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BENTHIC INJURY DOSE–RESPONSE MODELS FOR POLYCHLORINATED BIPHENYL–CONTAMINATED SEDIMENT USING EQUILIBRIUM PARTITIONING

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Abstract

The study goal was to develop a sediment polychlorinated biphenyl (PCB) dose–response model based on benthic invertebrate effects to PCBs. The authors 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 aquatic toxicity studies. The present study differs from all other EqP collective sediment investigations in that the authors examined a common dose–response gradient of effects for PCBs rather than a single, protective value. The authors reviewed the chronic aquatic toxicity literature to identify measured aqueous PCB concentrations and associated benthic invertebrate effects. The authors control-normalized the aquatic toxic effect data and expressed results from various studies as a common metric, percent injury. Then, they calculated organic carbon–normalized sediment PCB concentrations (mg/kg organic carbon) from the aqueous PCB toxicity data set using EqP theory based on the US Environmental Protection Agency's (EPIWEB 4.1) derivation of the water–organic carbon partition coefficient (K_{OC}). Lastly, the authors constructed a nonlinear dose–response numerical model for these synoptic sediment PCB concentrations and biological effects: $Y = 100/([1 + 10\{\log EC50 - \log X\}] \times \text{Hill slope})$**<ZAQ;1>** (EC50 = median effective concentration). These models were used to generate "look-up" tables reporting percent injury in benthic biota for a range of Aroclor-specific sediment concentrations. For example, the model using the EPIWEB K_{OC} estimate predicts mean benthic injury of 23.3%, 46.0%, 70.6%, 87.1%, and 95% for hypothetical sediment concentrations of 1 mg/kg, 2 mg/kg, 4 mg/kg, 8 mg/kg, and 16 mg/kg dry weight of Aroclor 1254, respectively (at 1% organic carbon). The authors recommend the model presented for screening but suggest, when possible, determining a site-specific K_{OC} that, along with the tables and equations, allows users to create their own protective dose–response sediment concentration.

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INTRODUCTION

Polychlorinated biphenyls (PCBs) are mixtures of synthetic compounds (congeners) which vary in chlorine content and spatial configuration. Congeners of PCBs can be grouped into isomeric homologs with the same chlorine content (i.e., monochlorobiphenyls, dichlorobiphenyls, up to decachlorobiphenyls) but different spatial configurations [1]. Polychlorinated biphenyls 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% [2,3]. Aroclors were used primarily as dielectric fluids in transformers and capacitors but also 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 [3–5].

Like most environmental contaminants, early regulatory control of PCBs focused on “end of the pipe” discharges. In the United States as well as other countries, technical support for regulatory control of PCBs and other contaminants appeared in the form of chemical-specific ambient water quality documents (e.g., US Environmental Protection Agency [4]) containing numerical criteria [6]. 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 that sorbed readily to sedimentary organic material such as PCBs. Today, PCBs are frequently identified as chemicals of concern at contaminated sediment sites in the United States and around the world [7–10].

In response to the increasing concern regarding contaminated sediments, the US Environmental Protection Agency (USEPA) embarked on a regulatory research program to develop sediment quality criteria analogous to water quality criteria [11]. Developing these sediment criteria eventually became part of the USEPA's strategy for managing contaminated sediments across its many regulatory programs [12]. Two methods, a theoretical method and an empirical method, were generally advocated for developing sediment criteria. First is the theoretical equilibrium partitioning (EqP) approach, which estimates a sediment concentration based on a porewater concentration protective of aquatic biota using the best available aquatic toxicity data and the sediment–water partitioning coefficient. The EqP approach is based on the assumption that the chemical sensitivity of benthic/epibenthic organisms is not significantly different from that of pelagic organisms, and this assumption has been supported by some applied research [13]. 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 data sets for numerical relationships between synoptic sediment chemistry and sediment toxicity data (largely 10-d amphipod bioassays). This empirical approach helps answer the question, "What is the likelihood this sediment will be toxic to benthic biota?" Both approaches have advantages and limitations, as discussed in Burton

[14]. 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 [13]. 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., effects range low, threshold effects level) as well as concentrations associated with a reasonable likelihood of effects (e.g., effects range medium, probable effects level, 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%) [15]. No analogous effects continuum has been developed for the EqP approach.

At hazardous waste sites in the United States, the ecological risks and potential injury of biological resources to PCBs are determined by conducting ecological risk assessments and natural resource damage assessments, respectively [16,17]. Both programs have the goal of identifying chemicals responsible for the risk or injury. Sediment guidelines or benchmarks are often used in both ecological risk assessments and natural resource damage assessments to estimate adverse effects of PCB-contaminated sediments on benthic invertebrates. Based on the empirical approach discussed, MacDonald et al. [18] proposed the following 3 consensus sediment quality guidelines for total PCBs: threshold effect concentration = 0.040 mg/kg dry weight, midrange effect concentration = 0.40

mg/kg dry weight, and extreme effect concentration = 1.7 mg/kg dry weight. Using the theoretical EqP approach, Fuchsman et al. [19] proposed protective organic carbon (OC)–normalized chronic sediment quality benchmarks for the following Aroclor mixtures: A1242 = 210 µg/g OC, A1248 = 490 µg/ g OC, A1254 = 1500 µg/ g OC, and A1260 = 3800 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 the present study, we used the theoretical EqP approach to generate a continuum of benthic injury dose responses for sediments contaminated with PCBs. We compare our approach with threshold values reported by Fuchsman et al. [19]. 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 percentage 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 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., Web of Knowledge, Aquatic Science & Fisheries Abstracts), review of published compilations of toxicity literature (e.g., USEPA [4]), and personal collections of papers. We excluded studies that had exposure concentrations greater than the Aroclor aqueous solubilities reported by

Mackay et al. [20]. In addition, we only considered studies in which investigators reported measured aqueous Aroclor exposure concentrations because actual concentrations can be one-half to 1 order of magnitude less than nominal concentrations [21–23]. We also avoided acute lethality exposures (e.g., ≤96-h median lethal concentration [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, and static-renewal), and 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. [24] used a control-normalized common metric of percent fish injury. A similar approach is used in the present study 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

$$\%\ \mathrm{CNR} = (\text{treatment response}/\text{control response}) \times 100 \tag{1}$$

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

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

Aqueous PCB dose–response curve

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 (Ver 5.01). The nonlinear log (stimulation) versus normalized response module with a variable Hill slope was the model selected for the present study. The numerical model for this curve is shown in Equation 3

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

<ZAQ;2>

where Y is the percent benthic injury, X is the aqueous Aroclor concentration (µg/L), EC50 is the effective Aroclor concentration that causes a response halfway (50%) between the baseline (0% benthic injury) and maximum response (100% benthic injury), and the Hill slope is the numerical value representing the steepness of the dose–response curve. Model outputs also include the lower and upper limits of the 95% confidence interval (CI) around the percent 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 articles contemporary to the toxicity literature we used [23,25,26].

EqP modeling

As noted (see section *Introduction*), EqP modeling can be used to predict sediment concentrations from aqueous concentrations. Using EqP, we modeled PCB concentrations in sediment from the aqueous concentrations used to construct the dose–response injury curve described (Equation 3). In its simplest form, EqP modeling for PCBs can be expressed by the following equation

$$\text{sediment concentration} = \text{interstitial water concentration} \times K_{OC} \times f_{OC} \times 0.001 \quad (4)$$

where the organic carbon–normalized PCB sediment concentration (mg/kg) 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} [27]. However, equations to calculate the K_{OC} from the K_{OW} for PCBs are available from the literature. For example, Hawthorne et al. [28] (from Schwarzenbach et al. [29]) provides

$$\log (K_{OC}) = 0.74 \log (K_{OW}) + 0.15 \quad (5)$$

and DiToro and McGrath [31] use

$$\log (K_{OC}) = 0.00028 + 0.983 \log (K_{OW}) \quad (6)$$

We note that Burgess et al. [30] used the DiToro and McGrath [31] K_{OW}–K_{OC} transformation equation in their seminal article on calculating EqP single-sediment benchmarks for non-ionic organic chemicals other than PCBs. Nevertheless, the K_{OC} selection is likely the most variable, and possibly divisive, selection within the EqP equation and therefore deserves more attention.

Selecting an appropriate K_{OW} *or* K_{OC} *for EqP modeling*

Uncertainties associated with the application of EqP theory to science and regulatory implementation have been examined and discussed [14,27,32]. The present study examines a major component of EqP modeling that significantly affects the development of a sediment PCB benthic injury curve: the selection of an appropriate K_{OW} value to calculate organic carbon–normalized sediment concentrations from aqueous PCB concentrations. Linkov et al. [33] demonstrated small changes in K_{OW} can result in significant differences 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 and 2), selecting an Aroclor-specific K_{OW} value was our principal approach for EqP modeling in the present investigation. The homolog approach used by Fuchsman et al. [19] is found in the *Discussion* section, as is a congener approach; however, neither matches with the Aroclor-based injury data from Tables 1 and 2. The handbook published by Mackay et al. [20] may be one of the most widely cited and respected sources for physical–chemical properties of organic chemicals. Table 3 is a summary of individual K_{OW} values for the 7 Aroclor mixtures reported by Mackay et al. [20]. Log K_{OW} values generally range between 2 and 3 orders of magnitude for each Aroclor (n = 8–13 per Aroclor). Descriptive statistics were calculated and are reported in Table 3 for the nonlogarithm expression of the K_{OW} 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 3). The mean and median K_{OW} 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, as these K_{OW} values are not sampled from a single population. Instead, they were compiled from disparate sources published by different investigators over numerous years using different analytical methods and partitioning techniques (e.g., shake-flask vs slow-stir methods). The median, which dampens the influence of very high and very low values, appears to be a better central tendency estimator for the highly variable Aroclor K_{OW} values reported by Mackay et al. [20]. In our first analysis, the median K_{OW} values and Equation 5 were used in EqP modeling from aqueous PCB concentrations to sediment Aroclor concentrations. We noted that the resulting log K_{OC} is conservative. For example, when using Equation 5 and the median log K_{OW} of

6.11 (1 288 250 L/kg) for Aroclor 1254 found in Table 3, the log K_{OC} is 4.6714 (46 925 L/kg).

Our second analysis used log K_{OC} from the USEPA Estimation Program Interface (EPI) Suite, **<ZAQ;3>**Ver 4.11. The transformation equation

$$\log (K_{OC}) = 0.55313 \log (K_{OW}) + 0.9251 + \text{correction factor} \tag{7}$$

is provided in the **<ZAQ;4>***KOCWIN User's Guide* [34]. The EPI Suite calculation of the Aroclor 1254 log (K_{OC}) is 4.8252 (66 865 L/kg), consistent with, but modestly higher than, the K_{OC} calculated using the median K_{OW} reported in Mackey et al. [20] and using Equation 5.

According to Hawthorne et al. [28], predicted and measured K_{OC} values reported in the literature likely underpredict K_{OC} calculated from measurements of the freely dissolved fraction in "real-world" contaminated sediments that can contain stronger sorbing phases than soil organic carbon, such as coal tar, soot, and possibly so-called black carbon. Therefore, we used a polyparameter linear free energy relationship approach to predict an Aroclor 1254 K_{OC} for coal tar organic carbon based on using the freely dissolved fraction [35; H.P.H. Arp, Norwegian Technical Institute, Oslo, Norway, personal communication]. Average homolog K_{OC} was calculated from individual congener coal tar polyparameter linear free energy relationship K_{OC} values, and the average homolog K_{OC} values were weighted by percent homolog composition (e.g., pentachlorobiphenyl is 59.12% of A1254 [5]) to calculate a coal tar log K_{OC} of 7.5 (31 622 777 L/kg) for

Aroclor 1254.

The K_{OC} selection is the biggest uncertainty in the EqP dose–response model, and the K_{OC} values using the 3 independent methods presented above are different. To build the dose–response relationship, we selected the relatively conservative log K_{OC} value of 4.8252 from the USEPA's EPI Suite. This K_{OC} is the best choice because it is consistent with the available aqueous toxicity data set (i.e., Aroclor measurements of whole unfiltered water containing both colloids and dissolved organic matter). An additional reason to choose this log K_{OC} is that it is supported by the USEPA, resulting in the use of a K_{OC} well below the freely dissolved PCB K_{OC} measured in impacted sediments.

RESULTS

Toxicity of aqueous PCBs to aquatic invertebrates

Our literature search identified 17 individual Aroclor chronic toxicity tests (in 6 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 1 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 for 2 studies that tested eastern oysters. Many exposures began with juvenile or early–life stage organisms. With 1 exception, all exposure scenarios involved flowing water with Aroclor metered in by pump or syringe (Table 1). In the 1 exception [23], static exposure water was renewed every 48 h. Although all experiments used a carrier solvent for the hydrophobic Aroclors, measured PCB concentrations were below median aqueous solubilities reported in Mackay et al. [20]. In all but 1 of the 17 experiments, survival was measured following chronic exposure to Aroclors (Table 1). In that 1 experiment, investigators monitored the number of larval and pupal cases produced by the freshwater midge *T. dissimilis* and stated these endpoints were a "measure of growth and survival." Various reproductive endpoints (e.g., young per initial adult) were measured in 5 of the experiments involving freshwater *D. magna* and *G. pseudolimnaeus*. Growth was measured in 3 experiments as new shell growth in young oysters or as weight of young scud (*G. pseudolimnaeus*) produced by exposed adults.

Aqueous PCB dose–response benthic injury curve

Crustacean survival following chronic Aroclor exposures was the most frequent (14 of 17 experiments) test organism–end point 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. Collectively, the 14 individual toxicity experiments represent a total of 58 paired observations of measured aqueous Aroclor concentrations and survival percentages. 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. The surrogate PCB concentration of 0.05 µg/L (=log –1.30 µg/L) was used for the control treatment concentrations in all but the 1 experiment discussed **<ZAQ;5>**above. We assumed 0% benthic injury for all control treatments. The nonlinear model indicated that aqueous Aroclor concentrations ≥15.6 µg/L were always associated with 100% benthic injury (i.e., 100% mortality).

The $\log_{10}$ expression of aqueous PCB concentrations is shown in Table 2 to facilitate observations of individual values in the dose–response curve (Figure 1) constructed per Equation 3 using the data in Table 2. 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 to 2.08. A Hill slope of 1.0 is typical in dose–response curves. The R^2 for this curve is 0.70.

The dose–response curve in Figure 1 using the left column of Table 2 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 [36]. This same observation has been reported for crustaceans in the literature we reviewed [37]. To quantify this relationship, survival and the number of young per initial adult were examined more closely in the 6 separate experiments reported by Nebeker and Puglisi [37] involving *D. magna* and *G. pseudolimneaus*. The young per initial adult 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 young per initial adult endpoints, total percent injury was calculated as the sum of percent injury values from individual treatments. Then, within each experiment, total percent injury for the survival endpoint was divided into the total percent injury for the young per initial adult endpoint to produce a survival:reproductive effects ratio. The ratios ranged between 0.92 and 1.52, with a mean of 1.25 (n = 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 2 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 recalculated using percent injury values that were adjusted upward by 25% (Table 2, right adjusted column) 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 3.29 µg/L (2.45–4.53 µg/L) compared with 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 1.50 (0.75–2.24) compared with 1.43 (0.78–2.07) for the survival-only curve in Figure 1. The r^2 for the curve in Figure 2, 0.69, is very similar to the survival-only curve (0.70). As seen in Figure 1, aqueous PCB concentrations in Figure 2 that are ≥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 curves for PCB-contaminated sediments using K_{OC} *from EPI Suite 4.1*

Benthic injury dose–response curves were developed for the Aroclor 1254 mixture. We include the limited Aroclor 1248 and 1242 toxicity data into this curve. At this time, it is not appropriate to develop curves for the other Aroclor mixtures (e.g., A1260, A1268) because the chronic aqueous toxicity data from the literature we reviewed (Table 1) are limited to these 3 Aroclors (primarily A1254) and because the paucity of comparative toxicity data renders extrapolation from these 3 Aroclors to other mixtures highly uncertain. Because 69% of the aquatic tests we obtained used A1254 as the test chemical, we focus on that Aroclor.

Table 4 reports the aqueous PCB dose–response information from Table 2 with t 2 inserted columns. One column is the organic carbon–normalized sediment concentrations modeled using EqP and the K_{OC} from Equation 7. The second additional column contains A1254 sediment concentrations expressed as the more familiar milligrams per kilogram dry weight, assuming 1% organic carbon. Data from Table 4 were used to construct a benthic injury dose–response curve in PRISM software for sediments containing A1254. Specifically, the organic carbon–normalized sediment concentrations and the percentage injury from Table 4 were the *X* and *Y* input parameters for Equation 3. This produced the benthic injury dose–response curve for A1254-contaminated sediments shown in Figure 3. Major descriptors for this curve include the EC50 (95% CI) of 222.6 mg/kg OC (163.5-303.0 mg/kg OC), Hill slope (95% CI) of 1.50 (0.74–2.24), r^2 (0.69), and number of points analyzed (n = 58).

Although we primarily model Aroclor 1254, we do provide some help where Aroclor 1248 or 1242 is the predominant Aroclor found in the sediment. For example, we found that the Hill slope (95% CI), R^2 and number of points analyzed are identical for all 3 Aroclors. The EC50 values, however, will decrease with decreasing degree of chlorination. The differences/similarities in EC50 values are driven directly and solely by the relative differences in their respective K_{OC}. For example, when using the EPA EPI Web 4.1, the log K_{OC} values for Aroclor 1254, 1248, and 1242 are 4.8252, 4.4989, and 4.5487, respectively. Hence the K_{OC} values are relatively close, but the user can expect somewhat more toxicity for similar PCB sediment concentrations when the PCB sediment chemistry is predominantly composed of Aroclor 1248 or 1242 when compared with the toxicity found in Aroclor 1254 as per gram of PCB in the sediment at equilibrium, relatively more PCBs would be able to partition to the "freely dissolved" water phase or to the organism.

Once the sediment dose–response curve is created, the PRISM software can create a table of graded *x,y* coordinates, which bracket the highest and lowest *x* values (organic carbon–normalized sediment concentrations) used to build each curve. We used this software feature to create look-up tables (n = 150 points) for A1254 (Table 5) that include the percent benthic injury (95% CI) corresponding to the range of sediment concentrations reported in Table 4.

Table 6 summarizes percent injury (95% CI) corresponding to a hypothetical arithmetic progression of sediment concentrations (mg/kg dry wt) for Aroclor A1254. For this series of sediment concentrations, predicted percent benthic injury in A1254-contaminated sediments would be 23.7%, 44.6%, 70.9%, 87.2%, and 95% for hypothetical sediment concentrations of 1 mg/kg, 2 mg/kg, 4 mg/kg, 8 mg/kg, and 16 mg/kg dry weight of Aroclor 1254, respectively (assuming

1% organic carbon). The predicted levels of injury in Table 6 assume no differences in the relative toxicity of A1254, A1248, and A1242. To the extent that the intrinsic toxicities of A1248 and/or A1242 are different from that of A1254, the predicted levels of injury generated with the EqP approach will be less accurate. However, as discussed, for samples exclusively comprised of Aroclor 1248 or A1242, we would expect somewhat more injury than that found in our 69% Aroclor 1254 PCB sediment PCB mixture model given the same total PCB concentration.

Other EqP choices to find benthic injury dose–response curves for PCB-contaminated sediments

By using the aquatic dose–response database provided in Table 2 and Figure 2, one can select preferred K_{OC} values to determine the PCB dose response. For example the median K_{OW} from Table 3 can be used in Equation 5 to calculate K_{OC} to estimate the sediment concentration for the EqP equation (Equation 4). This K_{OC} is approximately 30% lower and therefore would predict greater injury at the same A1254 concentrations.

The coal tar polyparameter linear free energy relationship approach for finding the K_{OC} for impacted sediments for our aquatic database was discussed previously. This K_{OC} relies on using freely dissolved concentration data from filtered water samples with removal of all colloidal material, resulting in a relatively high log K_{OC} of 7.5. Aquatic concentrations in Tables 1and 2 are from PCB concentrations measured in unfiltered water and therefore cannot be used with the polyparameter linear free energy relationship approach. Nevertheless, other K_{OC}

values may be used to develop new Tables 4, 5, and 6 by applying the dose–response model. However, PCB aqueous concentration measurements need to match the data set to which they are applied.

A better approach may be to determine a site-specific K_{OC}, although obtaining accurate measurements can be challenging. Using site-specific matching unfiltered porewater concentrations and organic carbon–normalized sediment concentrations allows one to calculate a site-specific K_{OC}. Then, using this site-specific K_{OC} and Equation 7 provides a new Table 4 that matches benthic injury and organic carbon–normalized sediment. Next, using Table 4 and the Prism software creates a new Table 5 that provides the aqueous concentration, the newly calculated EqP sediment concentration, and the associated benthic injury.

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 [38–40]. Although ecological risk assessments have typically relied heavily on point estimates for risk thresholds, and natural resource damage assessments more frequently rely on dose–response models, practitioners of both would benefit from a greater use of dose–response information [41]. 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., effects range low/medium, threshold effects levels/probable effects levels, threshold effect concentration/probable effect concentration, apparent effects thresholds, logistic regression [18,42–45] or theoretically via EqP [19,30]. By undertaking a site-specific (i.e., field-derived) EqP PCB sediment study of the Anniston Superfund Site in Alabama (USA), MacDonald et al. [46] calculated a toxicity threshold high range and low range. The former is defined as "the concentrations of contaminants of potential concern . . . or contaminants of potential concern mixtures that corresponded to a 10% reduction in survival, weight, biomass, emergence, or reproduction, compared with 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 porewater allows for an empirical dose response (i.e., reference envelope approach) resulting in a toxicity threshold high range sediment value of 2.08 mg/kg for total PCBs using 42-d *Hyalella azteca* reproduction. When using total homologs rather than total Aroclors, this toxicity threshold high range value gets reduced by approximately 0.5 mg/kg to 1.18 mg/kg and, when using the toxicity threshold low range, to as low as 0.5 mg/kg. Although these values represent a dose response from 1 specific study, they modestly fit our generic dose–response model as provided in Table 5.

Despite drawing PCB toxicity information from disparate literature sources (Table 1), the resulting pattern of dose response appears quite good (Figures 1–3) with reasonable R^2 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 [47]. Consequently, much of this discussion describes the toxicological and physicochemical uncertainties associated with data inputs to the benthic PCB dose–response models in the present article. 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 K_{OW} and K_{OC} values for the EqP model. The *Discussion* section 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 K_{OC} 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. Aroclors 1248 and 1242 represent 10% and 21%, respectively, of the paired observations used to create the dose–response curves. Consequently, predicting percentage benthic injury when other Aroclors are present is problematic. At least 3 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) [19,48,49]. This is likely 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 [50] and Mayer and Ellersieck [51]) must be viewed carefully because they often do not control for factors having substantial effects on comparative toxicity. 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 [36]. This difference in response occurs largely because the 3 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. [23] and Mayer [50]). Other factors such as duration of exposure, temperature, and feeding regime 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 that control for the previously mentioned confounding factors. Mayer [50] reported results of numerous static toxicity tests with A1242 and A1016 conducted with various life stages of *Palaemonetes pugio*. The 96-h LC50 values based on measured water concentrations were virtually identical for the 2 Aroclors. This is perhaps not too surprising given the fact that A1016 at 41.1% and A1242 at 43.7% [52] have similar degrees of chlorination. Ho et al. [22] exposed *Ampelisca abdita* and *Mysidopsis bahia* to A1242 and A1254 under static-renewal conditions. Based on measured water concentrations, 96-h LC50 values indicated that A1242 was 3 times to 4 times more toxic than A1254 to both species. On the other hand, McLeese and Metcalfe [53] reported that 96-h 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 [37] reported that, under static conditions, 96-h LC50 results (measured concentrations) indicated that A1242 was twice as toxic as A1248 to juvenile *G. pseudolimnaeus*. These results with 4 crustacean species suggest that A1242 is more acutely toxic or equally toxic to A1254 and A1248. Differences among the investigations may be the result, in part, of interspecific sensitivities.

We could find only 1 published report [37] 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 8 Aroclors with <24-h-old neonates of *D. magna*. Exposures continued for 21 d. The most toxic mixture was A1248, with a 21-d LC50 (95% CI) of 25 µg/L (21.4–29.2 µg/L) (Figure 4). Overlapping 95% CIs suggested that A1254 and A1260 are as toxic as A1248. The LC50 values and corresponding 95% CIs 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 *D. magna* than these 3 mixtures (Figure 4), mirroring published compilations discussed earlier. Aroclors 1242 and 1232 were about half as toxic as A1248 with

21-d 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 8 Aroclors (Figure 4). The 21-d 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 that 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

Dose–response curves developed in the present investigation are based on 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. [54] exposed 7-d-old *D. magna* for 21 d to 0 µg/L, 0.1 µg/L, 1.5 µg/L, 12 µg/L, and 15 µg/L Aroclor 1254 (measured concentrations) in a flow-through system. The 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, ecological consequences of this altered swimming behavior could result in death. Swimming behavior was not significantly affected in the 0.1 µg/L treatment.

Lehmann et al. [55] exposed adult freshwater clams (*Corbicula fluminea*) to 0 µg/L, 1 µg/L, 10 µg/L, and 100 µg/L Aroclor 1260 for 21 d 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 among the necrotic gonadal tissues likely reflects oxidative damage to lipid membranes. Additional evidence for PCB-induced oxidative stress is the significant alterations of γ-tocopherol and total reduced glutathione in all PCB-exposed clams.

Carnevali et al. [56] also reported PCB adverse effects 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 d 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-d exposure. Exposure to PCB resulted in abnormal arm growth in terms of both gross morphology and microscopic anatomy. Observations included massive cell migration/proliferation, hypertrophic development of celomic canals, rearrangement of differentiated tissues, and accelerated growth of regenerating tissue. The investigators concluded that the developmental anomalies observed were compatible with a pattern of endocrine disruption.

In experiments reported by Ryan et al. [57], fertilized eggs of a marine clam (*Mercenaria mercenaria*) were exposed for 48 h to 0 M, 3.05E-11 M, 3.05E-10 M, 3.05E-9 M, 3.05E-8 M, and 3.05E-7 M Aroclor 1254. Assuming that A1254 has a molecular weight of 327 [20], these nominal molar concentrations would be approximately 0 µg/L, 0.01 µg/L, 0.1 µg/L, 1.0 µg/L, 10 µg/L, 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-h 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 was significantly greater than that in controls (<10% abnormal larvae). We can conclude from the above 4 experiments involving test species from 3 distinct invertebrate phyla (mollusks, echinoderms, arthropods) that 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.

K_{OW} *values for Aroclor mixtures*

Linkov et al. [33] examined uncertainty associated with K_{OW} values for PCBs and the impact of this variation on calculating sediment concentrations protective of human health and the environment. They reported that log K_{OW} 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 1 case study. The monetary implication for sediment cleanup caused by this variation in K_{OW} values was not insignificant ($48 million). Detailed analysis by Linkov et al. [33] led them to conclude that the largest (but not the only) source of variation in K_{OW} values was measurement error. Specifically, they reported 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 K_{OW} values. The alternative slow-stir method for the experimental determination of K_{OW} for highly hydrophobic chemicals such as PCBs may generate more precise and accurate data [58]. To avoid the K_{OW} uncertainty described, one can alternatively measure a site-specific K_{OC} using site porewater and sediment.

K$_{OW}$ *values for PCB homologs*

In this report, we initially used K_{OW} values derived directly from Aroclors because the aqueous toxicity data were based on Aroclors. Fuchsman et al. [19] took an alternative "homolog approach" for calculating Aroclor-specific K_{OW} values whereby they selected 1) the percent composition of homologs for each Aroclor mixture and 2) a K_{OW} value for each homolog group. Using these values, they calculated an Aroclor-specific K_{OW} as the fractional sum of the homolog K_{OW} values as shown in Equation 8

$$K_{OW} - \text{total PCB} = 1/\sum (f\ \text{homolog}\ i / K_{OW}\ \text{homolog}\ i) \qquad (8)$$

where f homolog i is the proportion of homolog group i in a particular Aroclor mixture, K_{OW} 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. [19] selected values reported by DeVoogt and Brinkman [3] for a variety of Aroclors. These values are generally consistent with 5 other sources we identified with respect to identifying the dominant homolog group in each Aroclor mixture (Table 7). For example, all published sources indicate that pentachlorobiphenyl is the dominant homolog group in Aroclor 1254 (Table 7). However, the range of pentachlorobiphenyl in Table 7 among the various sources is not small (45–71%). Slight differences in the chlorination process [3,5,59] as well as manufacturing source (e.g., see A1254, source E in Table 7) 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 monochlorobiphenyls, dichlorobiphenyls, and trichlorobiphenyls (Table 7). At the other extreme, heavily chlorinated mixtures (Aroclors 1260 and 1262) are dominated by hexachlorobiphenyls, heptachlorobiphenyls, and octachlorobiphenyls. Mixtures with intermediate chlorination (Aroclors 1242, 1248, and 1254) are dominated by trichlorobiphenyls, tetrachlorobiphenyls, and pentachlorobiphenyls (Table 7). As noted above, the literature search indicated that these Aroclors with intermediate chlorination were often the most toxic mixtures to invertebrates.

For the second component in the homolog approach, Fuchsman et al. [19] selected K_{OW} values for each homolog group from those published by Mackay et al. [60] and Shiu and Mackay [2]. Table 8 is a summary of K_{OW} values for the 9 homolog groups (n = 3–7 per group) reported in the more recent publication by Mackay et al. [20]. Variation in K_{OW} values among the monochlorobiphenyl through heptachlorobiphenyl homolog groups is much smaller (≈an order of magnitude, coefficient of variation < 100%) compared with the variation in Aroclor K_{OW} values (Table 3). Mean and median K_{OW} values within these 7 homolog groups are generally similar, suggesting normally distributed K_{OW} values. In addition, median K_{OW} values for the monochlorobiphenyl through heptachlorobiphenyl homolog groups from Mackay et al. [20] are similar to values used by Fuchsman et al. [19] (Table 8). However, variations in K_{OW} values for the octachlorobiphenyl and nonachlorobiphenyl homolog groups from Mackay et al. [20] are much larger (coefficient of variation > 100%) than those for the other homolog groups. The K_{OW} values for these 2 homologs used by Fuchsman et al. [19] are larger than the median values from Mackay et al. [20]. The increased variation in these 2 homolog groups may be attributable to experimental error in determining K_{OW} values for highly hydrophobic chemicals, as discussed in Linkov et al. [33]. From a practical standpoint, K_{OW} results for the octachlorobiphenyl and nonachlorobiphenyl homolog groups have minimal impact, because these 2 groups only appear in highly chlorinated Aroclors (i.e., ≥A1260; Table 7).

The K_{OW} values calculated for Aroclor mixtures using the homolog approach are generally greater (except A1248) than the median K_{OW} values from Mackay et al. [20] (Table 3). The EqP modeling with higher K_{OW} values yields higher organic carbon–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 homologs or congeners. However, this is rarely the case, although we address the latter below. The homolog approach has the potential to introduce additional uncertainty associated with the selection of homolog percent composition and homolog K_{OW} values. Given the substantial influence selecting a K_{OW} has on modeling PCB sediment concentrations (see discussion of Linkov et al. [33]), perhaps a more propitious approach would be to focus on the quality of the K_{OW} information when selecting a specific value to use in EqP modeling.

Although the present investigation and that of Fuchsman et al. [19] both 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 2 studies other than the approach to select Aroclor-specific K_{OW} values discussed previously. Firstly, Fuchsman et al. [19] used acute toxicity information exclusively for A1254, then applied an acute:chronic ratio to produce a final chronic value. The acute toxicity information was almost exclusively 96-h LC50 values, whereas the present investigation used chronic toxicity data. Different modes of toxicity are likely operating in the 2 data sets (narcosis vs non-dioxin-like toxicity). Additionally, many of their acute studies did not measure actual exposure concentrations, and the reported nominal concentrations often exceeded the aqueous solubility of PCBs. The present investigation only used chronic toxicity data in which aqueous exposure concentrations were measured. Secondly, the present investigation also considered sublethal biological responses in 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. [19] used the K_{OW} as the K_{OC} value, as shown in Bucheli and Gustafsson [61], claiming that such equality is a conservative estimate of K_{OC}; but the K_{OW}–K_{OC} transformation equations shown earlier indicate otherwise. Perhaps the most significant difference between the present investigation and Fuchsman et al. [19] is that the latter reports a single sediment quality benchmark for PCBs, whereas we developed a numerical dose–response model generating a continuum of predictions.

K_{OC} *values using congeners*

If congener data are available, one can directly find the K_{OC} without using either the median K_{OW} value (Table 3) or a log K_{OW} to log K_{OC} transformation (e.g., Equation 5, 6, or 7) by using the calibrated quantitative structure–activity relationship model

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

where N_{CL} is the total number of chlorines and $N_{orthoCL}$ is the number of orthochlorines [28,62]. Whether one uses the K_{OC} for reference sediments or impacted sediments depends on the contamination history of the site. Knowledge of sorption of PCBs or other hydrophobic contaminants from the location can help determine whether the organic carbon sorbs similarly to natural or impacted organic matter. Afterward, much like after finding a site-specific K_{OC}, the user can calculate the organic carbon–normalized chronic sediment concentration from the sample-specific porewater value using Equation 4.

Another issue concerns how the lab measures the aqueous samples. One must take into account the colloidal material if unfiltered or if this aqueous PCB measure is from a filtered freely dissolved sample. The quantitative structure–activity relationship (Equation 9), as well as other equations for impacted sediments [28,62], were generally taken from the freely dissolved concentration.

Most other data, such as our data set, used nonimpacted sediments and water samples that were unfiltered or incompletely filtered, thus representing the total (particulate and dissolved) PCBs.

Recommended applications

The preceding discussion highlights important uncertainties that could affect predictions of benthic injury caused by PCB-contaminated sediments using the EqP modeling approach described in the present study. 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 [13,19,31]. As discussed in Burgess et al. [30], the EqP approach does not consider effects of co-occurring contaminants or the potential for trophic transfer. Benthic communities contain multiple trophic levels [63], which may not be protected by an EqP approach. On a case-specific basis, users 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 those associated with the comparative toxicity of different Aroclor mixtures to invertebrates; the acquired resistance to PCBs in laboratory animals used in 1970s toxicity studies; and the variation in, and methods used to calculate, Aroclor K_{OW} and/or K_{OC} values. We believe the latter is the most important uncertainty, and we address this throughout the present study.

We present the following general guidance for recommended application of the benthic injury curves when applied to field data that potentially report sediment PCB concentrations as mid-weight Aroclors.

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

First, if 1 or more of A1242, A1248, or A1254 are detected in sediment, calculate an organic carbon–normalized concentration for each detected result in a sample. Ignore results when flagged as less than the detection limit. Although this is less protective than other alternatives (e.g., assuming one-half detection limit), it avoids the other potentially more serious bias that could result from reporting of high detection limits. Second, sum the detected organic carbon–normalized concentrations of the Aroclors from step 1 to obtain a "total Aroclors" organic carbon–normalized expression for each sediment sample. Third, find the "total Aroclors" organic carbon–normalized concentration calculated in the second step in the sediment look-up table for A1254 (Table 5). Use the mean value corresponding to the "total Aroclors" concentration for the prediction of percentage benthic injury. Some may prefer to use the upper 95% CI value based on uncertainties discussed and the demonstrated effects of PCBs at very low concentrations on biologically important endpoints other than survival and reproduction, such as behavior, early–life stage growth, and development in 3 invertebrate phyla (see previous text in the section *Discussion*). Using the look-up table for A1254 is recommended because A1254 constitutes most (≈70%) of the data in the aqueous dose–response curves (Figures 2 and 3). 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" organic carbon–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). Aroclor 1260 also may be included in the group because it was as toxic as A1254 and A1248 in a chronic life cycle experiment with an aquatic crustacean [36] and, similar to A1254, has very profound and biologically significant adverse effects on 3 distinct invertebrate phyla (mollusks, echinoderms, arthropods) at very low aqueous concentrations [54–57]. Predicting benthic injury from other Aroclors is not recommended at this time since sufficient and appropriate dose–response and comparative toxicity information are not available.

The above approach 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% that matches the value the USEPA [64] uses 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.

This step-wise approach is not recommended if an Aroclor other than

A1242, A1248, or A1254 is the only PCB mixture detected in a sample.

SUMMARY AND OUTSTANDING ISSUES

The present investigation reviewed the aqueous PCB toxicity literature and used EqP modeling to generate an Aroclor-specific sediment dose–response curve (and associated look-up table) for estimating benthic injury in PCB-contaminated sediments. We used a K_{OW} to K_{OC} transformation equation, supported by the USEPA, that reflects an undissolved aqueous PCB concentration but matches that used by literature sources to determine PCB toxicity to invertebrates. With that, we believe Tables 5 and 6 are well-founded tools to determine likely sediment toxicity. Using familiar PCB sediment concentrations, one may predict benthic injury, as shown in Table 6. Although this approach remains viable, we note the following 5 outstanding issues that remain. 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 literature Aroclor K_{OW} and K_{OC} values with the goal of reducing source variation and selecting the most accurate K_{OW} and/or K_{OC} value(s). We recommend calculating a site-specific K_{OC}. One way to do this is by measuring the sediment and porewater distribution of specific PCB congeners or homologs with passive sampling, as in Hawthorne et al. [28; H.P.H. Arp, Norwegian Technical Institute, Oslo, Norway, personal communication].

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

Experimentally determine the comparative toxicity of 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 are most likely causing toxicity through the non-dioxin-like mode of action. Although a congener-specific equation (Equation 9) is found in the literature, we choose not to endorse it as it can only provide an unreasonably high K_{OC} given our aquatic database.

Recent studies [65,66] have used the 2-carbon model to note that thermoresistant black carbon is properly taken into account when calculating the sediment–water partitioning constant, K_D. Despite the possibility of the 1-carbon model (Equation 4) underpredicting K_{OC}, both Hawthorne et al. [28] and Martinez et al. [67] found no improvement when using the 2-carbon model to predict the sediment porewater. Hence, we currently choose to not use the additional black carbon measure in our model.

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Data Availability—Data, associated metadata, and calculation tools are available from the corresponding author (Ken.Finkelstein@NOAA.gov).

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Figure 1. Benthic injury curve (survival) for measured aqueous concentrations of polychlorinated biphenyls (PCBs; A1254, A1248, A1242). Dashed lines are 95% confidence interval around the mean (solid line). R^2 = 0.71, Hill slope = 1.43

Figure 2. Benthic injury curve (adjusted for reproductive effects) for measured aqueous concentrations of polychlorinated biphenyls (PCBs; A1254, A1248, A1242). Dashed lines are 95% confidence interval around the mean (solid line). R^2 = 0.69, Hill slope = 1.50.

Figure 3. Benthic injury curve for equilibrium partitioning–modeled, A1254-contaminated sediments using Table 4. Dashed lines are 95% confidence interval around the mean. R^2 = 0.69 Hill slope = 1.49. oc = organic carbon.

Figure 4. Median lethal concentrations (LC50s) at 21 d (measured polychlorinated biphenyl concentrations) for *Daphnia magna* in static aqueous exposures to 8 Aroclor mixtures as reported by Nebeker and Puglisi [36]. Error bars = 95% confidence interval.

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Table 1. Summary of individual nonacute experiments in the literature reporting measured aqueous polychlorinated biphenyl dose–response information for invertebrates

Test species [a]	Life stage, length (cm)	Aroclor	Exposure scenario	Measured exposure concentration (µg/L)	Biological test endpoints	Ref.
Pink shrimp	Juvenile, 2.5–3.8	1254	15 d; FT	0.0–19.0	Survival	[68]
Pink shrimp	Juvenile, 4.2–7.2	1254	17–32 d; FT	0.0–3.1	Survival	[68]
Pink shrimp	6.6–9.0	1254	53 d; FT	0.0–4.3	Survival	[68]
Pink shrimp	7.6–8.5	1254	18 d; FT	0.0–4.0	Survival	[68]
Pink shrimp	Adult, 9.5–12.5	1254	35 d; FT	0.0–3.5	Survival	[68]
Pink shrimp	Juvenile, 4–6	1254	20 d; FT	0.0–3.8	Survival	[25]
Grass shrimp	NR	1254	7 d; FT	0.0–9.1	Survival	[69]
Grass shrimp	NR	1254	16 d; FT	0.0–12.5	Survival	[69]
Grass shrimp	Larvae	1254	23–26 d; SR	0.0–15.6	Survival	[23]
Eastern oyster	Young, 2.6–5.7	1254	210 d; FT	0.0–0.64	Survival, growth	[70]
Eastern oyster	Young, 3.1–8.3	1254	168 d; FT	0.0–3.9	Survival, growth	[70]
Water flea	<24 h Neonates	1248	14 d; FT	0.0–7.5	Survival, reproduction	[37]

Water flea	<24 h Neonates	1254	14 d; FT	0.0–9.0	Survival, reproduction	[37]
Water flea	<24 h Neonates	1254	21 d; FT	0.0–33	Survival, reproduction	[37]
Amphipods	Juvenile	1242	56 d; FT	0.0–234	Survival, reproduction	[37]
Amphipods	Juvenile	1248	56 d; FT	0.0–18.0	Survival, reproduction, growth	[37]
Midge	1st to 4th instars	1254	NR: FT	0.0–33	Number of larval and pupal cases	[37]

[a] Pink shrimp, *Penaeus duorarum*; grass shrimp, *Palaemonetes pugio*; eastern oyster, *Crassostrea virginica*; water flea, *Daphnia magna*; amphipod, *Gammarus*

midge, *Tanytarsus dissimilis*.

FT = flow through; NR = not reported; SR = static renewal.

Table 2. Paired observations (n = 58) of measured aqueous PCB concentrations, percent benthic injury (survival), and percent benthic injury adjusted (for repr

Log10 measured aqueous PCB conc. (µg/L)	Measured aqueous PCB conc. (µg/L)	Benthic injury[b] (%)	Benthic injury adjusted[c] (%)	Source notes
–1.3010	0.05	0	0	A1254, Juvenile *Penaeus duorarum*, 15-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	0	0	A1254, *P. duorarum*, 17-d to 32-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	0	0	A1254, *P. duorarum*, 53-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	0	0	A1254, *P. duorarum*, 18-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	0	0	A1254, Adult *duorarum*, 35-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	0	0	A1254, *duorarum*, 20-d survival, controls, Duke et al. [25]
–1.3010	0.05	0	0	A1254, *Palaemonetes pugio*, 7-d survival, controls, Nimmo et al. [69]
–1.3010	0.05	0	0	A1254, *P. pugio*, 16-d survival, controls, Nimmo et al. [69]
–1.3010	0.05	0	0	A1248, *Daphnia magna*, 14-d survival, controls, Nebeker and Puglisi [37]

–1.3010	0.05	0	0	A1254, *D. magna*, 14-d survival, controls, Nebeker and Puglisi [37]
–1.3010	0.05	0	0	A1254, *D. magna*, 21-d survival, controls, Nebeker and Puglisi [37]
–1.3010	0.05	0	0	A1242, *Gammarus pseudolimnaeus*, 56-d survival, controls, Nebeker and Puglisi [37]
–1.3010	0.05	0	0	A1248, *G. pseudolimnaeus*, 56-d survival, controls, Nebeker and Puglisi [37]
–1.0000	0.10	0	0	A1254, *P. pugio*, 23-d to 26-d survival, controls, Roesijadi et al. [23]
–1.0000	0.10	7	9	A1254, *P. pugio*, 23-d to 26-d survival, Roesijadi et al. [23]
–1.0000	0.10	0	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.7696	0.17	4	5	A1254, *P. pugio*, 7-d survival, Nimmo et al. [69]
–0.7447	0.18	0	0	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
–0.5850	0.26	0	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.4318	0.37	0	0	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.3468	0.45	14	17	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
–0.2676	0.54	0	0	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
–0.2441	0.57	20	25	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]

–0.2076	0.62	0	0	A1254, *P. pugio*, 7-d survival, Nimmo et al. [69]
–0.0655	0.86	0	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.0362	0.92	0	0	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.0269	0.94	40	50	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
0.0792	1.20	13	16	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
0.1139	1.30	20	25	A1254, *P. pugio*, 16-d survival, Nimmo et al. [69]
0.2304	1.70	0	0	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.3424	2.20	0	0	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.3802	2.40	64	79	A1254, *P. duorarum*, 17-d to 32-d survival, Nimmo et al. [68]
0.3979	2.50	0	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.4472	2.80	0	0	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.4914	3.10	79	99	A1254, *P. duorarum*, 17-d to 32-d survival, Nimmo et al. [68]
0.5051	3.20	10	13	A1254, *P. pugio*, 23-d to 26-d survival, Roesijadi et al. [23]
0.5441	3.50	46	57	A1254, Adult *duorarum*, 35-d survival, Nimmo et al. [68]
0.5441	3.50	100	100	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
0.5798	3.80	72	90	A1254, *P. duorarum*, 20-d survival, Duke et al. [25]

0.5798	3.80	100	100	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.6021	4.00	35	44	A1254, *P. duorarum*, 18-d survival, Nimmo et al. [68]
0.6021	4.00	27	33	A1254, *P. pugio*, 16-d survival, Nimmo et al. [69]
0.6335	4.30	77	96	A1254, *P. duorarum*, 53-d survival, Nimmo et al. [68]
0.7076	5.10	17	21	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.8751	7.50	92	100	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.9395	8.70	0	0	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.9542	9.00	100	100	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.9542	9.00	100	100	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
0.9590	9.10	58	73	A1254, *P. pugio*, 7-d survival, Nimmo et al. [69]
0.9731	9.40	89	100	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
1.0969	12.50	40	50	A1254, *P. pugio*, 16-d survival, Nimmo et al. [69]
1.1931	15.60	100	100	A1254, *P. pugio*, 23-d to 26-d survival, Roesijadi et al. [23]
1.2553	18.00	100	100	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
1.2788	19.00	100	100	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
1.4150	26.00	100	100	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]

1.5185	33.00	100	100	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
1.9085	81.00	100	100	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
2.3692	234.00	100	100	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]

[a] The surrogate concentration of 0.05 µg/L was used for control treatments.

[b] Percent benthic injury based on the survival endpoint only. Same values as in Table 4.

[c] Percentage benthic injury adjusted upward by 25% based on the greater sensitivity of the reproduction endpoint.

PCB = polychlorinated biphenyl.

Table 3. Individual log K_{OW} values for 7 Aroclor mixtures reported by Mackay et al. [20][a]

	A1221		A1232		A1016		A1242		A1248		A1254		A1260	
K_{OW} values	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}
	2.78	603	3.18	1514	3.48	3020	0.70	5	5.60	398 107	4.08	12 023	4.34	21 878
	2.80	631	3.20	1585	4.30	19 953	3.54	3467	5.75	562 341	4.08	12 023	6.00	1 000 000
	2.81	646	3.23	1698	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 K_{OW}		12 357		35 234		260 886		273 280		1 052 762		3 405 454		8 400 277
SD		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 K_{OW}		12 023		30 200		204 174		194 984		1 129 463		1 288 250		6 008 543
Fuchsman et	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

al. [19] [b]

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[a] Descriptive statistics are based on the nonlogarithm expressions of the K_{OW} values.

[b] Log K_{OW} values for Aroclors A1242, A1248, 1254, and A1260 are those reported by Fuchsman et al. [19] using the homolog approach (see text for explanatio

K_{OW} values for Aroclors A1221, A1232, and A1026 were calculated per the homolog approach described in Fuchsman et al. [19] using the homolog log K_{OW} va

the homolog proportion by weight from the reference they cite [3]. The homolog approach for A1221 and A1232 used the log K_{OW} for biphenyl (3.9) from Mac

K_{OW} = octanol–water partition coefficient; SD = standard deviation; *CV* = coefficient of variation.

Table 4. Paired observations (n = 58) of A1254 sediment concentrations and percent benthic injury adjusted (for reproductive effects)[a]

Log10 measured aqueous PCB conc. (µg/L)	Measured aqueous PCB conc. (µg/L)	A1254 in sediment (mg/kg OC)	A1254 in sediment[b] (mg/kg)	Benthic injury adjusted[c] (%)	Source notes
–1.3010	0.05	3.3	0.03	0	A1254, Juvenile *Penaeus duorarum*, 15-d survival, controls, Nimmo et al. [6
–1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 17-d to 32-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 53-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 18-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	3.3	0.03	0	A1254, Adult *P. duorarum*, 35-d survival, controls, Nimmo et al. [68]
–1.3010	0.05	3.3	0.03	0	A1254, *P. duorarum*, 20-d survival, controls, Duke et al. [68]
–1.3010	0.05	3.3	0.03	0	A1254, *Palaemonetes pugio*, 7-d survival, controls, Nimmo et al. [69]
–1.3010	0.05	3.3	0.03	0	A1254, *P. pugio*, 16-d survival, controls, Nimmo et al. [69]
–1.3010	0.05	3.3	0.03	0	A1248, *Daphnia magna*, 14-d survival, controls, Nebeker and Puglisi [37]
–1.3010	0.05	3.3	0.03	0	A1254, *D. magna*, 14-d survival, controls, Nebeker and Puglisi [37]
–1.3010	0.05	3.3	0.03	0	A1254, *D. magna*, 21-d survival, controls, Nebeker and Puglisi [37]
–1.3010	0.05	3.3	0.03	0	A1242, *Gammarus pseudolimnaeus*, 56-d survival, controls, Nebeker and Puglis
–1.3010	0.05	3.3	0.03	0	A1248, *G. pseudolimnaeus*, 56-d survival, controls, Nebeker and Puglisi [3
–1.0000	0.10	6.7	0.07	0	A1254, *P. pugio*, 23-d to 26-d survival, controls, Roesijadi et al. [23]
–1.0000	0.10	6.7	0.07	9	A1254, *P. pugio*, 23-d to 26-d survival, Roesijadi et al. [23]

–1.0000	0.10	6.7	0.07	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.7696	0.17	11.4	0.11	5	A1254, *P. pugio*, 7-d survival, Nimmo et al. [69]
–0.7447	0.18	12.0	0.12	0	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
–0.5850	0.26	17.4	0.17	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.4318	0.37	24.7	0.25	0	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.3468	0.45	30.1	0.30	17	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
–0.2676	0.54	36.1	0.36	0	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
–0.2441	0.57	38.1	0.38	25	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
–0.2076	0.62	41.5	0.41	0	A1254, *P. pugio*, 7-d survival, Nimmo et al. [69]
–0.0655	0.86	57.5	0.58	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.0362	0.92	61.5	0.62	0	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
–0.0269	0.94	62.9	0.63	50	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
0.0792	1.20	80.2	0.80	16	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
0.1139	1.30	86.9	0.87	25	A1254, *P. pugio*, 16-d survival, Nimmo et al. [68]
0.2304	1.70	113.7	1.14	0	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.3424	2.20	147.1	1.47	0	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.3802	2.40	160.5	1.60	79	A1254, *P. duorarum*, 17-d to 32-d survival, Nimmo et al. [68]
0.3979	2.50	167.2	1.67	0	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.4472	2.80	187.2	1.87	0	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.4914	3.10	207.3	2.07	99	A1254, *P. duorarum*, 17-d to 32-d survival, Nimmo et al. [68]
0.5051	3.20	214.0	2.14	13	A1254, *P. pugio*, 23-d to 26-d survival, Roesijadi et al. [23]
0.5441	3.50	234.0	2.34	57	A1254, Adult *P. duorarum*, 35-d survival, Nimmo et al. [68]

0.5441	3.50	234.0	2.34	100	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
0.5798	3.80	254.1	2.54	90	A1254, *P. duorarum*, 20-d survival, Duke et al. [68]
0.5798	3.80	254.1	2.54	100	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.6021	4.00	267.5	2.67	44	A1254, *P. duorarum*, 18-d survival, Nimmo et al. [68]
0.6021	4.00	267.5	2.67	33	A1254, *P. pugio*, 16-d survival, Nimmo et al. [69]
0.6335	4.30	287.5	2.88	96	A1254, *duorarum*, 53-d survival, Nimmo et al. [68]
0.7076	5.10	341.0	3.41	21	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.8751	7.50	501.5	5.01	100	A1248, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.9395	8.70	581.7	5.82	0	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
0.9542	9.00	601.8	6.02	100	A1254, *D. magna*, 14-d survival, Nebeker and Puglisi [37]
0.9542	9.00	601.8	6.02	100	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
0.9590	9.10	608.5	6.08	73	A1254, *P. pugio*, 7-d survival, Nimmo et al. [69]
0.9731	9.40	628.5	6.29	100	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
1.0969	12.50	835.8	8.36	50	A1254, *P. pugio*, 16-d survival, Nimmo et al. [69]
1.1931	15.60	1043.1	10.43	100	A1254, *P. pugio*, 23-d to 26-d survival, Roesijadi et al. [23]
1.2553	18.00	1203.6	12.04	100	A1248, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
1.2788	19.00	1270.4	12.70	100	A1254, Juvenile *P. duorarum*, 15-d survival, Nimmo et al. [68]
1.4150	26.00	1738.5	17.38	100	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
1.5185	33.00	2206.6	22.07	100	A1254, *D. magna*, 21-d survival, Nebeker and Puglisi [37]
1.9085	81.00	5416.1	54.16	100	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]
2.3692	234.00	15 646.5	156.46	100	A1242, *G. pseudolimnaeus*, 56-d survival, Nebeker and Puglisi [37]

[a] Sediment concentrations (mg/kg OC and mg/kg using 1% organic carbon) predicted via equilibrium partitioning using measured aqueous polychlorinated bipl

concentrations from Table 2 and K_{OC} from EPI Web, Ver 4.1 (using Equation 7 to obtain 66.865 L/kg for K_{OC} or 4.8252 for log K_{OC})

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

[c] Percent benthic injury adjusted upward by 25% based on the greater sensitivity of the reproduction end point.

K_{OC} = water–organic carbon partition coefficient; PCB = polychlorinated biphenyl; OC = organic carbon.

Table 5. Look-up table for predicting percent benthic injury corresponding to a range of A1254 concentrations in sediment using the data from Table 4 and the software (Equation 3)

Log10 A1254 sediment conc. (mg/kg-oc)	A1254 sediment conc. (mg/kg OC)	A1254 sediment conc.[a] (mg/kg)	Benthic injury (%)	Lower 95% CI
0.519	3.30	0.03	0.20	–0.4
0.543	3.49	0.03	0.21	–0.4
0.568	3.70	0.04	0.23	–0.5
0.593	3.91	0.04	0.25	–0.5
0.617	4.14	0.04	0.27	–0.5
0.642	4.38	0.04	0.30	–0.6
0.667	4.64	0.05	0.33	–0.6
0.691	4.91	0.05	0.35	–0.6
0.716	5.20	0.05	0.38	–0.7
0.741	5.50	0.06	0.42	–0.7
0.765	5.82	0.06	0.46	–0.8

0.790	6.16	0.06	0.50	–0.8
0.815	6.52	0.07	0.54	–0.9
0.839	6.91	0.07	0.59	–0.9
0.864	7.31	0.07	0.64	–1.0
0.889	7.74	0.08	0.69	–1.0
0.913	8.19	0.08	0.75	–1.1
0.938	8.67	0.09	0.82	–1.2
0.963	9.17	0.09	0.89	–1.2
0.987	9.71	0.10	0.97	–1.3
1.012	10.28	0.10	1.05	–1.3
1.037	10.88	0.11	1.14	–1.4
1.061	11.51	0.12	1.24	–1.5
1.086	12.19	0.12	1.35	–1.6
1.111	12.90	0.13	1.47	–1.6
1.135	13.65	0.14	1.59	–1.7
1.160	14.45	0.14	1.73	–1.8

1.185	15.30	0.15	1.88	–1.9
1.209	16.19	0.16	2.04	–1.9
1.234	17.14	0.17	2.22	–2.0
1.259	18.14	0.18	2.41	–2.1
1.283	19.20	0.19	2.62	–2.1
1.308	20.32	0.20	2.84	–2.2
1.333	21.51	0.22	3.08	–2.2
1.357	22.77	0.23	3.34	–2.3
1.382	24.10	0.24	3.63	–2.3
1.407	25.51	0.26	3.93	–2.3
1.431	27.00	0.27	4.27	–2.4
1.456	28.58	0.29	4.62	–2.4
1.481	30.25	0.30	5.01	–2.3
1.505	32.01	0.32	5.43	–2.3
1.530	33.88	0.34	5.88	–2.2
1.555	35.87	0.36	6.36	–2.1

1.579	37.96	0.38	6.88	–2.0
1.604	40.18	0.40	7.44	–1.8
1.629	42.53	0.43	8.05	–1.6
1.653	45.01	0.45	8.69	–1.4
1.678	47.65	0.48	9.38	–1.1
1.703	50.43	0.50	10.13	–0.7
1.727	53.38	0.53	10.92	–0.3
1.752	56.50	0.56	11.77	0.2
1.777	59.80	0.60	12.67	0.7
1.801	63.30	0.63	13.64	1.4
1.826	67.00	0.67	14.66	2.1
1.851	70.91	0.71	15.75	2.9
1.875	75.06	0.75	16.90	3.8
1.900	79.44	0.79	18.11	4.9
1.925	84.09	0.84	19.40	6.0
1.949	89.00	0.89	20.75	7.2

1.974	94.20	0.94	22.17	8.6
1.999	99.71	1.00	23.66	10.0
2.023	105.54	1.06	25.22	11.6
2.048	111.71	1.12	26.84	13.3
2.073	118.24	1.18	28.53	15.1
2.097	125.15	1.25	30.28	17.0
2.122	132.46	1.32	32.09	19.0
2.147	140.20	1.40	33.95	21.0
2.171	148.40	1.48	35.87	23.2
2.196	157.07	1.57	37.83	25.4
2.221	166.25	1.66	39.84	27.6
2.245	175.97	1.76	41.87	29.9
2.270	186.26	1.86	43.94	32.2
2.295	197.14	1.97	46.02	34.5
2.319	208.67	2.09	48.13	36.7
2.344	220.86	2.21	50.23	38.9

2.369	233.77	2.34	52.34	41.0
2.393	247.44	2.47	54.44	43.1
2.418	261.90	2.62	56.52	45.1
2.443	277.21	2.77	58.58	47.1
2.467	293.41	2.93	60.61	48.9
2.492	310.56	3.11	62.60	50.8
2.517	328.71	3.29	64.56	52.5
2.541	347.93	3.48	66.46	54.3
2.566	368.26	3.68	68.31	55.9
2.591	389.79	3.90	70.11	57.6
2.615	412.57	4.13	71.85	59.2
2.640	436.68	4.37	73.52	60.8
2.665	462.21	4.62	75.13	62.3
2.690	489.23	4.89	76.67	63.8
2.714	517.82	5.18	78.15	65.3
2.739	548.09	5.48	79.55	66.8

2.764	580.12	5.80	80.89	68.3
2.788	614.03	6.14	82.16	69.7
2.813	649.92	6.50	83.36	71.1
2.838	687.91	6.88	84.50	72.4
2.862	728.12	7.28	85.57	73.7
2.887	770.68	7.71	86.58	75.0
2.912	815.72	8.16	87.53	76.3
2.936	863.40	8.63	88.42	77.5
2.961	913.87	9.14	89.26	78.6
2.986	967.28	9.67	90.04	79.8
3.010	1023.82	10.24	90.77	80.8
3.035	1083.66	10.84	91.45	81.9
3.060	1147.00	11.47	92.09	82.9
3.084	1214.05	12.14	92.68	83.9
3.109	1285.01	12.85	93.24	84.8
3.134	1360.12	13.60	93.75	85.7

3.158	1439.62	14.40	94.22	86.5
3.183	1523.76	15.24	94.67	87.3
3.208	1612.82	16.13	95.08	88.1
3.232	1707.10	17.07	95.46	88.8
3.257	1806.87	18.07	95.81	89.5
3.282	1912.49	19.12	96.13	90.1
3.306	2024.27	20.24	96.44	90.7
3.331	2142.59	21.43	96.72	91.3
3.356	2267.83	22.68	96.97	91.9
3.380	2400.38	24.00	97.21	92.4
3.405	2540.68	25.41	97.43	92.9
3.430	2689.19	26.89	97.63	93.3
3.454	2846.37	28.46	97.82	93.8
3.479	3012.74	30.13	97.99	94.2
3.504	3188.83	31.89	98.15	94.6
3.528	3375.22	33.75	98.30	94.9

3.553	3572.51	35.73	98.43	95.3
3.578	3781.32	37.81	98.56	95.6
3.602	4002.34	40.02	98.67	95.9
3.627	4236.27	42.36	98.78	96.2
3.652	4483.88	44.84	98.88	96.4
3.676	4745.97	47.46	98.97	96.7
3.701	5023.37	50.23	99.05	96.9
3.726	5316.99	53.17	99.13	97.1
3.750	5627.77	56.28	99.20	97.3
3.775	5956.72	59.57	99.26	97.5
3.800	6304.88	63.05	99.32	97.7
3.824	6673.40	66.73	99.38	97.8
3.849	7063.47	70.63	99.43	98.0
3.874	7476.32	74.76	99.47	98.1
3.898	7913.31	79.13	99.51	98.2
3.923	8375.85	83.76	99.55	98.4

3.948	8865.41	88.65	99.59	98.5
3.972	9383.61	93.84	99.62	98.6
3.997	9932.08	99.32	99.65	98.7
4.022	10 512.60	105.13	99.68	98.8
4.046	11 127.07	111.27	99.71	98.9
4.071	11 777.44	117.77	99.73	98.9
4.096	12 465.85	124.66	99.75	99.0
4.120	13 194.47	131.94	99.77	99.1
4.145	13 965.68	139.66	99.79	99.2
4.170	14 781.99	147.82	99.81	99.2
4.194	15 645.99	156.46	99.82	99.3

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

CI = confidence interval; OC = organic carbon.

Table 6. Comparison of benthic injury (95% CI) estimates for A1254 for a hypothetical arithmetic progression of sediment concentrations using the data from Ta

Sediment concentration (mg/kg dry wt)	A1254		
	Benthic injury (%)	Lower 95% CI	Upp
1	23.7	10.1	
2	46.6	35.0	
4	70.9	58.3	
8	87.2	75.8	
16	95.0	88.0	

CI = confidence interval.

Table 7. **<ZAQ;9>**Percent homolog composition, by weight, in 8 Aroclor mixtures as reported by 6 literature sources[a]

Aroclor	Source	Homolog groups									
		Biphenyl	Monochloro-	Dichloro-	Trichloro-	Tetrachloro-	Pentachloro-	Hexachloro-	Heptachloro-	Octachloro-	Nonachloro-
A1221											
	A	11	51	32	4	2	0.5				
	B	7	51	38	3						
	C	10	50	35	4	1					
	D		65.5	29.7	4.8						
	E		60.06	33.38	4.21	1.15	1.23				
A1232											
	B	6	26	29	24	15	0.5				
	C		26	29	24	15					
	D		31.3	23.7	23.4	15.7	5.8				
	E		27.55	26.83	25.64	10.58	9.39	0.21	0.03		

A1016									
	A	<0.1	1	20	57	21	1	<0.1	
	C		2	19	57	22			
	D			21.2	51.5	27.3			
	E		0.7	17.53	54.67	22.07	5.07		
A1242									
	A	<0.1	1	16	49	25	8	1	<0.1
	B		1	17	40	32	10	0.5	
	C		1	13	45	31	10		
	D			14.7	46	30.6	8.7		
	E		0.75	15.04	44.91	20.16	18.85	0.31	
	F			4	39	42	14		
A1248									
	A	<0.1	<0.1	0.5	1	21	48	23	6
	B			1	23	50	20	1	
	C			1	21	49	27	2	

	D			20.9	60.3	18.1	0.8			
	E	0.07	1.55	21.27	32.77	42.92	1.64	0.02		
A1254										
	B				16	60	23	1		
	C			1	15	53	26	4		
	D			1.8	17.1	49.3	27.8	3.9		
	E[a]	0.02	0.09	0.39	4.86	71.44	21.97	1.36		0.04
	E[b]		0.24	1.26	10.25	59.12	26.76	2.66	0.04	0.04
	F			0.5	36	45	18	1		
A1260										
	B					12	46	36	6	
	C					12	42	38	7	1
	D					9.2	46.9	36.9	6.3	0.7
	E	0.02	0.08	0.21	0.35	8.74	43.35	38.54	8.27	0.7
A1262										
	D					4.2	30.9	45.8	17.7	1.3

E	0.02	0.27	0.98	0.49	3.35	26.43	48.48	19.69	1.65

[a]Sources: A = Mieure et al. [71] as cited in US Environmental Protection Agency [4]; B = Webb and McCall [72] as cited in US Environmental Protection Agency [4]; C = DeVoogt and Brinkman [3]; D = Frame e

Toxic Substances and Disease Registry [5]; F = Hirwe et al. [73]. E[a] = Monsanto lot from abnormal late production (1974–1977); E[b] = General Electric lot.

Table 8. Individual, mean, and median log K_{OW} values for 9 homolog groups reported by Mackay et al. [20][a]

	Monochlorobiphenyl		Dichlorobiphenyl		Trichlorobiphenyl		Tetrachlorobiphenyl		Pentachlorobiphenyl		Hexachlorobipheny		Heptachlorobiphenyl		Octachlorobipheny		Nonachlorobiphenyl	
	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}	Log K_{OW}	K_{OW}
	4.3	19 953	4.9	79 433	5.5	316 228	5.6	398,107	6.2	1 584 893	6.7	5 011 872	6.7	5 011 872	7.1	12 589 254	7.2	15 848 932
	4.5	31 623	5.1	125893	5.5	316 228	5.9	794 328	6.3	1 995 262	6.7	5 011 872	7	10 000 000	7.5	31 622 777	7.9	79 432 823
	4.6	39 811	5.1	125 893	5.53	338 844	6.35	2 238 721	6.33	2 137 962	6.8	6 309 573	7.1	12 589 254	8.55	354 813 389	8.16	144 543 977
	4.6	45 709	5.13	134 896	5.76	575 440	6.5	3 162 278	6.4	2 511 886	7	10 000 000					9.14	1 380 384 265
	4.7	50 119	5.19	154 882	5.8	630 957			6.5	3 162 278	7.3	19 952 623						
	4.73	53 703	5.3	199 526	5.9	794 328			6.6	3 981 072								
									6.85	7 079 458								
Mean K_{OW}		40 153		136 754		495 338		1 648 359		3 207 544		9 257 188		9 200 375		133 008 473		405 052 499
SD		12 607		39 482		201 423		1 282 312		1 885 147		6 318 187		3 851 458		192 324 295		652 340 487
CV		31%		29%		41%		78%		59%		68%		42%		145%		161%
n		6		6		6		4		7		5		3		3		4
Median K_{OW}		42 760		130 394		457 142		1 516 525		2 511 886		6 309 573		10 000 000		31 622 777		111 988 400
Fuchsman et al. [19][b]	4.64	43 652	5.12	131 826	5.62	416 869	6.04	1 096 478	6.49	3 090 295	6.84	6 918 310	6.98	9 549 926	7.72	52 480 746	8.24	173 780 083

[a] Descriptive statistics are based on the non-logarithm K_{OW} expressions.

[b] Log K_{OW} values used by Fuchsman et al. [19] shown for comparison.

K_{OW} = octanol–water partition coefficient; SD = standard deviation; CV = coefficient of variation.