growth in young oysters or as weight of young scud (*Gammarus pseudolimnaeus*) produced by exposed adults.

Aqueous PCB Dose-Response Benthic Injury Curves

Crustacean survival following chronic Aroclor exposures was the most frequent (14 of 17 experiments) test organism-endpoint pairing in the literature we reviewed (Table 1). Consequently, an initial aqueous PCB dose-response curve was constructed based solely on crustacean survival data reported in these 14 experiments. Calculations of % CNR and % benthic injury for these experiments are shown in Table 3. Collectively the 14 individual toxicity experiments represent a total of 58 paired observations of measured aqueous Aroclor concentrations and % survival (Table 3). Most (69%) of the 58 paired observations are for A1254 (n=40). A1248 and A1242 are represented by 12 (21%) and 6 (10%) paired observations, respectively. Table 4 summarizes all 58 paired observations. The surrogate PCB concentration of 0.05 µg/L (see Materials and Methods) was used for the control treatment concentrations in all experiments discussed above. We assumed 0% benthic injury for all control treatments. The non-linear model indicated aqueous Aroclor concentrations equal to or greater than 15.6 µg/L were always associated with 100% benthic injury (i.e., 100% mortality).

The $\log_{10}$ expression of aqueous PCB concentrations are also shown in Table 4 to facilitate observations of individual values in the dose-response curve (Figure 1) constructed per equation (3)

using the data in Table 4. The curve (Figure 1) has an EC50 (95% CI) of 4.09 µg/L (3.05-5.49 µg/L). The unitless Hill slope is 1.43 with a 95% CI of 0.77-2.08. A Hill slope of 1.0 is typical in dose-response curves. The R-squared for this curve is 0.70.

The dose-response curve in Figure 1 is based on survival of crustaceans exposed to aqueous solutions of Aroclors. However, it is a frequent observation in the aquatic toxicity literature, that sublethal effects occur at concentrations below those causing death (Rand 1995). This same observation has been reported for crustaceans in the literature we reviewed (Nebeker and Puglisi 1974). To quantify this relationship, survival and the number of Young per Initial Adult (YpIA) were examined more closely in the six separate experiments reported by Nebeker and Puglisi (1974) involving *Daphnia magna* and *Gammarus pseudolimneaus*. The YpIA reproductive endpoint was selected over others (i.e., Total Young Produced, Young Produced per Surviving Adult) because it is less influenced by different survival rates and because the number of initial adults varied among treatments. For both the survival and YpIA endpoints, total % injury was calculated as the sum of % injury values from individual treatments (Table 6). Then, within each experiment, total % injury for the survival endpoint was divided into the total % injury for the YpIA endpoint to produce a Survival:Reproductive Effects ratio (Table 6). The ratios ranged between 0.92 and 1.52 with a mean of 1.25 (n=6) (Table 6). This suggests that, on average, the reproductive endpoint is about 25% more sensitive than survival in these experiments reporting the chronic effects of PCBs to two crustacean species. None of the other publications described in Table 1 report both survival and reproduction.

The aqueous PCB dose-response injury curve based on survival (Figure 1) was re-calculated using % injury values that were adjusted upward by 25% (Table 7) to account for the adverse effects of PCBs on offspring production. As expected, the resultant curve (Figure 2) has a slightly lower EC50 (95% CI) of 3.33 µg/L (2.45-4.53 µg/L) compared to Figure 1; 4.09 µg/L (3.05-5.49 µg/L). The unitless Hill slope (95% CI) for the curve in Figure 2 is slightly higher 1.49 (0.75-2.24) compared to 1.43 (0.77-2.08) for the survival-only curve in Figure 1. The R-squared for the curve in Figure 2, 0.69, is very similar to the survival-only curve (0.70). As was seen in Figure 1, aqueous PCB concentrations in Figure 2 that are equal to or greater than 15.6 µg/L ($\log_{10}$ = 1.19 µg/L) were always associated with 100% injury. Concentrations equal to or less than the surrogate value of 0.05 µg/L ($\log_{10}$ = -1.30 µg/L) were always associated with 0% injury.

Benthic Injury Dose-Response Curve for PCB-Contaminated Sediments Using Koc from EPI Suite 4.1

A benthic injury dose-response curve was developed for Aroclor 1254 with the limited toxicity data for Aroclor 1248 and Aroclor 1242 also included. At this time, it is not appropriate to develop curves for the other Aroclor mixtures (e.g. A1260, A1268) because: 1) the chronic aqueous toxicity data from the literature we reviewed (Table 1) are limited to these three Aroclors (primarily A1254) and 2) the paucity of comparative toxicity data renders extrapolation from these three Aroclors to other mixtures highly uncertain (see Discussion). Because 69% of the aquatic toxicity tests we obtained used A1254 as the test chemical, we focus on that Aroclor.

Table 8 reports the aqueous PCB dose-response information from Table 7 with the additional sediment columns. The first additional column presents the oc-normalized sediment concentrations (mg/kg-oc) modeled using EqP and the Koc from Equation 7. The second additional column contains A1254 sediment concentrations expressed as the more familiar mg/kg dry wt. assuming 1% organic carbon. Data from Table 8 were used to construct a benthic injury dose-response curve in PRISM software for sediments containing A1254. Specifically, the oc-normalized sediment concentrations and the % injury from Table 8 were the X and Y input parameters for equation (3). This produced the benthic injury dose-response curve for A1254-contaminated sediments as shown in Figure 3. Major descriptors for this curve include the EC50 (95% CI) 222.6 mg/kg-oc (163.5-303.0 mg/kg-oc), Hill slope (95% CI) 1.49 (0.74-2.24), R-squared (0.69) and number of points analyzed (n=58).

Although we focus on Aroclor 1254, the Hill slope (95% CI), R-squared and the number of data points would be the same for Aroclors 1248 and 1242. The EC50 values, however, change according to the relative difference in their respective Koc values. For example, when using the EPA EPI Web 4.1, the log Koc for Aroclors 1254, 1248, and 1242 are 4.8252, 4.4989, and 4.5487, respectively. The Koc values are relatively close, but the lower Koc values would predict higher injury for similar PCB sediment concentrations when the PCB sediment mixture is predominantly composed of Aroclor 1248 or Aroclor 1242, when compared to Aroclor 1254.

Once the sediment dose-response curve is created, the PRISM software can create a table of graded XY coordinates that bracket the highest and lowest X-values (oc-normalized sediment concentrations) used to build each curve. We used this software feature to create lookup tables (n=150 points) for A1254 (Table 9) that includes the % benthic injury (95% CI) corresponding to the range of sediment concentrations reported in Table 8.

Table 10 summarizes % injury (95% CI) corresponding to a hypothetical geometric progression of sediment concentrations (mg/kg dry wt.) for A1254. For this series of sediment concentrations, predicted % benthic injury in A1254-contaminated sediments would be 23.3%, 46.0%, 70.6%, 87.1% and 95.0% for hypothetical sediment concentrations of 1, 2, 4, 8, 16 mg/kg dry wt., respectively (assuming 1% organic carbon).

Other EqP Choices to Find Benthic Injury Dose-Response Curves for PCB-Contaminated Sediments

By using the aquatic dose response database provided in Table 7 and Figure 2, one can select preferred Koc values to determine the PCB dose response (cf. Tables 8, 10 and 11). For example, the median K_{ow} from Table 5 can be used in Equation 5 to calculate Koc to estimate the sediment concentration for the EqP equation (Equation 4). This Koc is approximately 30% lower and therefore would predict greater injury at the same A1254 concentrations.

The PP-LFER approach for finding the Koc for our aquatic database was discussed previously. This Koc relies on using freely dissolved concentration data from filtered water samples with

removal of all colloidal material, resulting in a relatively high log Koc of 7.5. The aquatic concentrations reported in aquatic toxicity datasets used to develop the dose-response model are from PCB concentrations measured in unfiltered water and therefore cannot be used with the PP_LFER approach. PCB aqueous concentration measurements and the selected Koc need to be paired appropriately for analysis.

Another approach for determining Koc is to make site-specific measurements. Matching site-specific unfiltered pore water concentrations and oc-normalized sediment concentrations allows one to calculate a site-specific Koc that could be used instead of the EPA EPIWIN Koc. However, obtaining accurate measurements for the extremely low PCB concentrations in the dissolved pore-water phase can be challenging.

DISCUSSION

There have been recent appeals in the environmental toxicological community to stop using point estimates to quantify chemical hazard and instead use a dose-response or exposure-response curve (Landis and Chapman 2011; Jager 2011). While ERAs have typically relied heavily on point estimates for risk thresholds, and NRDAs more frequently rely on dose-response models, practitioners of both would benefit from a greater use of dose-response information (Gala et al. 2009). To our knowledge, our investigation is the first to derive a common sediment dose-response curve for aquatic invertebrates by coupling literature-derived aqueous dose-response information for PCBs with EqP modeling.

In the sediment toxicity community, point estimates predominate whether derived empirically (e.g., ERLs/ERMs , TELs/PELs, TEC/PECs, AETs, Logistic Regression(Long and Morgan 1990, Smith et al.1996, MacDonald et al. 2000, Barrick et al. 1988, Field et al. 2002, among others) or theoretically via EqP (Fuchsman et al. 2006, Burgess et al. 2013). By undertaking a site-specific (i.e. field derived) EqP PCB sediment study of the Anniston Superfund Site in Alabama, MacDonald et al. (2014) calculated a toxicity threshold high range (TT_{HR}) and low range (TT_{LR}). The former is defined as "the concentrations of contaminants of potential concern (COPCs) or COPC mixtures that corresponded to a 10-percent reduction in survival, weight, biomass, emergence, or reproduction, compared to the lower limit of the reference envelope". The latter corresponds to that lower limit of the reference envelope for the selected toxicity test endpoint. Using measured pore water allows for an empirical dose –response (i.e., reference envelope approach) resulting in a TT_{HR} sediment values of 2.08 mg/kg for total PCBs using 42-d *Hyalella azteca* reproduction. When using total homologs rather than total Aroclors this TT_{HR} value gets reduced by about one half to 1.18 mg/kg and when using the TT_{LR} as low as 0.5 mg/kg. Although these values represent a dose-response from one specific study they modestly fit our generic dose-response model as provided in Tables 9 and10.

Despite drawing PCB toxicity information from disparate literature sources (Table 1), the resulting pattern of dose-response appears quite good (Figures 1, 2, 3) with reasonable R-squared values (0.69-0.71). These PCB dose-response curves for invertebrates are a type of ecological model. To

have greater value to scientists, environmental managers and decision-makers, predictions generated by ecological models should be accompanied by a description of their associated uncertainty (Li and Wu 2006). Consequently, much of the discussion below describes the toxicological and physico-chemical uncertainties associated with data inputs to the benthic PCB dose-response models presented here. Toxicological factors include the comparative toxicity of the Aroclor mixtures, the limited availability of the aqueous toxicity literature and older studies that use potentially pre-exposed PCB-resistant test organisms, as well as the use of unfiltered water for aquatic testing. The latter has an extremely important influence on the selection of Kow and Koc values for the EqP model. The Discussion concludes with recommendations for how to apply the benthic dose-response models to field results with PCB-contaminated sediments and an overview of outstanding technical issues that need further work. As emphasized previously, the choice of Koc is the key factor in calculating a protective sediment concentration.

Comparative Toxicity of Aroclor Mixtures to Aquatic Invertebrates

The aqueous dose-response curves for PCBs (Figures 1 and 2) are based largely (69%) on the adverse effects on survival and reproduction in crustaceans following chronic exposure to Aroclor 1254. A1248 and A1242 represent 10% and 21%, respectively, of the paired observations used to create the dose-response curves. Consequently, predicting % benthic injury when other Aroclors are present is problematic. At least three published compilations of aqueous toxicity tests with PCBs report that mortality is highest in Aroclor mixtures of intermediate chlorination (e.g., A1242, A1248, A1254) and lowest in the higher and lower chlorinated mixtures; e.g., A1268 and A1221, respectively (Nagpal 1992, Dobson and van Esch. 1993, Fuchsman et al. 2006). Likely, these results occur because higher weighted Aroclors are hydrophobic and lower weighted Aroclors are more water soluble. However, generalizations from these and similar published compilations (e.g., Mayer 1987, Mayer and Ellersieck 1986) must be viewed carefully because factors that have substantial effects on comparative toxicity are not adequately considered. For example, organisms exposed in flowing-water systems exhibited greater apparent sensitivity to PCBs (e.g., lower LC50 values) than those in static-renewal or static-exposure systems (Nebeker and Puglisi 1974). This difference in response occurs largely because the three systems generally create constant, pulsed and declining PCB exposure concentrations, respectively.

Life stage of the test species can also have substantial effects on survival. Juvenile and early life stages are generally more sensitive than adult organisms of the same species (e.g., Roesijadi et al. 1976, Mayer 1987). Other factors such as duration of exposure, temperature and feeding regime all can have profound influence on the outcomes of PCB toxicity tests. Consequently, generalizations about comparative Aroclor toxicity require careful consideration of test variables that could influence apparent sensitivity.

Relatively few reports have been published which control for the above confounding factors. Mayer (1987) reports the results of numerous static toxicity tests with A1242 and A1016 conducted with various life stages of *Palaemonetes pugio*. The 96h LC50 values based on measured water concentrations were virtually identical for the two Aroclors. This is perhaps not too surprising

given that both A1016 at 41.1% and A1242 at 43.7% (Frame et al. 1996) have similar degrees of chlorination. Aroclor 1016, a distillation product of A1242, was introduced in 1971 by Monsanto as a more biodegradable dielectric fluid for use in capacitors (DeVoogt and Brinkman 1989). Ho et al. (1997) exposed *Ampelisca abdita* and *Mysidopsis bahia* to A1242 and A1254 under static renewal conditions. Based on measured water concentrations, 96 hour LC50 values indicated A1242 was 3-4 times more toxic than A1254 to both species. On the other hand, McLeese and Metcalfe (1980) reported that 96 hour LC50 values for A1242 and A1254, based on measured exposure concentrations, were virtually identical for *Crangon septemspinosa* exposed under static renewal conditions. Nebeker and Puglisi (1974) reported that, under static conditions, 96 hour LC50 results (measured concentrations) indicated A1242 was twice as toxic as A1248 to juvenile *Gammarus pseudolimnaeus*. These results with four crustacean species suggest A1242 is more acutely toxic, or equally toxic, to A1254 and A1248. The differences among the investigations may be due, in part, to interspecific sensitivities.

We could find only one published report (Nebeker and Puglisi,1974) that evaluated the relative chronic toxicity of a wide range of Aroclors (i.e., A1221, A1232, A1242, A1248, A1254, A1260, A1262 and A1268) in a consistent manner. They initiated static exposures to the eight Aroclors with <24 hour old neonates of *Daphnia magna*. Exposures continued for 21 days. The most toxic mixture was A1248 with a 21-day LC50 (95% CI) of 25 µg/L (21.4-29.2 µg/L) (Figure 4). Overlapping 95% CI suggested A1254 and A1260 are as toxic as A1248. The LC50 values and corresponding 95% CI for A1254 and A1260 are 31 µg/L (25.8-37.2 µg/L) and 36 µg/L (27.7-46.8 µg/L), respectively. Aroclors with more or less chlorination were less toxic to *Daphnia magna* than these three mixtures (Figure 4) mirroring published compilations discussed earlier. Aroclor 1242 and A1232 were about half as toxic as A1248 with 21-day LC50 values (95% CI) of 67 µg/L (55.4-81 µg/L) and 72 µg/L (62.6-82.8 µg/L), respectively. The least and most heavily chlorinated PCB mixtures (A1221 and A1268) were also the least toxic among the eight Aroclors (Figure 4). The 21-day LC50 values (95% CI) for A1221 and A1268 were 180 µg/L (158-205 µg/L) and 253 µg/L (222-288 µg/L), respectively. Taken together, these comparative Aroclor toxicity investigations suggest the aqueous PCB dose-response curves in Figures 1 and 2, which are based largely on A1254, should not be used to extrapolate toxicity to the least and most heavily chlorinated PCB mixtures (i.e., A1221, A1232, A1262, A1268). Extrapolation to Aroclors of intermediate chlorination (e.g., A1242, A1248) may represent a more acceptable degree of uncertainty. To reduce these uncertainties, chronic toxicity tests should be conducted with appropriately sensitive species in a manner that allows one to determine the relative toxicity of Aroclor mixtures representing a range of chlorination.

Observations with Other Endpoints Including Low PCB Exposures

The dose-response curves developed in this investigation are based on the effects of PCBs on crustacean survival and reproduction. While crustaceans are often considered more sensitive to environmental contaminants than other invertebrate phyla, additional investigators have reported significant adverse effects of PCBs at very low concentrations on endpoints other than survival and reproduction. Schmidt et al. (2006) exposed 7-day old *Daphnia magna* for 21 days to 0, 0.1, 1.5,

12, and 15 µg/L Aroclor1254 (measured concentrations) in a flow-through system. PCBs had no effects on survival, growth, reproduction or enzymes essential to preventing or repairing cellular oxidative damage (glutathione peroxidase activity and glutathione S-transferase). However, swimming behavior (speed and position in the water column) was significantly affected in the 1.5 µg/L PCB treatment. Affected organisms would slowly swim upward in the exposure chamber and then sink to the deeper layers. During the last days of exposure, swimming speed and antennal movement diminished further. Under field conditions, the ecological consequences of this altered swimming behavior would be death. Swimming behavior was not significantly affected in the 0.1 µg/L treatment.

Lehmann et al. (2007) exposed adult freshwater clams (*Corbicula fluminea*) to 0, 1, 10 and 100 µg/L Aroclor 1260 for 21 days under static renewal conditions (twice weekly). These were nominal concentrations so actual exposure concentrations were likely much lower. Although there was no effect of PCBs on clam survival, a number of biochemical and histological endpoints were significantly altered at all nominal PCB concentrations. Tissue necrosis, gonadal atrophy, cellular inflammation and pigmented macrophage aggregates increased in a dose-responsive manner in the PCB-exposed clams. Necrosis occurs when tissue damage caused by chemical exposure exceeds cellular repair capacity. The accumulation of macrophage aggregates amongst the necrotic gonadal tissues likely reflects oxidative damage to lipid membranes. Additional evidence for PCB-induced oxidative stress was the significant alterations of γ-tocopherol and total reduced glutathione (GSH) in all PCB-exposed clams.

Candia Carnevali et al. (2001) also reported adverse effects PCBs on histology and invertebrate cellular development but at much lower aqueous concentrations. They monitored arm regeneration in the marine crinoid (*Antedon mediterranea*) exposed to Aroclor 1260 for 14 days under static conditions. From the dosing description provided, the nominal exposure concentration appeared to be 624 ng/L. The initial measured concentration was 77 ng/L or about an order of magnitude lower than the target nominal concentration. Measured exposure concentrations declined with time to 4 ng/L with a mean of 14 ng/L over the 14 day exposure. PCB exposure resulted in abnormal arm growth both in terms of gross morphology and microscopic anatomy. Observations included massive cell migration/proliferation, hypertrophic development of coelomic canals, rearrangement of differentiated tissues, and accelerated growth of regenerating tissue. The investigators concluded that the developmental anomalies they observed were compatible with a pattern of endocrine disruption.

In experiments reported by Ryan et al. (2001), fertilized eggs of a marine clam (*Mercenaria mercenaria*) were exposed for 48 hours to 0, 3.05E-11, 3.05E-10, 3.05E-9, 3.05E-8, 3.05E-7 M Aroclor 1254. Assuming A1254 has a molecular weight of 327 (Mackay et al. 2006), these nominal molar concentrations would be approximately 0, 0.01, 0.1, 1.0, 10 and 100 µg/L on a mass concentration basis. Actual exposure concentrations were probably far lower than these nominal values and likely declined during the static 48 hour test. At the end of the exposure period, the proportion of abnormal larvae exhibited a very clear dose-response pattern ranging from 21.7%

abnormal larvae in the lowest PCB treatment to 43.6% in the highest. The proportion of abnormal clam larvae in all PCB treatments were significantly greater than controls (<10% abnormal larvae). We can conclude from the above four experiments involving test species from three distinct invertebrate phyla (Mollusks, Echinoderms, Arthropods) that very low concentrations of aqueous solutions of PCBs (A1254 and A1260) can have very profound and biologically significant adverse effects on endpoints other than survival and reproduction. The benthic injury model we developed based on crustacean survival and reproduction was not able to capture these other endpoints and species.

Development of PCB-Resistant Populations

Organisms exposed to non-lethal concentrations of environmental contaminants may acquire genetic and/or non-genetic resistance that may enhance their net survival potential (Meyer and DiGiulio 2003). Evolution of chemical resistance by aquatic organisms can occur rapidly (years or a few generations) rather than hundreds or thousands of years (Klerks and Levinton 1989). For example, Xie and Klerks (2003) developed a cadmium-resistant laboratory population of the least killifish (*Heterandria formosa*) over just six generations. Ward and Robinson (2005) induced increased resistance to cadmium in a laboratory population of *Daphnia magna* after just eight generations.

The PCB chronic toxicity experiments summarized in Table 1 were all published in the 1970s, approximately 40 years ago. During that time period, it was not uncommon to discover elevated PCB concentrations in the food fed to laboratory test species. Most investigators at that time, however, did not analyze food materials for contaminants. Moreover, this was also prior to the advent of high resolution gas chromatography (GC) with glass capillary columns that enabled quantification of lower PCB concentrations. Therefore, food and tissue samples containing low PCB concentrations may have been reported as below detection limits even if analyzed. In these older papers, a contaminated food source was often manifested by the bioaccumulation of PCBs in the tissues of control animals. Bengtsson (1979) reported PCBs in control minnows (*Phoxinum phoxinus*) at twice the level normally observed in field- collected fish. The investigators attributed this observation to the level of PCBs (0.88 µg/g dry weight or dw) in their dried fish food (*Tubifex*). Nebeker et al. (1974) reported elevated PCBs in fish food ranging between 0.8-1.5 µg/g and 0.3-0.5 µg/g for Aroclors 1254 and 1248, respectively. PCB concentrations in their control fathead minnows (*Pimephales promelas*) were correspondingly high, routinely exceeding 1 µg/g at the end of 9-month life cycle exposure experiments. Mac and Seelye (1981) exposed lake trout fry (*Salvelinus namaycush*) to Aroclor 1254 for 52 days to evaluate the effects on survival and growth. During the experiment, they observed PCBs in control fish increased from 0.4 µg/g dw initially to 1.6 µg/g dw by the end of the test. They attributed this increase to low levels of PCBs in water (<10 µg/L) and food (0.06 µg/g wet weight, or ww). Nebeker and Puglisi (1974), who evaluated the chronic effects of PCBs on freshwater invertebrates, observed high levels of PCB contamination in the invertebrate food source. During 56 day exposures, they reported elevated PCBs in control

amphipods (*Gammarus pseudolimnaeus*) ranging between 4.0-7.0 µg/g and 6.0-8.0 µg/g for Aroclors 1254 and 1248, respectively (Nebeker and Puglisi 1974). They did not report PCB residues in other invertebrate test species.

Field populations of aquatic organisms inhabiting PCB-contaminated environments have demonstrated an ability to acquire resistance to PCBs' toxic effects (Nacci et al. 2009, Wirgin et al. 2011). In one instance, the increased resistance was the result of rapid evolution at the AHR locus (Wirgin et al. 2011). Those investigators speculated that non-AHR-dependent modalities for acquiring PCB resistance were also likely. The two field investigations cited above dealt with the acquisition of PCB resistance in fish. We could find no analogous reports documenting PCB resistance in aquatic invertebrates. However, a number of studies have demonstrated acquired resistance in field populations of aquatic crustaceans chronically exposed to organochlorine pesticides (Naqvi and Ferguson 1970, Albaugh 1972, Olima et al. 1997, Brausch and Smith 2009). Experiments reported by Nebeker and Puglisi (1974) represent 30 of the 58 (52%) paired observations in the aqueous dose-response curve (Tables 4 and 6, Figures 1 and 2). Elevated PCB concentrations in their food source and in controls leads us to speculate that one or more of these test species may have evolved some level of PCB resistance prior to experimental PCB exposures. To the extent this speculation is true, the benthic injury curves developed from these studies may under-predict benthic injury in native invertebrate populations.

Kow Values for Aroclor Mixtures

Linkov et al. (2005) examined the uncertainty associated with Kow values for PCBs and the impact of this variation on calculating sediment concentrations which are protective of human health and the environment. He reported that log Kow values available from or recommended by the USEPA ranged between 3.90 and 8.23 for total PCBs and between 3.34 and 6.98 for A1254. This large orders-of-magnitude variation translated into a 5-fold range of protective PCB sediment concentrations in one case study. The monetary implication for sediment cleanup caused by this variation in Kow values was not insignificant ($48 million). Detailed analysis by Linkov et al. (2005) led them to conclude that the largest (but not the only) source of variation in Kow values was measurement error. Specifically, they report that the most common way to measure octanol-water partitioning in the 1970s and 1980s, the shake-flask method, could produce microemulsions of octanol in the water phase leading to low-biased Kow values. The alternative slow-stir method for the experimental determination of Kow for highly hydrophobic chemicals such as PCBs may generate data that are more precise and accurate (Tolls et al. 2003). As previously mentioned, a site-specific Koc measurement using site pore water and sediment could reduce uncertainty associated with these values.

Kow Values for PCB Homologs

In this report, we initially used Kow values derived directly from Aroclors because the aqueous toxicity data was based on Aroclors. Fuchsman et al. (2006) took an alternative homolog approach for calculating Aroclor-specific Kows. In their approach, they selected: 1) the percent composition of homologs for each Aroclor mixture and 2) a Kow value for each homolog group.

Using these values, they calculated an Aroclor-specific Kow as the fractional sum of the homolog Kow values as shown in equation (8)

$$K_{ow\text{-Total PCB}} = 1/\sum (f_{homolog\ i} / K_{ow\text{-homolog i}}) \quad (8)$$

where $f_{\text{homolog } i}$ is the proportion of homolog group *i* in a particular Aroclor mixture, $K_{ow\text{-homolog } i}$ is the K_{ow} for homolog group *i* and $\sum$ is the sum of decimal fractional quotients for all homolog groups in the Aroclor mixture. For the first component (percent composition of homologs), Fuchsman et al. (2006) selected values reported by DeVoogt and Brinkman (1989) for a variety of Aroclors. These values are generally consistent with five other sources we identified with respect to identifying the dominant homolog group in each Aroclor mixture (Table 11). For example, all published sources indicate pentachlorobiphenyl is the dominant homolog group in Aroclor 1254 (Table 11). However, the range of percent pentachlorobiphenyl in Table 11 among the various sources is not small (45%-71%). Slight differences in the chlorination process (ATSDR 2000, Eisler and Belisle 1996, DeVoogt and Brinkman 1989) as well as manufacturing source (e.g., see A1254, Source E in Table 11) can also contribute to the variation in percent homolog composition observed in the various Aroclor mixtures. The lightly chlorinated mixtures (Aroclors 1221 and 1232) are dominated by monochloro-, dichloro- and trichlorobiphenyls (Table 11). At the other extreme, heavily chlorinated mixtures (Aroclors 1260 and 1262) are dominated by hexachloro-, hepta- and octachlorobiphenyls. Mixtures with intermediate chlorination (Aroclors 1242, 1248 and 1254) are dominated by trichloro-, tetrachloro- and pentachlorobiphenyls (Table 11). As noted above, the literature search indicated these Aroclors with intermediate chlorination were often the most toxic mixtures to invertebrates.

For the second component in the homolog approach, Fuchsman et al. (2006) selected Kow values for each homolog group from those published by Mackay et al. (1992) and Shiu and Mackay (1986). Table 12 is a summary of Kow values for the nine homolog groups (n=3-7 per group) reported in the more recent publication by Mackay et al. (2006). Variation in Kow values among the mono- through heptachlorobiphenyl homolog groups is much smaller (≈an order of magnitude; %CV<100%) compared to the variation in Aroclor Kow values (Table 5). The mean and median Kow values within these seven homolog groups are generally similar suggesting normally distributed Kow values. In addition, the median Kow values for the mono- through heptachlorobiphenyl homolog groups from Mackay et al. (2006) are similar to values used by Fuchsman et al. (2006) (Table 12). However, variations in Kow values for the octa- and nonachlorobiphenyl homolog groups from Mackay et al. (2006) are much larger (%CV>100%) than the other homolog groups. The Kow values for these two homologs used by Fuchsman et. al. (2006) is larger than the median values from Mackay et al. (2006). The increased variation in these two homolog groups may be due to experimental error in determining Kow values for highly hydrophobic chemicals, as discussed in Linkov et al. (2005). From a practical standpoint, Kow results for the octa- and nonachlorobiphenyl homolog group have minimal impact because these two groups appear only in highly chlorinated Aroclors (i.e., ≥A1260) (Table 11).

Kow values calculated for Aroclor mixtures using the homolog approach are generally greater (except A1248) than the median Kow values from Mackay et al. (2006) (Table 5). EqP modeling with higher Kow values yields higher oc-normalized sediment concentrations, which are less protective of the biological resource for a given aqueous PCB concentration. The homolog approach may be desirable if PCB sediment concentrations are expressed only as homolog or congeners. However, the selection of homolog percent composition and homolog Kow values may introduce additional uncertainty. Given the substantial influence that Kow selection has on modeling PCB sediment concentrations (see discussion of Linkov et al. 2005), perhaps a better approach would be to focus on the quality of the Kow information when a specific value is selected for use in EqP modeling.

While this investigation and that of Fuchsman et al. (2006), used aqueous PCB toxicity information gathered from the literature and EqP modeling to predict adverse effects of PCB- contaminated sediments, important differences exist between the two studies other than the approach to select Aroclor-specific Kow values discussed above. Fuchsman et al. (2006) used acute toxicity information exclusively for A1254, then applied an acute:chronic ratio to produce a Final Chronic Value (FCV). The acute toxicity information was almost exclusively 96h LC50 values, whereas this investigation used toxicity data from chronic exposures. Different modes of toxicity are likely operating in the two datasets (narcosis vs non-dioxin-like toxicity). Many of their acute studies did not measure actual exposure concentrations, and the reported nominal concentrations often exceeded the aqueous solubility of PCBs. In contrast, this investigation used only chronic toxicity data in which aqueous exposure concentrations were measured. Secondly, this investigation also considered sublethal biological responses in the dose-response curves (i.e., reproduction), as well as other studies that documented sublethal effects at very low aqueous PCB concentrations. Thirdly, Fuchsman et al. (2006) used the Kow as the Koc value as shown in Bucheli and Gustafsson (2001), claiming that such equality is a conservative estimate of Koc, but the Kow-Koc transformation equations shown earlier indicate otherwise. Perhaps the most significant difference between this investigation and Fuchsman et al. (2006) is that the latter study reports a single sediment quality benchmark for PCBs, while we developed a numerical dose-response model generating a continuum of predictions.

Koc Values Using Congeners

If congener data are available, one can directly determine the Koc without using either the median Kow value (Table 5) or a log Kow to log Koc transformation (e.g., Equations 5, 6 or 7) by using the calibrated QSAR model:

$$\log (Koc) = 0.53(N_{cl} - N_{orthoCl}) + 4.98 \quad (9)$$

where N_{CL} is the total number of chlorines and $N_{orthoCL}$ is the number of ortho-chlorines (Hawthorne et al., 2011; Arp, et al., 2009). In this case, much like after finding a site-specific Koc, one can calculate the oc-normalized chronic sediment concentration from the sample-specific pore water value by using Equation 4. See Appendix A for an example.

The issue of how the aqueous sample was measured, including colloidal material (unfiltered) or just the freely dissolved (filtered) concentration, must be taken into account. The equation above uses the latter. Note that the log (Koc) is nearly a value of 5 before one even starts to calculate total and ortho-chlorines. Hence, this equation cannot be used with our data set that uses total (particulate and dissolved) PCBs.

PCB Analysis and Weathering

As noted in the Introduction, PCBs are complex mixtures of up to 209 theoretically possible congeners that can be grouped into ten homolog groups of similar molecular weight but different spatial configurations. Commercial Aroclor mixtures of PCBs with very different homolog proportions were manufactured to meet different industrial needs. Once released into the environment, PCB mixtures are subject to environmental degradation ("weathering"). Weathering may produce an analytical signature that can be quite different from the original manufactured product. This can be especially problematic when field samples are also contaminated with more than one commercial Aroclor mixture. For these reasons, the chemical analysis of PCBs can be complex and confounding. PCB exposure concentrations reported in the aqueous toxicity literature were from commercial PCB sources.

The USEPA standard method 8082A for the analysis of PCBs uses gas chromatography (GC) with glass capillary columns for high resolution separation and electron capture detectors (USEPA 2007). This method indicates it is appropriate for identifying seven Aroclor mixtures (A1016, A1221, A1232, A1242, A1248, A1254, A1260) and 19 individual congeners (IUPAC #1, 5, 18, 31, 44, 52, 66, 87, 101, 110, 138, 141, 151, 153, 170, 180, 183, 187, 206). The analyst compares the sample chromatogram to the Aroclor standard and chooses which Aroclor (or Aroclors) is most similar to residue in the sample. To assist the analyst, Method 8082A provides tables listing congeners and chromatographic peaks that are present (or absent) in the seven Aroclor mixtures. This analysis can be very challenging for highly weathered samples and/or those samples containing multiple Aroclor mixtures. Method 8082A states that analyzing a more complete suite of congeners for weathered samples may be beneficial. Results can then be reported as the concentration for each congener and/or the sum of all congener concentrations expressed as a total PCB value.

Recommended Applications

The above discussion highlights important uncertainties that could affect predictions of benthic injury due to PCB-contaminated sediments when one uses the EqP modeling approach described in this report. Some of these uncertainties may be more (or less) important than others depending on the site-specific data and their intended use. These uncertainties also diminish the veracity of the frequently cited causal nature advantage of sediment quality benchmarks based on EqP (Fuchsman et al. 2006, DiToro and McGrath 2000, USEPA 2008). As discussed in Burgess et al. (2013), the EqP approach does not consider effects of co-occurring contaminants, nor the potential for trophic transfer. Benthic communities contain multiple trophic levels (Commito and Ambrose 1985), which may not be protected by an EqP approach. On a case-specific basis, one must employ

technically sound best professional judgment to assess the relative importance of each of these uncertainties. At the present time, it is our judgment that the most frequently encountered and quantitatively most important uncertainties are likely to be: a) those associated with the comparative toxicity of different Aroclor mixtures to invertebrates, b) the acquired resistance to PCBs in laboratory animals used in 1970s toxicity studies and c) the variation in, and methods used to calculate, Aroclor Kow and/or Koc values. We believe the latter is the most important uncertainty and address this throughout the paper.

We present the following steps as general guidance for recommended application of the benthic injury curves when applied to field data that potentially report sediment PCB concentrations in different ways. These steps include reporting of PCBs by A) multiple Aroclors; B) single Aroclor; C) PCB congeners; D) PCB homologs; and E) total PCBs.

A. Step-wise approach for predicting % benthic injury when multiple or individual Aroclors (A1242, A1248, A1254) are detected in sediment

1) If one or more Aroclors A1242, A1248, and/or A1254 are detected in sediment, calculate an oc-normalized concentration for each detected result in a sample. Ignore results that are flagged as less than the detection limit. While this approach is less protective than other alternatives (e.g., assuming ½ DL), it avoids the other potentially more serious bias that could result from reporting high detection limits.

2) Sum the detected oc-normalized concentrations of the Aroclors from Step 1 to obtain a "Total Aroclors" oc-normalized expression for each sediment sample.

3) Find the "Total Aroclors" oc-normalized concentration calculated in Step 2 in the sediment look-up table for A1254 (Table 9). Use the mean value corresponding to the "Total Aroclors" concentration for the prediction % benthic injury. Some may prefer to use the Upper 95% CI value based on uncertainties discussed above and the demonstrated effects of PCBs at very low concentrations on biologically important endpoints other than survival and reproduction, e.g., behavior, early life stage growth and development in three invertebrate phyla (see Discussion). Using the look up table for A1254 is recommended because A1254 constitutes most (≈70%) data in the aqueous dose-response curve (Figure 2). To the extent a sediment sample is dominated by A1242 results, benthic injury estimates will likely be biased upward.

Three Aroclors for the "Total Aroclors" oc-normalized expression (A1254, A1248, A1242) are included in this approach because they form the toxicological basis for the aqueous and sediment dose-response curves (Figures 1-3). A1260 also may be included in the group because it was as toxic as A1254 and 1248 in a chronic life cycle experiment with an aquatic crustacean (Nebeker and Puglisi 1974). Likewise, similar to A1254, it has a very profound and biologically significant adverse effects on three distinct invertebrate phyla (Mollusks, Echinoderms, Arthropods) at very low aqueous concentrations (Schmidt et al. 2006; Lehmann et al. 2007; Candia Carnevali et al.

2001; Ryan et al. 2001). Predicting benthic injury from other Aroclors is not recommended at this time because sufficient and appropriate dose-response and comparative toxicity information are not available.

The approach above requires sample-specific organic carbon data to normalize sediment PCB concentrations. In the absence of sample-specific data, one could use other site-specific sources of sediment organic carbon and perhaps calculate area-wide averages. In lieu of site-specific sediment carbon data, one could use the default value of 1%, which is used by the USEPA (2004) in their National Sediment Quality Survey when organic carbon is not reported. In either case, one must realize that the absence of sample-specific organic carbon data represents a potentially large source of uncertainty that may bias the benthic injury predictions. For example, if the organic carbon value is 10% rather than the 1% default, the estimated injury is reduced by a factor of 10.

The step-wise approach above is not recommended if an Aroclor other than A1242, A1248 or A1254 is the only PCB mixture detected in a sample.

B. Step-wise approach for predicting % benthic injury when sediment concentrations are reported as PCB congeners

1a) If sediment analytical results are reported only as the concentration of individual PCB congeners, the analytical lab should be queried to see if results were also expressed (but not reported) as Aroclors. If they did quantify on the basis of Aroclors, proceed with the Aroclor approaches described above.

1b) If the lab did not express analytical results as Aroclors or if it is not possible to query the laboratory (e.g., because dataset is old and unavailable), then group the congeners by homologs, sum the concentrations within each homolog group and calculate the relative proportion that each homolog group represents. Then proceed to the homolog group approach (C) described below.

Or 2) If congeners are available, then calculate the Koc using

$$\log (Koc) = 0.53(N_{cl} - N_{orthoCl}) + 4.98 \quad (9)$$

where N_{CL} is the total number of chlorines and $N_{orthoCL}$ is the number of ortho-chlorines (Hawthorne et al. 2011; c.f., Arp et al. 2009). In this case, much like after finding a site-specific Koc, one can calculate the oc-normalized chronic sediment concentration from the sample-specific pore water value using Equation 4. Then use this aquatic number and Table 7 and 8 to determine the percentage of benthic injury with the assumption that the sediment is primarily composed of Aroclor 1242, 1248 and 1254 (also see Figures 2 and 4). Later, create Table 9 as previously discussed. For an example of this method see Appendix A. Note, however, that Equation 9 limits the Koc to no lower than 4.98. Hence, we note that this equation assumes a dissolved water column measurement.

C. Step-wise approach for predicting % benthic injury when sediment concentrations are reported as PCB homolog groups

1) If analytical results are reported only as the concentration of homolog groups, the analytical lab should be queried to see if results were also expressed (but not reported) as Aroclors. If they did quantify on the basis of Aroclors, proceed with one of the Aroclor approaches described above. Like above, if you know the homolog groups and the concentration of each homolog then you will know the chlorination (and concentration) and can estimate the Aroclor.

2) If the lab did not express analytical results as Aroclors or if it is not possible to query the laboratory (e.g., because dataset is old and unavailable), then group the congeners by homolog, sum the concentrations within each homolog group and calculate the relative proportion each homolog group represents.

3) Compare the pattern of relative homolog proportions to results in Table 11 of this report to see which Aroclors the sample most closely resembles. At this point, collaboration with chemists experienced with PCB analysis using USEPA Method 8082A may be valuable. It also may be instructive to conduct a source characterization. For example, it may be very helpful to know which Aroclors have been released (or not released) into the area under investigation.

4) Once the Aroclors are identified, proceed with one of the Aroclor approaches described above. For reasons discussed earlier, the homolog Kow approach used by Fuchsman et al. (2006) is not recommended.

D. Step-wise approach for predicting % benthic injury when sediment concentrations are reported as total PCBs

1) If analytical results are reported only as total PCBs, the analytical lab should be queried to see if results were also expressed (but not reported) as individual Aroclors. If they did quantify on the basis of individual Aroclors, proceed with one of the Aroclor approaches described above.

2) In the event that the lab did not express analytical results as Aroclors or if it is not possible to query the laboratory (e.g., because dataset is old and unavailable), one must determine on a case-by-case basis what the total PCBs expression is believed to represent. Again, source characterization as described above may prove valuable. Additionally, it may be useful to examine (if available) other site-specific sediment PCB data. In USEPA Method 8082A, “total PCBs” is used to refer to both the sum of congener concentrations and the sum of Aroclor concentrations.

Summary and Outstanding Issues

This investigation reviewed the aqueous PCB toxicity literature and used EqP modeling to generate Aroclor-specific sediment dose-response curves (and associated lookup tables) for estimating benthic injury in PCB-contaminated sediments. We used a Kow-to-Koc transformation equation supported by the USEPA that is based on undissolved aqueous PCB concentrations. This approach matches the literature sources used to determine PCB toxicity to invertebrates. As a result, we believe that Tables 10 and 11 are well-founded tools to determine likely sediment toxicity. While this approach remains worthwhile, a number of outstanding issues remain, as listed below. Addressing these issues in a technically sound and sufficient manner will reduce the uncertainties associated with the recommended approach for predicting benthic injury resulting from exposure to PCB-contaminated sediments.

- Examine more closely the cause of large variations in reported Aroclor Kow and Koc values with the goal of reducing that source variation and selecting the most accurate Kow and/or Koc value(s).

- Apply and validate the recommended approach to sediment datasets from PCB-contaminated sites. This exercise would likely highlight the strengths and limitations of the recommended approach.

- Experimentally determine the comparative toxicity of individual Aroclors, mixtures of Aroclors, and weathered Aroclors representing a range of chlorination/hydrophobicity, to appropriately sensitive invertebrates.

- Evaluate the available congener-specific toxicity data for invertebrates with the goal of identifying those congeners that most likely cause toxicity through the non-dioxin-like mode of action.

- Recent studies (Lohmann et al, 2005, Werner, et al, 2010) have used the two-carbon model to ensure that thermo-resistant black carbon is properly taken into account when calculating the sediment-water partitioning constant, K_D. Despite the possibility of the one-carbon model (Equation 4) underpredicting Koc, both Hawthorne et al (2011) and Martinez et al. (2013) found no improvement when using the two-carbon model to predict the sediment pore water. Hence, we have not included the additional black carbon measure in our model.

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TABLES AND FIGURES

Table 1. Summary of individual non-acute experiments in the literature reporting measured aqueous PCB dose-response information for invertebrates.

Test Species[a]	Lifestage, Length (cm)	Aroclor	Exposure Scenario[b]	Measured Exposure Concentrations(µg/L)	Biological Test Endpoints	Reference
Pink shrimp	juvenile, 2.5-3.8	1254	15 days; FT	0.0 - 19.0	Survival	Nimmo et al. (1971)
Pink shrimp	juvenile, 4.2-7.2	1254	17-32 days; FT	0.0 - 3.1	Survival	Nimmo et al. (1971)
Pink shrimp	6.6-9.0	1254	53 days; FT	0.0 - 4.3	Survival	Nimmo et al. (1971)
Pink shrimp	7.6-8.5	1254	18 days; FT	0.0 - 4.0	Survival	Nimmo et al. (1971)
Pink shrimp	adult, 9.5-12.5	1254	35 days; FT	0.0 - 3.5	Survival	Nimmo et al. (1971)
Pink shrimp	juvenile, 4-6	1254	20 days; FT	0.0 - 3.8	Survival	Duke et al. (1970)
Grass shrimp	NR[c]	1254	7 days; FT	0.0 - 9.1	Survival	Nimmo et al. (1974)
Grass shrimp	NR[c]	1254	16 days; FT	0.0 - 12.5	Survival	Nimmo et al. (1974)
Grass shrimp	larvae	1254	23-26 days; SR	0.0 - 15.6	Survival	Roesijadi et al. (1976)
Eastern oyster	young, 2.6-5.7	1254	210 days; FT	0.0 - 0.64	Survival, Growth	Lowe et al. (1972)
Eastern oyster	young, 3.1-8.3	1254	168 days; FT	0.0 - 3.9	Survival, Growth	Lowe et al. (1972)
Water flea	<24 h neonates	1248	14 day; FT	0.0 - 7.5	Survival, Reproduction	Nebeker & Puglisi (1974)
Water flea	<24 h neonates	1254	14 day; FT	0.0 - 9.0	Survival, Reproduction	Nebeker & Puglisi (1974)
Water flea	<24 h neonates	1254	21 day; FT	0.0 - 33	Survival, Reproduction	Nebeker & Puglisi (1974)
Amphipods	juvenile	1242	56 day; FT	0.0 - 234	Survival, Reproduction	Nebeker & Puglisi (1974)
Amphipods	juvenile	1248	56 day; FT	0.0 - 18.0	Survival, Reproduction, Growth	Nebeker & Puglisi (1974)
Midge	1st to 4th instars	1254	NR: FT	0.0 - 33	Number of larval and pupal cases	Nebeker & Puglisi (1974)

[a] pink shrimp - *Penaeus duorarum*, grass shrimp - *Palaemonetes pugio*, Eastern oyster - *Crassostrea virginica*, water flea - *Daphnia magna*, amphipod - *Gammarus pseudolimnaeus*, midge - *Tanytarsus dissimilis*

[b] FT - flow through, SR - static renewal

[c] NR - not reported

Table 2. Individual and median aqueous solubilities (mg/L or g/m3) for seven Aroclor mixtures reported by Mackay et al. (2006).

Aroclor	**1221**	**1232**	**1016**	**1242**	**1248**	**1254**	**1260**
	0.59	1.45	0.049	0.045	0.043	0.0001	0.0027
	3.5	1.45	0.085	0.085	0.052	0.01	0.003
	3.5	407	0.22	0.085	0.054	0.01	0.0144
	3.52		0.25	0.097	0.054	0.0115	0.025
	5		0.332	0.1	0.056	0.012	0.025
	15		0.34	0.1	0.06	0.012	0.08
	15		0.4	0.1329	0.1	0.0242	
	40		0.42	0.2	0.1	0.031	
			0.49	0.2	0.32	0.035	
			0.84	0.23		0.04	
			0.906	0.23		0.042	
			0.906	0.24		0.043	
			0.906	0.25		0.043	
			0.91	0.277		0.045	
				0.3		0.045	
				0.34		0.05	
				0.34		0.056	
				0.34		0.057	
				0.703		0.06	
				0.703		0.07	
				0.703		0.07	
				0.703		0.07	
				0.75		0.07	
						0.07	
						0.14	
						0.3	
Median	**4.26**	**1.45**	**0.41**	**0.24**	**0.056**	**0.044**	**0.022**
n	8	3	14	23	9	26	6

Table 3. Calculation of % Control-Normalized Response (% CNR) and % injury for each PCB treatment in 14 of the 17 experiments identified in Table 1 which report the chronic effects of PCBs on crustacean survival.

Reference	**A1254 Exposure[a]**	**15 day**	**% CNR[b]**	**% Injury[c]**
Nimmo et al. (1971)		**% Survival**	**% Survival**	**Survival**
	Juvenile *Penaeus duorarum*, rostrum-telson length 2.5-3.8 cm			
	0.00	88	100	0
	0.57	70	80	20
	0.94	49	56	44
	9.40	10	11	89
	19.00	0	0	100

Reference	**A1254 Exposure[a]**	**17-32 day**	**% CNR[b]**	**% Injury[c]**
Nimmo et al. (1971)		**% Survival**	**% Survival**	**Survival**
	Juvenile *Penaeus duorarum*, rostrum-telson length 4.2-7.2 cm			
	0.00	96	100	0
	2.40	35	36	64
	3.10	20	21	79

Reference	**A1254 Exposure[a]**	**53 day**	**% CNR[b]**	**% Injury[c]**
Nimmo et al. (1971)		**% Survival**	**% Survival**	**Survival**
	Penaeus duorarum, rostrum-telson length 6.6-9.0 cm			
	0.00	74	100	0
	4.30	17	23	77

Reference	**A1254 Exposure[a]**	**18 day**	**% CNR[b]**	**% Injury[c]**
Nimmo et al. (1971)		**% Survival**	**% Survival**	**Survival**
	Penaeus duorarum, rostrum-telson length 7.6-8.5 cm			
	0.00	91	100	0
	4.00	59	65	35

Reference	**A1254 Exposure[a]**	**35 day**	**% CNR[b]**	**% Injury[c]**
Nimmo et al. (1971)		**% Survival**	**% Survival**	**Survival**
	Adult *Penaeus duorarum*, rostrum-telson length 9.5-12.5 cm			
	0.00	92	100	0
	3.50	50	54	46

Reference	**A1254 Exposure[a]**	**20 day**	**% CNR[b]**	**% Injury[c]**
Duke et al. (1970)		**% Survival**	**% Survival**	**Survival**
	Penaeus duorarum, rostrum-telson length 4-6 cm			
	0.00	100	100	0
	3.80	28	28	72

Reference Nimmo et al. (1974)	**A1254 Exposure[a]**	**7 day % Survival**	**% CNR[b] % Survival**	**% Injury[c] Survival**
	Palemonetes pugio			
	0.00	96	100	0
	0.17	92	96	4
	0.62	96	100	0
	9.10	40	42	58

Reference Nimmo et al. (1974)	**A1254 Exposure[a]**	**16 day % Survival**	**% CNR[b] % Survival**	**% Injury[c] Survival**
	Palemonetes pugio			
	0.00	75	100	0
	1.30	60	80	20
	4.00	55	73	27
	12.50	45	60	40

Reference Roesijadi et al. (1976)	**A1254 Exposure[a]**	**23-26 day % Survival**	**% CNR[b] % Survival**	**% Injury[c] Survival**
	Palemonetes pugio, larvae			
	0.00	93	100	0
	0.05[e]	100	108	0[d]
	3.20	90	97	3
	15.60	0	0	100

Reference Nebeker and Puglisi (1974)	**A1248 Exposure[a]**	**14 day % Survival**	**% CNR[b] % Survival**	**% Injury[c] Survival**
	Daphnia magna, initiated with <24h old neonates			
	0.00	60	100	0
	0.10	74	123	0[d]
	0.26	87	145	0[d]
	0.86	92	153	0[d]
	2.50	65	108	0[d]
	7.50	5	8	92

Reference Nebeker and Puglisi (1974)	**A1254 Exposure[a]**	**14 day % Survival**	**% CNR[b] % Survival**	**% Injury[c] Survival**
	Daphnia magna, initiated with <24h old neonates			
	0.00	53	100	0
	0.37	80	151	0[d]
	0.92	93	175	0[d]
	1.70	60	113	0[d]
	3.80	0	0	100
	9.00	0	0	100

Reference Nebeker and Puglisi (1974)	**A1254 Exposure**[a]	**21 day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**
	Daphnia magna, initiated with <24h old neonates			
	0.00	80	100	0
	0.45	69	86	14
	1.20	70	88	13
	3.50	0	0	100
	9.00	0	0	100
	33.00	0	0	100

Reference Nebeker and Puglisi (1974)	**A1242 Exposure**[a]	**56 day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**
	Gammarus pseudolimnaeus, initiated with juvenile scuds			
	0.00	48	100	0
	2.80	77	160	0[d]
	8.70	52	108	0[d]
	26.00	0	0	100
	81.00	0	0	100
	234.00	0	0	100

Reference Nebeker and Puglisi (1974)	**A1248 Exposure**[a]	**56 day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**
	Gammarus pseudolimnaeus, initiated with juvenile scuds			
	0.00	64	100	0
	0.18	73	114	0[d]
	0.54	71	111	0[d]
	2.20	73	114	0[d]
	5.10	53	83	17
	18.00	0	0	100

[a] The first row of numbers in each experiment is the Control treatment. All PCB exposure concentrations are measured aqueous values expressed as µg/L. See Table 1 for additional experimental details.

[b] % CNR-Percent Control-Normalized Response. See Materials and Methods for explanation.

[c] See Materials and Methods for explanation of % injury.

[d] The response in some experimental treatments outperformed the control so injury in these treatments was set to 0%.

[e] value is one half the detection limit

Table 4. Paired observations (n=58) of measured aqueous PCB concentrations and % benthic injury (survival endpoint) from the experimental results in Table 3. The surrogate PCB concentration of 0.05 µg/L was used for control treatments (see Materials and Methods). Source Notes describe the experimental treatment for each paired observation. For additional experimental details see Table 1.

Log_{10} Measured Aqueous PCB Concentration (µg/L)	Measured Aqueous PCB Concentration (µg/L)	Benthic Injury (%)	Source Notes
-1.3010	0.05	0	A1254, Juvenile *P. duorarum*, 15 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	A1254, *P. duorarum*, 17-32 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	A1254, *P. duorarum*, 53 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	A1254, *P. duorarum*, 18 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	A1254, Adult *P. duorarum*, 35 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	A1254, *P. duorarum*, 20 day survival, controls, Duke et al. (1970)
-1.3010	0.05	0	A1254, *P. pugio*, 7 day survival, controls, Nimmo et al. (1974)
-1.3010	0.05	0	A1254, *P. pugio*, 16 day survival, controls, Nimmo et al. (1974)
-1.3010	0.05	0	A1248, *D. magna*, 14 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	A1254, *D. magna*, 14 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	A1254, *D. magna*, 21 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	A1242, *G. pseudolimnaeus*, 56 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	A1248, *G. pseudolimnaeus*, 56 day survival, controls, Nebeker & Puglisi (1974)
-1.0000	0.05	0	A1254, *P. pugio*, 23-26 day survival, controls, Roesijadi et al. (1976)
-1.0000	0.05	0	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
-1.0000	0.10	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.7696	0.17	4	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
-0.7447	0.18	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
-0.5850	0.26	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.4318	0.37	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.3468	0.45	14	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
-0.2676	0.54	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
-0.2441	0.57	20	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
-0.2076	0.62	0	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
-0.0655	0.86	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.0362	0.92	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.0269	0.94	40	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
0.0792	1.20	13	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)

Log_{10} Measured Aqueous PCB Concentration (µg/L)	Measured Aqueous PCB Concentration (µg/L)	Benthic Injury (%)	Source Notes
0.1139	1.30	20	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
0.2304	1.70	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.3424	2.20	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.3802	2.40	64	A1254, *P. duorarum*, 17-32 day survival, Nimmo et al. (1971)
0.3979	2.50	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.4472	2.80	0	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.4914	3.10	79	A1254, *P. duorarum*, 17-32 day survival, Nimmo et al. (1971)
0.5051	3.20	3	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
0.5441	3.50	46	A1254, Adult *P. duorarum*, 35 day survival, Nimmo et al. (1971)
0.5441	3.50	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.5798	3.80	72	A1254, *P. duorarum*, 20 day survival, Duke et al. (1970)
0.5798	3.80	100	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.6021	4.00	35	A1254, *P. duorarum*, 18 day survival, Nimmo et al. (1971)
0.6021	4.00	27	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
0.6335	4.30	77	A1254, *P. duorarum*, 53 day survival, Nimmo et al. (1971)
0.7076	5.10	17	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.8751	7.50	92	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.9395	8.70	0	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.9542	9.00	100	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.9542	9.00	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.9590	9.10	58	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
0.9731	9.40	89	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
1.0969	12.50	40	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
1.1931	15.60	100	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
1.2553	18.00	100	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
1.2788	19.00	100	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
1.4150	26.00	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
1.5185	33.00	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
1.9085	81.00	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
2.3692	234.00	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)

Table 5. Individual Log Kow values for seven Aroclor mixtures reported by Mackay et al. (2006). Descriptive statistics are based on the non-logarithm expressions of the Kow values. Aroclor Kow values reported by Fuchsman et al. (2006) (A1260, A1254, A1248, A1242) or calculated using the homolog approach described in Fuchsman et al. (2006) (A1016, A1232, A1221) are shown for comparison.

Aroclor Mixtures	**A1221**		**A1232**		**A1016**		**A1242**		**A1248**		**A1254**		**A1260**	
Kow Values	**Log Kow**	**Kow**	**Log Kow**	**Kow**	**Log Kow**	**Kow**	**Log Kow**	**Kow**	**Log Kow**	**Kow**	**Log Kow**	**Kow**	**Log Kow**	**Kow**
	2.78	603	3.18	1,514	3.48	3,020	0.70	5	5.60	398,107	4.08	12,023	4.34	21,878
	2.80	631	3.20	1,585	4.30	19,953	3.54	3,467	5.75	562,341	4.08	12,023	6.00	1,000,000
	2.81	646	3.23	1,698	4.38	23,988	4.00	10,000	5.80	630,957	6.00	1,000,000	6.11	1,288,250
	4.00	10,000	4.10	12,589	4.40	25,119	4.11	12,882	6.00	1,000,000	6.00	1,000,000	6.30	1,995,262
	4.08	12,023	4.48	30,200	5.31	204,174	4.50	31,623	6.10	1,258,925	6.03	1,071,519	6.61	4,073,803
	4.09	12,303	4.54	34,674	5.48	301,995	5.29	194,984	6.11	1,288,250	6.10	1,258,925	6.90	7,943,282
	4.09	12,303	4.54	34,674	5.58	380,189	5.58	380,189	6.11	1,288,250	6.11	1,288,250	6.91	8,128,305
	4.10	12,589	4.62	41,687	5.80	630,957	5.60	398,107	6.30	1,995,262	6.47	2,951,209	7.14	13,803,843
	4.70	50,119	5.20	158,489	5.88	758,578	5.74	549,541			6.50	3,162,278	7.15	14,125,375
							5.80	630,957			6.72	5,248,075	7.50	31,622,777
							5.90	794,328			6.79	6,165,950		
											6.80	6,309,573		
											7.17	14,791,084		
Mean Kow		12,357		35,234		260,886		273,280		1,052,762		3,405,454		8,400,277
Stdev.		15,184		48,947		282,851		291,871		519,822		4,067,023		9,642,659
% CV		123%		139%		108%		107%		49%		119%		115%
Count		9		9		9		11		8		13		10
Median Kow		12,023		30,200		204,174		194,984		1,129,463		1,288,250		6,008,543
Fuchsman et al. (2006)[a]	4.57	37,308	4.82	65,948	5.46	288,397	5.59	389,045	5.95	891,251	6.43	2,691,535	6.85	7,079,458

[a] Log Kow values for Aroclors A1242, A1248, 1254 and A1260 are those reported by Fuchsman et al. (2006) using the homolog approach (see text for explanation). Kow values for Aroclors A1221, A1232 and A1026 were calculated per the homolog approach described in Fuchsman et al. (2006) using the homolog Log Kow values they report and the homolog proportion by weight from the reference they cite (DeVoogt and Brinkman 1989). The homolog approach for A1221 and A1232 used the Log Kow for biphenyl (3.9) from Mackay et al. (2006).

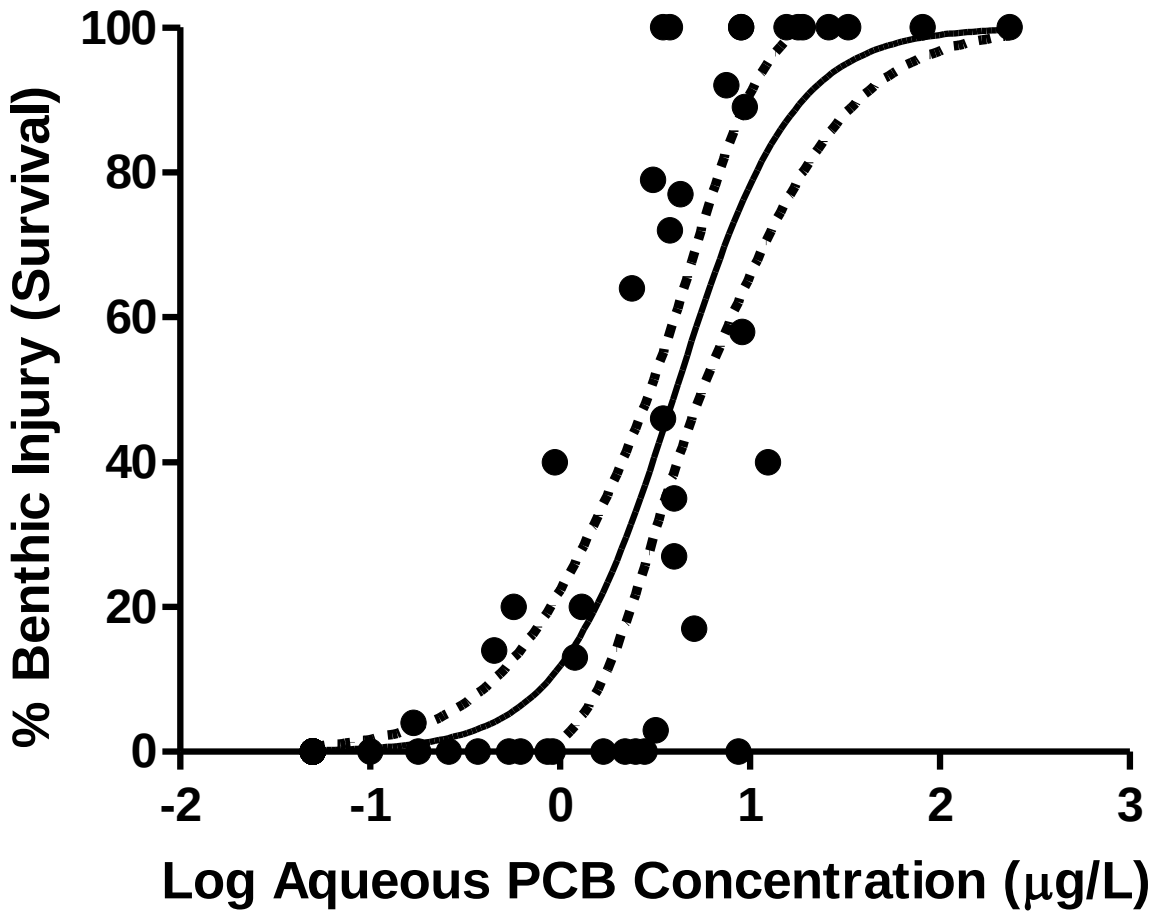

Figure 1. Benthic injury curve (survival) for measured aqueous concentrations of PCBs (A1254, A1248, A1242). Dashed lines are 95% CI around the mean (solid line). R-squared = 0.7 Hill slope = 1.43

Table 6. Calculation of the Chronic Survival:Reproductive (S:R) Effects Ratios (values in bold) for six experiments reported by Nebeker and Puglisi (1974). Mean (n=6) Chronic S:R Effects Ratio = 1.25.

Reference Nebeker and Puglisi (1974)	**A1248 Exposure**[a]	**14-day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**	**Young per Initial Adult**	**% CNR**[b] **YpIA**	**% Injury**[c] **YpIA**
	Daphnia magna , initiated with <24h old neonates						
	0.00	60	100	0	16	100	0
	0.10	74	123	0[d]	13	81	19
	0.26	87	145	0[d]	27	169	0[d]
	0.86	92	153	0[d]	24	150	0[d]
	2.50	65	108	0[d]	12	75	25
	7.50	5	8	92	0.7	4	96
		Total % Injury		92			139
					Chronic S:R Effects Ratio		**1.52**

Reference Nebeker and Puglisi (1974)	**A1254 Exposure**[a]	**14-day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**	**Young per Initial Adult**	**% CNR**[b] **YpIA**	**% Injury**[c] **YpIA**
	Daphnia magna , initiated with <24h old neonates						
	0.00	53	100	0	19	100	0
	0.37	80	151	0[d]	34	179	0[d]
	0.92	93	175	0[d]	18	95	5
	1.70	60	113	0[d]	12	63	37
	3.80	0	0	100	0	0	100
	9.00	0	0	100	0	0	100
		Total % Injury		200			242
					Chronic S:R Effects Ratio		**1.21**

Reference Nebeker and Puglisi (1974)	**A1254 Exposure**[a]	**21-day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**	**Young per Initial Adult**	**% CNR**[b] **YpIA**	**% Injury**[c] **YpIA**
	Daphnia magna , initiated with <24h old neonates						
	0.00	80	100	0	38	100	0
	0.45	69	86	14	52	137	0[d]
	1.20	70	88	13	39	103	0[d]
	3.50	0	0	100	0	0	100
	9.00	0	0	100	0	0	100
	33.00	0	0	100	0	0	100
		Total % Injury		326			300
					Chronic S:R Effects Ratio		**0.92**

Reference Nebeker and Puglisi (1974)	**A1242 Exposure**[a]	**56-day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**	**Young per Initial Adult**	**% CNR**[b] **YpIA**	**% Injury**[c] **YpIA**
	Gammarus pseudolimnaeus , initiated with juvenile scuds						
	0.00	48	100	0	3.25	100	0
	2.80	77	160	0[d]	3.28	101	0[d]
	8.70	52	108	0[d]	0	0	100
	26.00	0	0	100	0	0	100
	81.00	0	0	100	0	0	100
	234.00	0	0	100	0	0	100
		Total % Injury		300			400
					Chronic S:R Effects Ratio		**1.33**

Reference Nebeker and Puglisi (1974)	**A1248 Exposure**[a]	**56-day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**	**Young per Initial Adult**	**% CNR**[b] **YpIA**	**% Injury**[c] **YpIA**
	Gammarus pseudolimnaeus , initiated with juvenile scuds						
	0.00	64	100	0	7.33	100	0
	0.18	73	114	0[d]	7.93	108	0[d]
	0.54	71	111	0[d]	13.9	190	0[d]
	2.20	73	114	0[d]	16.2	221	0[d]
	5.10	53	83	17	3.76	51	49
	18.00	0	0	100	0	0	100
		Total % Injury		117			149
					Chronic S:R Effects Ratio		**1.27**

Reference Nebeker and Puglisi (1974)	**Mixture of Aroclors**[e]	**21 day % Survival**	**% CNR**[b] **% Survival**	**% Injury**[c] **Survival**	**Young per Initial Adult**[f]	**% CNR**[b] **YpIA**	**% Injury**[c] **YpIA**
	Daphnia magna , initiated with <24h old neonates						
	0 %	92	100	0	38	100	0
	0.5 %	92	100	0	36	94	6
	1 %	87	95	5	29	77	23
	5 %	97	105	0[d]	38	100	0
	10 %	93	101	0[d]	33	87	13
	20%	17	18	82	5	13	87
	40 %	0	0	100	0	0	100
		Total % Injury		187			229
					Chronic S:R Effects Ratio		**1.22**

Mean (n=6) Chronic S:R Effects Ratio = 1.25

[a] The first row of numbers in each experiment is the Control treatment. All PCB exposure concentrations are measured aqueous values expressed as µg/L. See Table 1 for additional experimental details.

[b] % CNR-Percent Control-Normalized Response. See Materials and Methods for explanation.

[c] See Materials and Methods for explanation of % injury.

[d] The response in some experimental treatments outperformed the control so injury in these treatments was set to 0%.

[e] Mixture of Aroclors consisted of the following LC50 nominal concentrations (µg/liter): A1221, 89; A1232, 53; A1242, 48; A1248, 16; A1254, 18; A1260, 22; A1262, 24; A1268, 162.

[f] In the Aroclor mixture experiment, YpIA was calculated as the average of reported total young produced in 3 tests divided by the number of initial adults

Mean S:R Effects Ratio = 1.25 (n=6)

Table 7. Paired observations (n=58) of measured aqueous PCB concentrations and % benthic injury (survival) and % benthic injury adjusted for reproductive effects. The surrogate PCB concentration of 0.05 µg/L was used for control treatments (see Materials and Methods). Source Notes describe the experimental treatment for each paired observation. For additional experimental details see Table 1.

Log10 Measured Aqueous PCB Concentration (µg/L)	Measured Aqueous PCB Concentration (µg/L)	Benthic Injury[a] (%)	Benthic Injury Adjusted[b] (%)	Source Notes
-1.3010	0.05	0	0	A1254, Juvenile *P. duorarum*, 15 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	0	A1254, *P. duorarum*, 17-32 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	0	A1254, *P. duorarum*, 53 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	0	A1254, *P. duorarum*, 18 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	0	A1254, Adult *P. duorarum*, 35 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	0	0	A1254, *P. duorarum*, 20 day survival, controls, Duke et al. (1970)
-1.3010	0.05	0	0	A1254, *P. pugio*, 7 day survival, controls, Nimmo et al. (1974)
-1.3010	0.05	0	0	A1254, *P. pugio*, 16 day survival, controls, Nimmo et al. (1974)
-1.3010	0.05	0	0	A1248, *D. magna*, 14 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	0	A1254, *D. magna*, 14 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	0	A1254, *D. magna*, 21 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	0	A1242, *G. pseudolimnaeus*, 56 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	0	A1248, *G. pseudolimnaeus*, 56 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	0	0	A1254, *P. pugio*, 23-26 day survival, controls, Roesijadi et al. (1976)
-1.3010	0.05	0	0	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
-1.0000	0.10	0	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.7696	0.17	4	5	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
-0.7447	0.18	0	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
-0.5850	0.26	0	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.4318	0.37	0	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.3468	0.45	14	17	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
-0.2676	0.54	0	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
-0.2441	0.57	20	25	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
-0.2076	0.62	0	0	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
-0.0655	0.86	0	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.0362	0.92	0	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.0269	0.94	40	50	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
0.0792	1.20	13	16	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.1139	1.30	20	25	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)

Log10 Measured Aqueous PCB Concentration (µg/L)	Measured Aqueous PCB Concentration (µg/L)	Benthic Injury[a] (%)	Benthic Injury Adjusted[b] (%)	Source Notes
0.2304	1.70	0	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.3424	2.20	0	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.3802	2.40	64	79	A1254, *P. duorarum*, 17-32 day survival, Nimmo et al. (1971)
0.3979	2.50	0	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.4472	2.80	0	0	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.4914	3.10	79	99	A1254, *P. duorarum*, 17-32 day survival, Nimmo et al. (1971)
0.5051	3.20	3	4	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
0.5441	3.50	46	57	A1254, Adult *P. duorarum*, 35 day survival, Nimmo et al. (1971)
0.5441	3.50	100	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.5798	3.80	72	90	A1254, *P. duorarum*, 20 day survival, Duke et al. (1970)
0.5798	3.80	100	100	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.6021	4.00	35	44	A1254, *P. duorarum*, 18 day survival, Nimmo et al. (1971)
0.6021	4.00	27	33	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
0.6335	4.30	77	96	A1254, *P. duorarum*, 53 day survival, Nimmo et al. (1971)
0.7076	5.10	17	21	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.8751	7.50	92	100	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.9395	8.70	0	0	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.9542	9.00	100	100	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.9542	9.00	100	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.9590	9.10	58	73	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
0.9731	9.40	89	100	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
1.0969	12.50	40	50	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
1.1931	15.60	100	100	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
1.2553	18.00	100	100	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
1.2788	19.00	100	100	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
1.4150	26.00	100	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
1.5185	33.00	100	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
1.9085	81.00	100	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
2.3692	234.00	100	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)

[a] % Benthic injury based on the survival endpoint only. Same values as in Table 4.

[b] % Benthic injury adjusted upwards by 25% based on the greater sensitivity of reproduction endpoint. See text and calculations in Table 6.

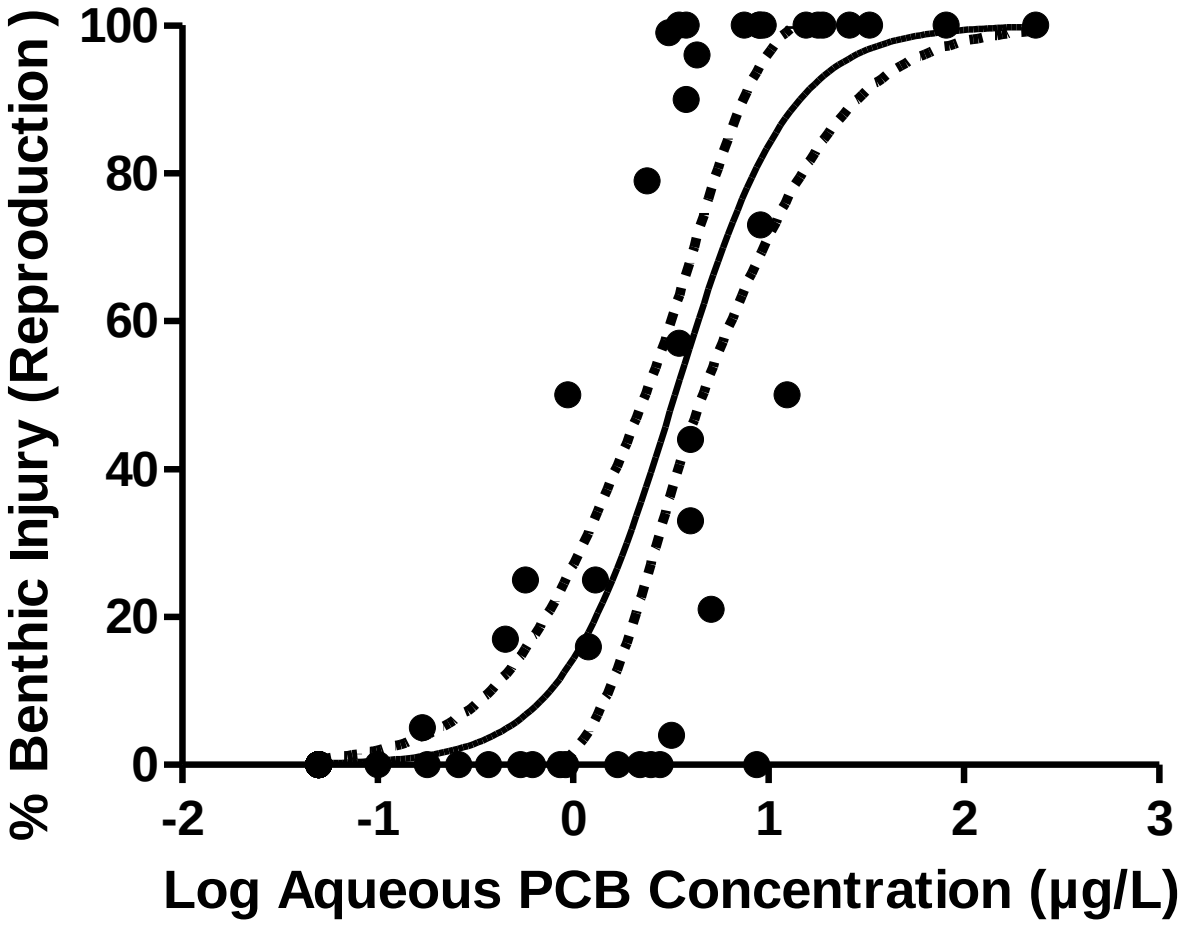

Figure 2. Benthic injury curve (adjusted for reproductive effects) for measured aqueous concentrations of PCBs (A1254, A1248, A1242). Dashed lines are 95% CI around the mean (solid line). R-squared = 0.69 Hill slope = 1.49

Table 8. Paired observations (n=58) of A1254 sediment concentrations and % benthic injury adjusted (for reproductive effects). Sediment concentrations (mg/kg-oc, and mg/kg using 1% organic carbon) predicted via EqP using measured aqueous PCB concentrations from Table 7 and Koc from EPI Web 4.1 (using Equation 7 to obtain 66.865 L/kg for Koc or 4.8252 for log Koc).

Log10 Measured Aqueous PCB Concentration (µg/L)	Measured Aqueous PCB Concentration (µg/L)	A1254 in Sediment (mg/kg-oc)	A1254 in Sediment[a] (mg/kg)	Benthic Injury Adjusted[b] (%)	Source Notes
-1.3010	0.05	3.3	0.03	0	A1254, Juvenile *P. duorarum*, 15 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 17-32 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 53 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 18 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	3.3	0.03	0	A1254, Adult *P. duorarum*, 35 day survival, controls, Nimmo et al. (1971)
-1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 20 day survival, controls, Duke et al. (1970)
-1.3010	0.05	3.3	0.03	0	A1254, *P. pugio*, 7 day survival, controls, Nimmo et al. (1974)
-1.3010	0.05	3.3	0.03	0	A1254, *P. pugio*, 16 day survival, controls, Nimmo et al. (1974)
-1.3010	0.05	3.3	0.03	0	A1248, *D. magna*, 14 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	3.3	0.03	0	A1254, *D. magna*, 14 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	3.3	0.03	0	A1254, *D. magna*, 21 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	3.3	0.03	0	A1242, *G. pseudolimnaeus*, 56 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	3.3	0.03	0	A1248, *G. pseudolimnaeus*, 56 day survival, controls, Nebeker & Puglisi (1974)
-1.3010	0.05	3.3	0.03	0	A1254, *P. pugio*, 23-26 day survival, controls, Roesijadi et al. (1976)
-1.3010	0.05	3.3	0.03	0	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
-1.0000	0.10	6.7	0.07	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.7696	0.17	11.4	0.11	5	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
-0.7447	0.18	12.0	0.12	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
-0.5850	0.26	17.4	0.17	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.4318	0.37	24.7	0.25	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.3468	0.45	30.1	0.30	17	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
-0.2676	0.54	36.1	0.36	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
-0.2441	0.57	38.1	0.38	25	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
-0.2076	0.62	41.5	0.41	0	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
-0.0655	0.86	57.5	0.58	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.0362	0.92	61.5	0.62	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
-0.0269	0.94	62.9	0.63	50	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
0.0792	1.20	80.2	0.80	16	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.1139	1.30	86.9	0.87	25	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
0.2304	1.70	113.7	1.14	0	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)

Log10 Measured Aqueous PCB Concentration (µg/L)	Measured Aqueous PCB Concentration (µg/L)	A1254 in Sediment (mg/kg-oc)	A1254 in Sediment[a] (mg/kg)	Benthic Injury Adjusted[b] (%)	Source Notes
0.3424	2.20	147.1	1.47	0	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.3802	2.40	160.5	1.60	79	A1254, *P. duorarum*, 17-32 day survival, Nimmo et al. (1971)
0.3979	2.50	167.2	1.67	0	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.4472	2.80	187.2	1.87	0	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.4914	3.10	207.3	2.07	99	A1254, *P. duorarum*, 17-32 day survival, Nimmo et al. (1971)
0.5051	3.20	214.0	2.14	4	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
0.5441	3.50	234.0	2.34	57	A1254, Adult *P. duorarum*, 35 day survival, Nimmo et al. (1971)
0.5441	3.50	234.0	2.34	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.5798	3.80	254.1	2.54	90	A1254, *P. duorarum*, 20 day survival, Duke et al. (1970)
0.5798	3.80	254.1	2.54	100	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.6021	4.00	267.5	2.67	44	A1254, *P. duorarum*, 18 day survival, Nimmo et al. (1971)
0.6021	4.00	267.5	2.67	33	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
0.6335	4.30	287.5	2.88	96	A1254, *P. duorarum*, 53 day survival, Nimmo et al. (1971)
0.7076	5.10	341.0	3.41	21	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.8751	7.50	501.5	5.01	100	A1248, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.9395	8.70	581.7	5.82	0	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
0.9542	9.00	601.8	6.02	100	A1254, *D. magna*, 14 day survival, Nebeker & Puglisi (1974)
0.9542	9.00	601.8	6.02	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
0.9590	9.10	608.5	6.08	73	A1254, *P. pugio*, 7 day survival, Nimmo et al. (1974)
0.9731	9.40	628.5	6.29	100	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
1.0969	12.50	835.8	8.36	50	A1254, *P. pugio*, 16 day survival, Nimmo et al. (1974)
1.1931	15.60	1,043.1	10.43	100	A1254, *P. pugio*, 23-26 day survival, Roesijadi et al. (1976)
1.2553	18.00	1,203.6	12.04	100	A1248, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
1.2788	19.00	1,270.4	12.70	100	A1254, Juvenile *P. duorarum*, 15 day survival, Nimmo et al. (1971)
1.4150	26.00	1,738.5	17.38	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
1.5185	33.00	2,206.6	22.07	100	A1254, *D. magna*, 21 day survival, Nebeker & Puglisi (1974)
1.9085	81.00	5,416.1	54.16	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)
2.3692	234.00	15,646.5	156.46	100	A1242, *G. pseudolimnaeus*, 56 day survival, Nebeker & Puglisi (1974)

[a] Sediment concentration (mg/kg) assuming 1% oc.

[b] % Benthic injury adjusted upwards by 25% based on greater sensitivity of reproduction endpoint. See text and calculations in Table 6.

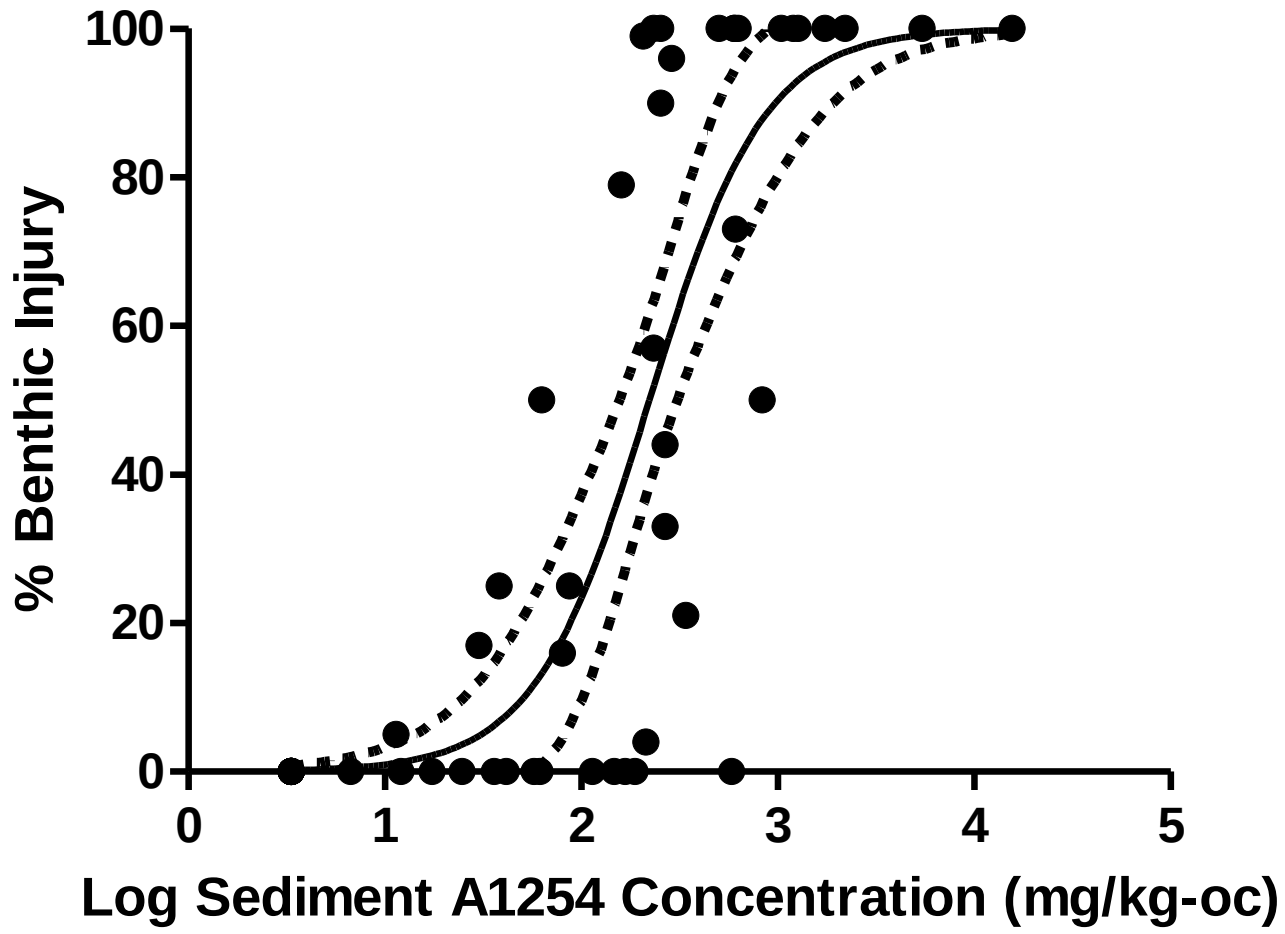

Figure 3. Benthic injury curve for EqP-modeled A1254-contaminated sediments using Table 8. Dashed lines are 95% CI around the mean. R-squared = 0.69 Hill slope = 1.49

Table 9. Look-up table for predicting % benthic injury corresponding to a range of A1254 concentrations in sediment using the data from Table 8 and the PRISM® software (Equation 3).

Log10 A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration[a] (mg/kg)	Benthic Injury (%)	Lower 95% CI	Upper 95% CI
0.524	3.34	0.03	0.2	-0.4	0.8
0.548	3.53	0.04	0.2	-0.4	0.9
0.573	3.74	0.04	0.2	-0.5	0.9
0.598	3.96	0.04	0.2	-0.5	1.0
0.622	4.19	0.04	0.3	-0.5	1.1
0.647	4.44	0.04	0.3	-0.6	1.2
0.672	4.69	0.05	0.3	-0.6	1.2
0.696	4.97	0.05	0.3	-0.7	1.3
0.721	5.26	0.05	0.4	-0.7	1.4
0.745	5.56	0.06	0.4	-0.7	1.6
0.770	5.89	0.06	0.4	-0.8	1.7
0.795	6.23	0.06	0.5	-0.8	1.8
0.819	6.60	0.07	0.5	-0.9	1.9
0.844	6.98	0.07	0.6	-0.9	2.1
0.869	7.39	0.07	0.6	-1.0	2.2
0.893	7.82	0.08	0.7	-1.0	2.4
0.918	8.28	0.08	0.7	-1.1	2.6
0.943	8.76	0.09	0.8	-1.2	2.8
0.967	9.27	0.09	0.9	-1.2	3.0
0.992	9.81	0.10	0.9	-1.3	3.2
1.016	10.39	0.10	1.0	-1.4	3.4
1.041	10.99	0.11	1.1	-1.4	3.7
1.066	11.63	0.12	1.2	-1.5	3.9
1.090	12.31	0.12	1.3	-1.6	4.2
1.115	13.03	0.13	1.4	-1.7	4.5
1.140	13.79	0.14	1.6	-1.7	4.9
1.164	14.60	0.15	1.7	-1.8	5.2
1.189	15.45	0.15	1.8	-1.9	5.6
1.214	16.35	0.16	2.0	-2.0	6.0
1.238	17.31	0.17	2.2	-2.1	6.4
1.263	18.32	0.18	2.4	-2.1	6.8
1.287	19.38	0.19	2.6	-2.2	7.3
1.312	20.52	0.21	2.8	-2.3	7.8
1.337	21.71	0.22	3.0	-2.3	8.4
1.361	22.98	0.23	3.3	-2.4	8.9
1.386	24.32	0.24	3.6	-2.4	9.5

Log10 A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration[a] (mg/kg)	Benthic Injury (%)	Lower 95% CI	Upper 95% CI
1.411	25.74	0.26	3.9	-2.5	10.2
1.435	27.24	0.27	4.2	-2.5	10.8
1.460	28.83	0.29	4.5	-2.5	11.5
1.485	30.52	0.31	4.9	-2.5	12.3
1.509	32.30	0.32	5.3	-2.4	13.1
1.534	34.18	0.34	5.8	-2.4	13.9
1.558	36.18	0.36	6.2	-2.3	14.8
1.583	38.29	0.38	6.8	-2.2	15.7
1.608	40.52	0.41	7.3	-2.0	16.7
1.632	42.89	0.43	7.9	-1.8	17.7
1.657	45.39	0.45	8.5	-1.6	18.7
1.682	48.04	0.48	9.2	-1.3	19.8
1.706	50.84	0.51	10.0	-1.0	20.9
1.731	53.81	0.54	10.7	-0.6	22.1
1.756	56.95	0.57	11.6	-0.1	23.3
1.780	60.28	0.60	12.5	0.4	24.5
1.805	63.79	0.64	13.4	1.0	25.8
1.829	67.52	0.68	14.4	1.8	27.1
1.854	71.46	0.71	15.5	2.5	28.5
1.879	75.63	0.76	16.7	3.4	29.9
1.903	80.04	0.80	17.9	4.4	31.3
1.928	84.72	0.85	19.2	5.5	32.8
1.953	89.66	0.90	20.5	6.8	34.2
1.977	94.89	0.95	21.9	8.1	35.7
2.002	100.43	1.00	23.4	9.5	37.2
2.027	106.29	1.06	24.9	11.1	38.8
2.051	112.50	1.12	26.6	12.8	40.3
2.076	119.06	1.19	28.2	14.5	41.9
2.100	126.01	1.26	30.0	16.4	43.5
2.125	133.37	1.33	31.8	18.4	45.1
2.150	141.15	1.41	33.6	20.5	46.8
2.174	149.39	1.49	35.6	22.7	48.5
2.199	158.11	1.58	37.5	24.9	50.2
2.224	167.34	1.67	39.5	27.1	51.9
2.248	177.10	1.77	41.6	29.4	53.7
2.273	187.44	1.87	43.6	31.7	55.6
2.297	198.38	1.98	45.7	34.0	57.5
2.322	209.96	2.10	47.8	36.2	59.4
2.347	222.21	2.22	49.9	38.4	61.4

Log10 A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration[a] (mg/kg)	Benthic Injury (%)	Lower 95% CI	Upper 95% CI
2.371	235.18	2.35	52.0	40.6	63.5
2.396	248.91	2.49	54.2	42.7	65.6
2.421	263.43	2.63	56.2	44.7	67.8
2.445	278.81	2.79	58.3	46.7	70.0
2.470	295.08	2.95	60.4	48.5	72.2
2.495	312.30	3.12	62.4	50.4	74.3
2.519	330.53	3.31	64.3	52.1	76.5
2.544	349.82	3.50	66.2	53.9	78.6
2.568	370.24	3.70	68.1	55.6	80.7
2.593	391.85	3.92	69.9	57.2	82.6
2.618	414.72	4.15	71.7	58.8	84.5
2.642	438.92	4.39	73.3	60.4	86.3
2.667	464.54	4.65	75.0	61.9	88.0
2.692	491.65	4.92	76.5	63.5	89.6
2.716	520.35	5.20	78.0	65.0	91.0
2.741	550.72	5.51	79.4	66.4	92.4
2.766	582.86	5.83	80.8	67.9	93.6
2.790	616.88	6.17	82.0	69.3	94.8
2.815	652.88	6.53	83.3	70.7	95.8
2.839	690.99	6.91	84.4	72.1	96.7
2.864	731.32	7.31	85.5	73.4	97.6
2.889	774.00	7.74	86.5	74.7	98.3
2.913	819.18	8.19	87.5	76.0	99.0
2.938	866.99	8.67	88.4	77.2	99.5
2.963	917.59	9.18	89.2	78.4	100.0
2.987	971.14	9.71	90.0	79.5	100.5
3.012	1,027.82	10.28	90.7	80.6	100.9
3.037	1,087.81	10.88	91.4	81.7	101.2
3.061	1,151.30	11.51	92.1	82.7	101.4
3.086	1,218.50	12.18	92.7	83.6	101.7
3.110	1,289.61	12.90	93.2	84.6	101.8
3.135	1,364.88	13.65	93.7	85.5	102.0
3.160	1,444.54	14.45	94.2	86.3	102.1
3.184	1,528.85	15.29	94.6	87.1	102.2
3.209	1,618.09	16.18	95.1	87.9	102.2
3.234	1,712.53	17.13	95.4	88.6	102.2
3.258	1,812.47	18.12	95.8	89.3	102.3
3.283	1,918.26	19.18	96.1	90.0	102.2
3.308	2,030.22	20.30	96.4	90.6	102.2

Log10 A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration (mg/kg-oc)	A1254 Sediment Concentration[a] (mg/kg)	Benthic Injury (%)	Lower 95% CI	Upper 95% CI
3.332	2,148.71	21.49	96.7	91.2	102.2
3.357	2,274.12	22.74	97.0	91.8	102.2
3.381	2,406.85	24.07	97.2	92.3	102.1
3.406	2,547.32	25.47	97.4	92.8	102.1
3.431	2,696.00	26.96	97.6	93.3	102.0
3.455	2,853.35	28.53	97.8	93.7	101.9
3.480	3,019.88	30.20	98.0	94.1	101.9
3.505	3,196.14	31.96	98.2	94.5	101.8
3.529	3,382.68	33.83	98.3	94.9	101.7
3.554	3,580.12	35.80	98.4	95.2	101.7
3.579	3,789.06	37.89	98.6	95.5	101.6
3.603	4,010.21	40.10	98.7	95.8	101.5
3.628	4,244.27	42.44	98.8	96.1	101.5
3.652	4,491.98	44.92	98.9	96.4	101.4
3.677	4,754.15	47.54	99.0	96.6	101.3
3.702	5,031.63	50.32	99.1	96.8	101.3
3.726	5,325.30	53.25	99.1	97.1	101.2
3.751	5,636.10	56.36	99.2	97.3	101.1
3.776	5,965.06	59.65	99.3	97.5	101.1
3.800	6,313.21	63.13	99.3	97.6	101.0
3.825	6,681.69	66.82	99.4	97.8	101.0
3.850	7,071.65	70.72	99.4	97.9	100.9
3.874	7,484.38	74.84	99.5	98.1	100.9
3.899	7,921.22	79.21	99.5	98.2	100.8
3.923	8,383.53	83.84	99.6	98.3	100.8
3.948	8,872.83	88.73	99.6	98.5	100.7
3.973	9,390.70	93.91	99.6	98.6	100.7
3.997	9,938.78	99.39	99.7	98.7	100.6
4.022	10,518.84	105.19	99.7	98.8	100.6
4.047	11,132.79	111.33	99.7	98.9	100.6
4.071	11,782.54	117.83	99.7	98.9	100.5
4.096	12,470.25	124.70	99.8	99.0	100.5
4.121	13,198.06	131.98	99.8	99.1	100.5
4.145	13,968.35	139.68	99.8	99.1	100.4
4.170	14,783.63	147.84	99.8	99.2	100.4
4.194	15,646.46	156.46	99.8	99.3	100.4

[a] Sediment concentration (mg/kg) assuming 1% organic carbon

Table 10. Comparison of benthic injury (95% CI) estimates for A1254 for a hypothetical arithmetic progression of sediment concentrations using the data from Table 9.

Sediment Concentration (mg/kg dw)[a]	A1254		
	Benthic Injury (%)	Lower 95% CI	Upper 95% CI
1	23.3	9.4	37.1
2	46.0	34.3	57.71
4	70.6	57.8	83.3
8	87.1	75.4	98.7
16	95.0	87.8	102.2

[a] assuming 1% organic carbon

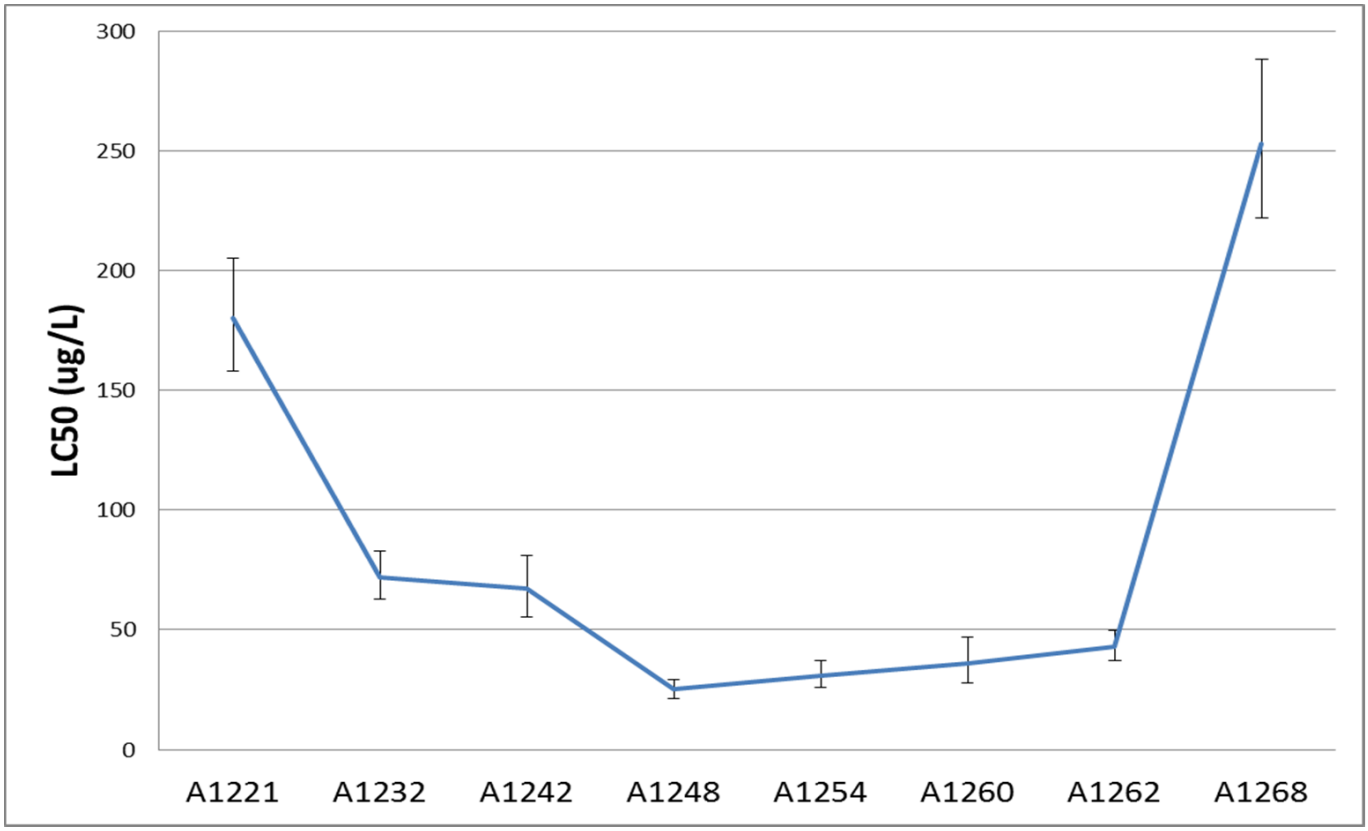

Figure 4. 21-day LC50s (measured PCB concentrations) for *D. magna* in static aqueous exposures to eight Aroclor mixtures as reported by Nebeker and Puglisi (1974). (Error bars = 95% CI)

Table 11. Percent homolog composition, by weight (%), in eight Aroclor mixtures as reported by six literature sources denoted by capital letters.

Homolog Groups	A1221					A1232				A1016				A1242					
	A	B	C	D	E	B	C	D	E	A	C	D	E	A	B	C	D	E	F
Biphenyl	11	7	10			6				<0.1				<0.1					
Monochloro-	51	51	50	65.5	60.06	26	26	31.3	27.55	1	2		0.7	1	1	1		0.75	
Dichloro-	32	38	35	29.7	33.38	29	29	23.7	26.83	20	19	21.2	17.53	16	17	13	14.7	15.04	4
Trichloro-	4	3	4	4.8	4.21	24	24	23.4	25.64	57	57	51.5	54.67	49	40	45	46	44.91	39
Tetrachloro-	2		1		1.15	15	15	15.7	10.58	21	22	27.3	22.07	25	32	31	30.6	20.16	42
Pentachloro-	0.5				1.23	0.5		5.8	9.39	1			5.07	8	10	10	8.7	18.85	14
Hexachloro-									0.21	<0.1				1	0.5			0.31	
Heptachloro-									0.03					<0.1					
Octachloro-																			
Nonachloro-																			

Homolog Groups	A1248					A1254						A1260				A1262	
	A	B	C	D	E	B	C	D	E[a]	E[b]	F	B	C	D	E	D	E
Biphenyl	<0.1																
Monochloro-	<0.1				0.07				0.02						0.02		0.02
Dichloro-	0.5	1	1		1.55				0.09	0.24					0.08		0.27
Trichloro-	1	23	21	20.9	21.27		1	1.8	0.39	1.26	0.5				0.21		0.98
Tetrachloro-	21	50	49	60.3	32.77	16	15	17.1	4.86	10.25	36				0.35		0.49
Pentachloro-	48	20	27	18.1	42.92	60	53	49.3	71.44	59.12	45	12	12	9.2	8.74	4.2	3.35
Hexachloro-	23	1	2	0.8	1.64	23	26	27.8	21.97	26.76	18	46	42	46.9	43.35	30.9	26.43
Heptachloro-	6				0.02	1	4	3.9	1.36	2.66	1	36	38	36.9	38.54	45.8	48.48
Octachloro-										0.04		6	7	6.3	8.27	17.7	19.69
Nonachloro-									0.04	0.04			1	0.7	0.7	1.3	1.65

Sources: A - Mieure et al. (1976) as cited in US EPA (1980); B - Webb and McCall (1973) as cited in US EPA (1980); C - DeVoogt and Brinkman (1989); D - Frame et al. (1996); E - ATSDR (2000); F - Hirwe et al. (1974)

E^a - Monsanto lot from abnormal late production (1974-1977); E^b - General Electric lot

Table 12. Individual, mean and median Log Kow values for nine homolog groups reported by Mackay et al. (2006). Descriptive statistics are based on the non-logarithm Kow expressions. Log Kow values used by Fuchsman et al. (2006) are shown for comparison.

Homolog Groups	Monochlorobiphenyl		Dichlorobiphenyl		Trichlorobiphenyl		Tetrachlorobiphenyl		Pentachlorobiphenyl	
Kow Values	Log Kow	Kow	Log Kow	Kow	Log Kow	Kow	Log Kow	Kow	Log Kow	Kow
	4.3	19,953	4.9	79,433	5.5	316,228	5.6	398,107	6.2	1,584,893
	4.5	31,623	5.1	125,893	5.5	316,228	5.9	794,328	6.3	1,995,262
	4.6	39,811	5.1	125,893	5.53	338,844	6.35	2,238,721	6.33	2,137,962
	4.6	45,709	5.13	134,896	5.76	575,440	6.5	3,162,278	6.4	2,511,886
	4.7	50,119	5.19	154,882	5.8	630,957			6.5	3,162,278
	4.73	53,703	5.3	199,526	5.9	794,328			6.6	3,981,072
									6.85	7,079,458
Mean Kow		40,153		136,754		495,338		1,648,359		3,207,544
Stdev		12,607		39,482		201,423		1,282,312		1,885,147
% CV		31%		29%		41%		78%		59%
n		6		6		6		4		7
Median Kow		42,760		130,394		457,142		1,516,525		2,511,886
Fuchsman et al. (2006)	4.64	43,652	5.12	131,826	5.62	416,869	6.04	1,096,478	6.49	3,090,295

Homolog Groups	Hexachlorobipheny		Heptachlorobiphenyl		Octachlorobipheny		Nonachlorobiphenyl	
Kow Values	Log Kow	Kow	Log Kow	Kow	Log Kow	Kow	Log Kow	Kow
	6.7	5,011,872	6.7	5,011,872	7.1	12,589,254	7.2	15,848,932
	6.7	5,011,872	7	10,000,000	7.5	31,622,777	7.9	79,432,823
	6.8	6,309,573	7.1	12,589,254	8.55	354,813,389	8.16	144,543,977
	7	10,000,000					9.14	1,380,384,265
	7.3	19,952,623						
Mean Kow		9,257,188		9,200,375		133,008,473		405,052,499
Stdev		6,318,187		3,851,458		192,324,295		652,340,487
% CV		68%		42%		145%		161%
n		5		3		3		4
Median Kow		6,309,573		10,000,000		31,622,777		111,988,400
Fuchsman et al. (2006)	6.84	6,918,310	6.98	9,549,926	7.72	52,480,746	8.24	173,780,083

APPENDIX A

To calculate a site specific Koc when congener data is available one can use Equation 9.

$$\log (Koc) = 0.53(N_{cl} - N_{orthoCl}) + 4.98 \quad (9)$$

where N_{CL} is the total number of chlorines and $N_{orthoCL}$ is the number of ortho-chlorines (Hawthorne et al., 2011; c.f., Arp, et al., 2009).

As a demonstration, we use a field sample from Newark Bay in New York Harbor to find the Koc. From the 2007 Passaic-Newark Bay Phase 2 Remedial Investigation - whose data is shown in the NOAA New York-New Jersey Query Manager database - we selected at random Station NB2SED116 found off the northern tip of Staten Island with a total PCB concentration of 3668 µg/kg. To find the Koc using Equation 9 one needs to first find the average number of chlorines in a sample. To do so first find the concentration of each homolog group and calculate the percent of each by comparing to the total PCB concentration. See Table 1 below that shows the weighted Cl contribution calculation of 4.4.

Table A-1: Concentration and percent of total sample PCBs in µg/kg per homolog group for Sample Station NB2SED116 from Newark Bay. The specific number of chlorines per homolog group for this PCB sample are shown in Column 4 using a weighted approach with the sum total at bottom. CL-1 and CL-10 were not used due to low concentrations.

Chlorine Group	Group Concentration (µg/kg)	Percent of Total (%)	Weighted Cl Contribution
CL-1	9	0.2 – Not used	0
CL-2	29	6.0	0.1
CL-3	83	27	0.8
CL-4	1100	30	1.2
CL-5	644	18	0.9
CL-6	386	11	0.7
CL-7	190	5	0.4
CL-8	76	2	0.2
CL-9	37	1	0.1
CL-10	12	0.3 – Not used	0
Total = 3,668 µg/kg			Total Weighted Cl's = 4.4

Following the calculation of the total chlorines, NCL, one then calculates the number of ortho-chlorines, NorthoCL, using Table A-2. Here, the weighted ortho-chlorine contribution per congener is calculated by finding the percent of total PCBs per congener and multiplying by the number of ortho-chlorines present in that congener. Table A-2 shows that the total weighted ortho-chlorine is 1.6.

Table A-2: Concentration and percent of total sample PCBs in µg/kg per congener for Sample Station NB2SED116 from Newark Bay. Total concentration is 3,668 µg/kg. The number of ortho-chlorines from this sample is based on the congeners that contribute the ortho-chlorine (2-6). The number of ortho-chlorines per congener from this PCB sample is shown in Column 5 using a weighted approach with the sum total at bottom. Congeners making up equal to or less than 0.1 percent of the sample were not used because their weighted ortho-chlorine contribution is insignificant.

Congener Number	Concentration µg/kg	Percent of Total	Number of Ortho-Chlorines	Weighted Ortho-Chlorine Contribution
1	4.3	0.1	1	0.001
2	1.3	<0.1 not used	0	0
3	3.8	0.1	0	0
4	12.0	0.3	2	0.006
5	24.0	0.7	1	0.007
6	11.2	0.3	1	0.003
7	2.0	<0.1 not used	1	0
8	24.0	0.7	1	0.007
9	2.0	<0.1 not used	1	0
10	11.0	0.3	1	0.003
11	59.1	1.6	0	0
12	8.3	0.2	0	0
13	8.3	0.2	0	0
14	0.2	<0.1 not used	0	0
15	67.0	1.8	0	0
16	36.3	1.0	2	0.02
17	57.1	1.5	2	0.03
18	108.0	2.9	2	0.058
19	11.5	0.3	3	0.009
20	85.6	2.3	1	0.023
21	NA		1	0
22	67.6	1.8	1	0.018
23	0.3	<0.1 not used	1	0
24	6.1	0.2	2	0
25	29.3	0.8	1	0.008
26	41.4	1.1	1	0.011
27	6.1	0.2	2	0.004
28	223.0	6.1	1	0.061
29	0.9	<0.1 not used	1	0
30	0.2	<0.1 not used	2	0
31	219.0	6.0	1	0.06
32	36.3	1.0	2	0.02
33	NA		1	0
34	1.4	<0.1 not used	1	0
35	5.0	0.1 not used	0	0
36	0.1	<0.1 not used	0	0
37	47.4	1.3	0	0
38	0.7	<0.1 not used	0	0

Congener Number	Concentration µg/kg	Percent of Total	Number of Ortho-Chlorines	Weighted Ortho-Chlorine Contribution
39	0.4	<0.1 not used	0	0
40	19.6	0.5	2	0.01
41	53.5	1.5	2	0.03
42	24.7	0.7	2	0.014
43	58.0	1.5	2	0.03
44	128.0	3.5	2	0.07
45	19.3	0.5	3	0.015
46	8.6	0.2	3	0.006
47	50.4	1.4	2	0.028
48	12.0	0.3	2	0.006
49	58.0	1.5	2	0.03
50	0.6	<0.1 not used	3	0
51	7.5	0.2	3	0.006
52	68.5	1.9	2	0.038
53	20.4	0.6	3	0.018
54	0.4	<0.1 not used	4	0
55	1.3	<0.1 not used	1	0
56	33.7	0.9	1	0.009
57	0.8	<0.1 not used	1	0
58	0.5	<0.1 not used	1	0
59	24.7	0.7	2	0.014
60	33.7	0.9	1	0.009
61	68.0	1.9	1	0.019
62	0.0	<0.1 not used	2	0
63	5.5	0.2	1	0.002
64	53.5	1.5	2	0.030
65	0.1	<0.1 not used	2	0
66	60.0	1.6	1	0.016
67	4.6	0.1 not used	1	0
68	0.8	<0.1 not used	1	0
69	68.5	1.9	2	0.038
70	68.0	1.9	1	0.019
71	NA		2	0
72	NA		1	0
73	0.0	<0.1 not used	2	0
74	57.5	1.6	1	0.016
75	12.0	0.3	2	0.006
76	60.0	1.6	1	0.016
77	14.3	0.4	0	0
78	0.0	<0.1 not used	0	0
79	1.0	<0.1 not used	0	0
80	0.0	<0.1 not used	0	0
81	0.4	<0.1 not used	0	0
82	12.8	0.3	2	0.006
83	0.1	<0.1 not used	2	0
84	21.1	0.6	3	0.018
85	9.1	0.2	2	0.004

Congener Number	Concentration µg/kg	Percent of Total	Number of Ortho-Chlorines	Weighted Ortho-Chlorine Contribution
86	0.8	<0.1 not used	2	0
87	15.8	0.4	2	0.008
88	9.7	0.3	3	0.009
89	1.8	<0.1 not used	3	0
90	49.0	1.4	2	0.028
91	9.7	0.3	3	0.009
92	21.1	0.6	2	0.012
93	0.0	<0.1 not used	3	0
94	1.0	<0.1 not used	3	0
95	41.0	1.1	3	0.033
96	1.4	<0.1 not used	4	0
97	32.5	0.9	2	0.018
98	41.0	1.1	3	0.033
99	48.8	1.3	2	0.026
100	0.9	<0.1 not used	3	0
101	49.0	1.3	2	0.026
102	0.9	<0.1 not used	3	0
103	1.2	<0.1 not used	3	0
104	0.1	<0.1 not used	4	0
105	28.3	0.8	1	0.008
106	40.8	1.1	1	0.011
107	3.4	0.1 not used	1	0
108	2.7	<0.1 not used	1	0
109	3.4	0.1 not used	2	0
110	115.0	3.9	2	0.078
111	1.0	<0.1 not used	1	0
112	2.7	<0.1 not used	2	0
113	1.0	<0.1 not used	2	0
114	1.9	<0.1 not used	1	0
115	1.0	<0.1 not used	2	0
116	9.1	0.2	2	0.004
117	15.8	0.4	2	0.008
118	40.8	1.1	1	0.011
119	2.8	<0.1 not used	2	0
120	0.3	<0.1 not used	1	0
121	0.0	<0.1 not used	2	0
122	1.1	<0.1 not used	1	0
123	1.6	<0.1 not used	1	0
124	3.5	0.1 not used	1	0
125	NA		1	0
126	0.5	<0.1 not used	0	0
127	0.0	<0.1 not used	0	0
128	5.7	0.2	2	0.004
129	3.1	<0.1 not used	2	0
130	4.9	0.1 not used	2	0
131	0.0	<0.1 not used	3	0
132	11.2	0.3	3	0.009

Congener Number	Concentration µg/kg	Percent of Total	Number of Ortho-Chlorines	Weighted Ortho-Chlorine Contribution
133	1.3	<0.1 not used	2	0
134	2.1	<0.1 not used	3	0
135	12.1	0.3	3	0.009
136	11.3	0.3	4	0.012
137	3.8	0.1 not used	2	0
138	77.6	2.1	2	0.042
139	37.5	1.0	3	0.03
140	0.6	<0.1 not used	3	0
141	13.7	0.4	2	0.008
142	1.3	<0.1 not used	3	0
143	2.1	<0.1 not used	3	0
144	4.2	0.1 not used	3	0
145	0.0	<0.1 not used	4	0
146	6.0	0.2	2	0.004
147	2.3	<0.1 not used	3	0
148	0.2	<0.1 not used	3	0
149	37.5	1.0	3	0.03
150	0.3	<0.1 not used	4	0
151	21.6	0.6	3	0.018
152	0.1	<0.1 not used	4	0
153	77.3	2.1	2	0.042
154	1.9	<0.1 not used	3	0
155	2.7	<0.1 not used	4	0
156	7.4	0.2	1	0.002
157	1.7	<0.1 not used	1	0
158	4.2	0.1 not used	2	0
159	0.0	<0.1 not used	1	0
160	4.2	0.1 not used	2	0
161	11.2	0.3	2	0.006
162	5.7	0.2	1	0.002
163	NA		2	0
164	NA		2	0
165	6.5	0.2	2	0.004
166	0.3	<0.1 not used	2	0
167	3.1	<0.1 not used	1	0
168	0.1	<0.1 not used	2	0
169	0.0	<0.1 not used	0	0
170	18.7	0.5	2	0.01
171	5.3	0.2	3	0.006
172	3.2	<0.1 not used	2	0
173	0.5	<0.1 not used	3	0
174	21.3	0.6	3	0.018
175	1.3	<0.1 not used	3	0
176	3.3	<0.1 not used	4	0
177	12.6	0.3	3	0.009
178	5.3	0.2	3	0.006
179	11.5	0.3	4	0.012

Congener Number	Concentration µg/kg	Percent of Total	Number of Ortho-Chlorines	Weighted Ortho-Chlorine Contribution
180	48.8	1.3	2	0.026
181	0.5	<0.1 not used	3	0
182	17.3	0.5	3	0.015
183	14.1	0.4	3	0.012
184	0.2	<0.1 not used	4	0
185	2.5	<0.1 not used	3	0
186	0.0	<0.1 not used	4	0
187	17.2	0.5	3	0.015
188	0.1	<0.1 not used	4	0
189	0.7	<0.1 not used	1	0
190	3.9	0.1 not used	2	0
191	0.8	<0.1 not used	2	0
192	0.0	<0.1 not used	2	0
193	2.2	<0.1 not used	2	0
194	12.6	0.3	2	0.006
195	4.7	0.1 not used	3	0
196	11.3	0.3	3	0.009
197	0.5	<0.1 not used	4	0
198	1.4	<0.1 not used	3	0
199	21.4	0.6	3	0.018
200	2.2	<0.1 not used	4	0
201	2.5	<0.1 not used	4	0
202	5.7	0.2	4	0.008
203	11.3	0.3	3	0.009
204	0.0	<0.1 not used	4	0
205	0.4	<0.1 not used	2	0
206	26.1	0.7	3	0.021
207	2.5	<0.1 not used	4	0
208	8.6	0.2	4	0.008
209	12.6	0.3	4	0.012
	Total = 3,668 µg/kg			Total Weighted Ortho-Cl's = 1.6

Table A-3 uses the calculated weighted total chlorine (Table A-1) and the weighted total ortho-chlorine (Table A-2) to calculate the log (Koc) for Sample Station NB2SED116 from Newark Bay using Equation 9. This measurement is made as an example of how one can determine Koc with congener data.

Table A-3: Calculation of Koc using the data from Tables B-1 and B-2 and Equation #9

$$\log (K_{OC}) = 0.53(N_{CL} - N_{OrthoCL}) + 4.98 \quad (9)$$

Where:

N_{CL} = 4.4 from Table B-1

$N_{OrthoCL}$ = 1.6 from Table B-2

Log K_{OC} = 0.53 (4.4-1.6) + 4.98

Log Koc = 0.53 (2.8) + 4.98

Log Koc =1.484 + 4.98 = 6.464* = Koc

*Based on a dissolved water column measure with no colloidal material

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