# Use of Food Web Models to Evaluate Bioaccumulation Data

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## Introduction

A typical use of bioaccumulation factors is to derive clean up levels or criteria/standards for water and sediment. The target sediment or water concentration (TSC or TWC) is established by dividing a maximum allowable tissue level (MATL) by either a biota-to-sediment accumulation factor (BSAF) or a bioaccumulation factor (BAF). Where possible, the BSAF and the BAF are defined by measurement (USEPA, 1995). The implicit assumption is that the BSAF and the BAF are estimates of an invariant steady-state relationship between tissue concentration and sediment or water concentration. By that we mean the following: the BSAF and BAF are applicable to conditions that differ from the measurement conditions such that achieving a sediment concentration equal to the TSC or a water concentration equal to the TWC will result in a tissue concentration equal to the MATL.

## Applicability of Measured BSAFs and BAFs

Measured BSAFs and BAFs can be applied to the clean up level or criteria/standards problem only if they describe the invariant steady-state relationship that is implied by their use. Numerous examples exist where this is evidently not the case.

### *BSAFs and BAFs vary with location*

In the Hudson River, the polychlorinated biphenyl (PCB) BAFs measured in 1990 for largemouth bass decline from ca. $40x10^6$ to $10x10^6$ L/kg lipid with distance from the PCB source. Conversely, the BSAFs increase from about 1 to 2 g OC/g lipid (see page 4-9). In Green Bay, the PCB BSAFs for carp increase with distance from the source by factors of 5 to 10 (see page 4-9). The ratio of ppDDE (p,p'-DDE) in kelp bass to ppDDE in white croaker from the Southern California Bight increases with distance from the source, changing by more than a factor of 7 (see page 4-10).

### *BSAFs and BAFs vary with time*

At Stillwater in the upper Hudson River, largemouth bass BAFs vary among years from about $3x10^6$ to $30x10^6$ L/kg lipid. Similarly, the BSAFs vary from about 2 to 4 g OC/g lipid (see page 4-10).

### *BSAFs and BAFs vary among species at similar trophic levels*

Green Bay carp and alewife are at similar trophic levels, as indicated by similar levels of PCB accumulation relative to particles at the base of the food web (see page 4-11). Yet, alewife have much lower PCB concentrations. Southern California Bight dover sole and white croaker both consume benthic invertebrates, yet the PCB and ppDDE BSAFs of the sole are 2 to 3 times lower than those of the croaker (see page 4-11).

To explore the potential causes of the variability in BSAFs and BAFs, consider that they are presumed to reflect a steady-state relationship among contaminant concentrations in biota ($v$), dissolved water ($c_{d1}$), and/or sediment ($r_2$). In general, both sediments and water column may contribute to fish contaminant loads, so

$$v = ac_{dl} + br_2$$

Because the use of a BSAF or a BAF implies an invariant relationship between the biota and media considered (i.e., sediment or dissolved water), a constant relationship must exist between dissolved water and sediment:

$$r_2 = K_{ws}c_{dl}$$

where $K_{ws}$ is the water-sediment partition coefficient.

These equations yield the following expressions for BSAF and BAF:

$$BSAF = \frac{a}{K_{ws}} + b$$

$$BAF = a + bK_{ws}$$

The coefficients a and b are functions of food web structure, bioenergetics, and toxicokinetics. The partition coefficient $K_{ws}$ is a function of contaminant loading and all



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of the fate and transport processes. Lack of steady-state conditions is an obvious cause for BSAF and BAF variability. BSAF and BAF variation with location could also be attributable to variations in $K_{ws}$ or food web structure. BSAF and BAF variation with time may result from variations in $K_{ws}$ or in bioenergetics that result from physiological changes (e.g., lipid content). BSAF and BAF variation among species may be due to food web structure, bioenergetics, or toxicokinetic differences.

Interpretation of BSAF and BAF data must involve an assessment of whether the implicit assumption of an invariant steady-state condition is accurate. Is a measured BSAF or BAF value appropriate for regulatory application or should it be adjusted or discarded? Such interpretation is hampered because of the probable site-specificity of BSAFs and BAFs and the many factors that can invalidate the invariant steady-state assumption.

## Use of Food Web Models to Validate Bioaccumulation Data

Food web models provide a means for validation because they mechanistically describe the bioaccumulation process and can ascribe causality to observed relationships between biota and sediment or water. The utility of models as validation tools for data is predicated on the accuracy of the models. Two issues are important: (1) is the bioaccumulation process sufficiently well characterized to permit the use of models as diagnostic tools? and (2) is the uncertainty of model calculations small enough to allow discrimination among measured BSAF or BAF values? A model of PCBs in Green Bay and DDE and PCBs in Southern California Bight illustrate the robustness of the models. In Green Bay, a single model structure with one set of bioenergetic and toxicokinetic parameters accurately reproduced congener and ΣPCB concentrations in five fish species in five locations that extend over an order of magnitude gradient in exposure concentrations (see page 4-14).

Monte Carlo analysis of a model of ppDDE in dover sole indicates that model uncertainty is not greater than the uncertainty of field BAF data, about a factor of 2 (see page 4-16).

## Example

Green Bay carp PCB data were used as an example of spatial variability in estimated BSAF values. To interpret these data a bioaccumulation model was developed using the same toxicokinetic parameters as used for the other Green Bay species. The computed BSAFs are consistent with those observed in Zone 3B. In contrast, the model was not capable of reproducing the Fox River and Zone 4 BSAF data while maintaining parameter values within experimental limits (see page 4-17). Thus, the modeling suggests that the Zone 3B data represent a steady-state relationship between carp and sediment. Further, it appears that in the other zones the carp were not at steady state with the sediments, possibly because the sampled sediments do not properly describe the exposure concentrations seen by the carp.

Southern California Bight ppDDE and PCB data in three species of birds were used to assess from what location the birds received their contaminants. To interpret these data, a bioaccumulation model was developed using the same toxicokinetic framework for all three species. Measured prey and predator concentrations were consistent for the peregrine falcon and bald eagle, suggesting that our view of the feeding behaviors and feeding locations of these species is reasonable. However, prey and predator levels were not consistent for the double-crested cormorant on Santa Barbara Island, suggesting that the cormorants feed in less contaminated areas than previously assumed.

## Conclusions

- Food web models provide a means to interpret bioaccumulation data.
- Models are necessary to test assumptions implicit in data-based BSAF and BAF values used for regulatory purposes.
- Two potential applications of models are:
  (1) to refine the database of BAF and BSAF values used for regulatory purposes and
  (2) to increase confidence in regulatory decisions having substantial economic implications.

## References

USEPA. 1995. *Great Lakes Water Quality Initiative technical support document for the procedure to determine bioaccumulation factors.* EPA-820-B-95-005. U. S. Environmental Protection Agency, Washington, DC.

- A typical use of bioaccumulation factors is in the derivation of clean up levels or criteria/standards for water and sediment:

*Sediment Target Level (STL in mg/kg)*

$$STL = v_c / BSAF$$

*Water Column Target Level (WTL in µg/l)*

$$WTL = v_c / BAF$$

- Where possible, the BSAF and the BAF are defined by measurement.

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- The implicit assumption is that the BASF and BAF values are estimates of an invariant steady-state relationship between tissue concentration and sediment or water concentration

  i.e., achieving a sediment concentration equal to the STL or a water column concentration equal to the WTL will result in a tissue concentration equal to $v_c$

The steady-state relationship among contaminant concentrations in biota (v), dissolved water ($c_{d1}$) and sediment ($r_2$) is:

$$v = ac_{d1} + br_2 \quad (1)$$

If *a* and *b* are both non-zero, an invariant relationship requires that:

$$c_{d1} = K_{ws} r_2 \quad (2)$$

which yields:

$$BSAF = aK_{ws} + b \quad (3)$$

$$BAF = a + \frac{b}{K_{ws}} \quad (4)$$

and, thus, requires that a, b and $K_{ws}$ are invariant

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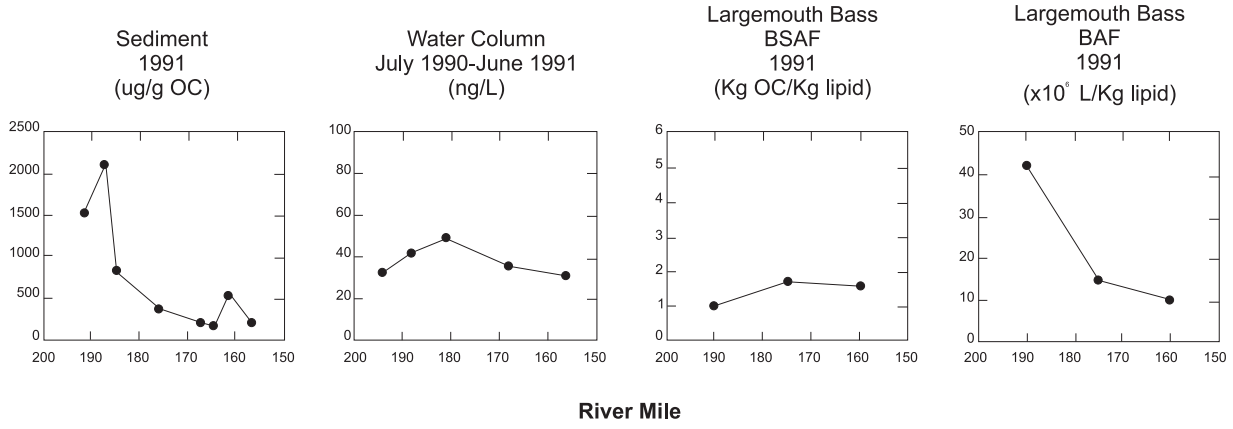
The constraints are restrictive, because:

- Equation (1) is only valid at steady-state
- *a* and *b* are functions of food web structure, bioenergetics and toxicokinetics
- $K_{ws}$ is a function of contaminant loading and all of the fate and transport processes

Thus, it is probable that many BSAF and BAF values calculated from measurements do not reflect an invariant, steady-state condition.

*How can we interpret BSAF and BAF data?*




Total PCBs in the upper Hudson River: Spatial Patterns
Sediment, water column and largemouth bass in 1991

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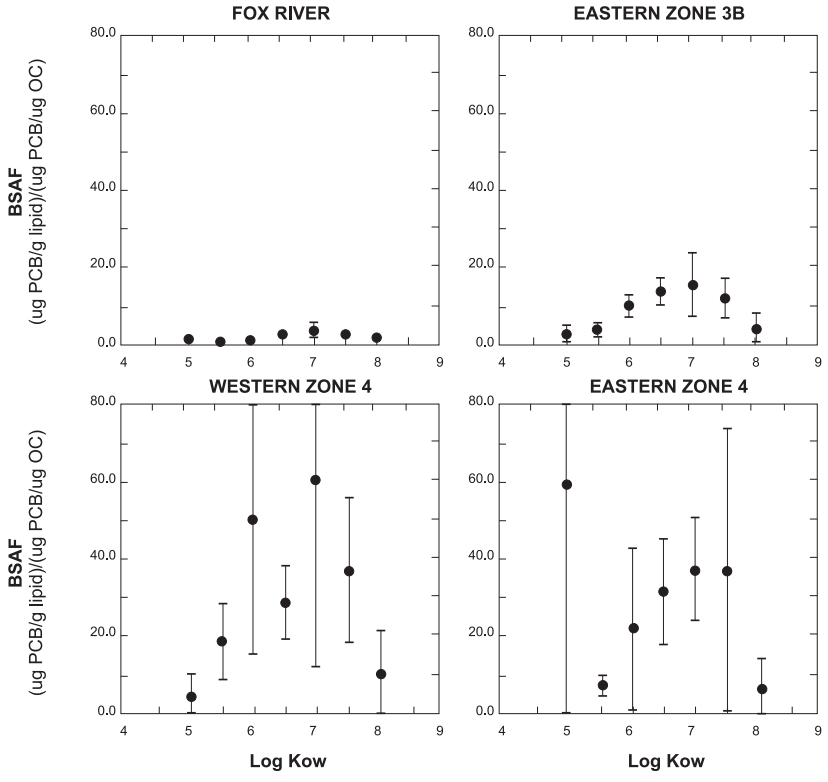
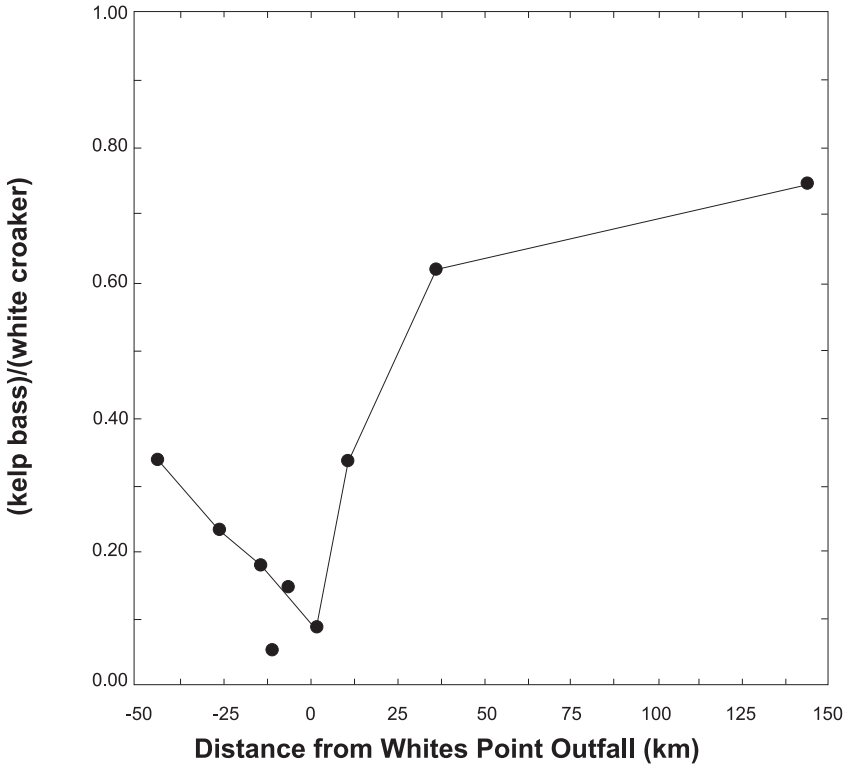
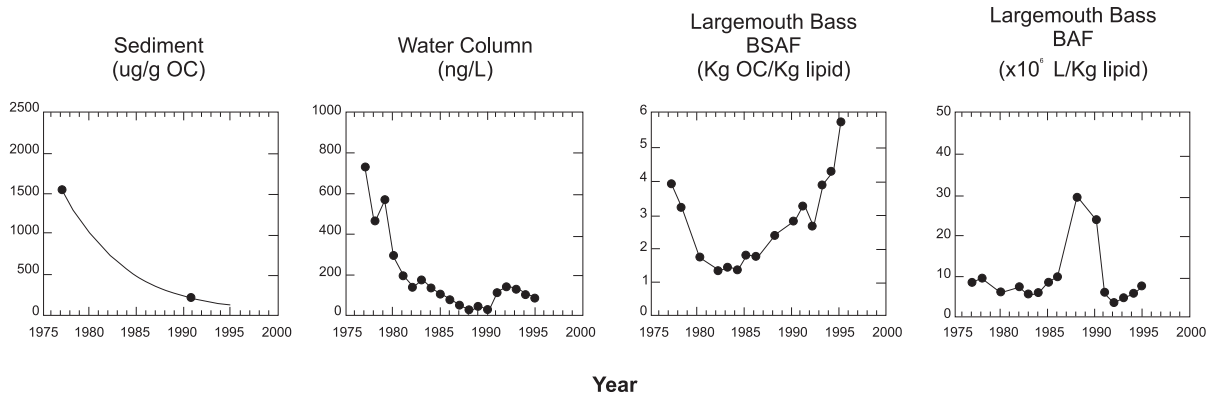


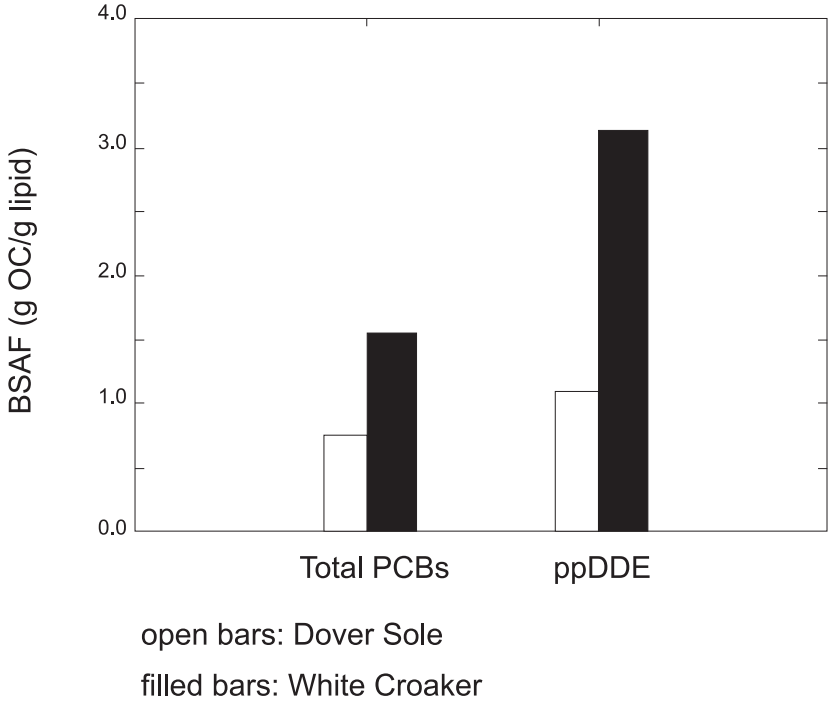

Bioaccumulation Factors for PCBs in Green Bay Carp
PCB Congeners Grouped into 0.5 Log Kow Bins
Data are Arithmetic Means and 95% Confidence Intervals



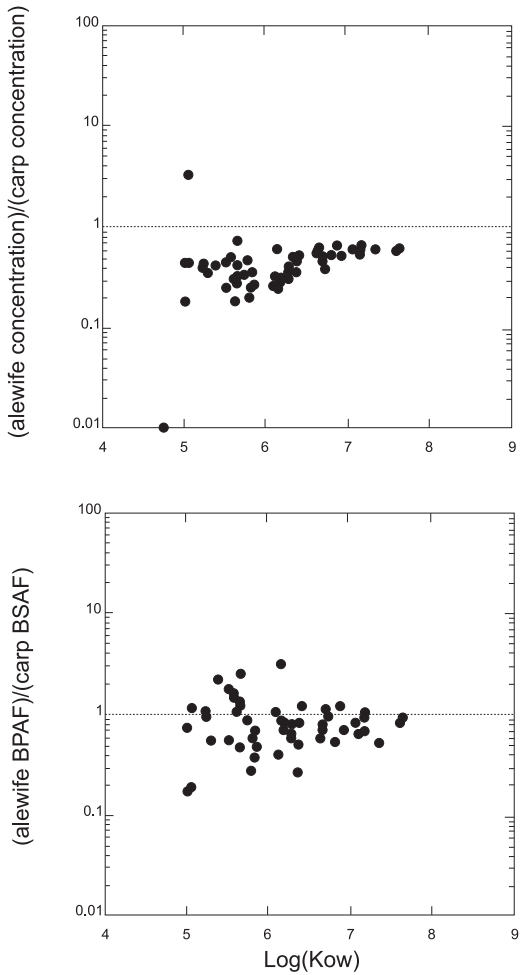

Ratio of (kelp bass)/(white croaker) lipid-based ppDDE concentrations in the Southern California Bight.




Total PCBs in the upper Hudson River: Temporal Patterns
Sediment, water column and largemouth bass from Stillwater



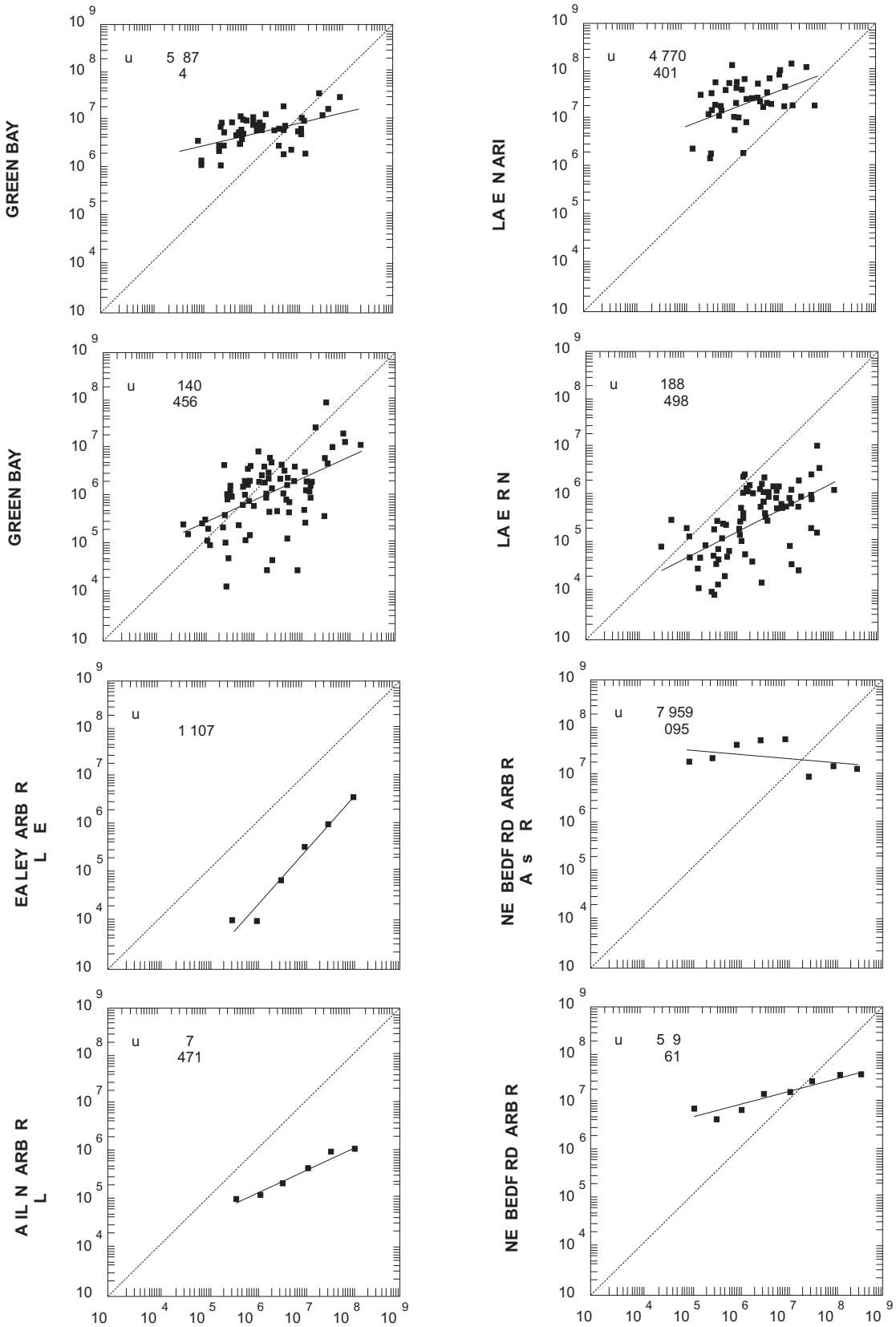

**Total PCBs and ppDDE BSAFs in fish from the Southern California Bight**




**PCB levels in a pelagic forage fish (alewife) and a benthic fish (carp) in Green Bay zone 3B. Top panel: Ratio of lipid-based concentrations. Bottom panel: Ratio of alewife BPAF/carp BSAF**

$$\text{BPAF} = \frac{\mu\text{g PCB/g lipid alewife}}{\mu\text{g PCB/g OC phytoplankton}}$$

$$\text{BSAF} = \frac{\mu\text{g PCB/g lipid carp}}{\mu\text{g PCB/g OC sediment}}$$




Water-Sediment partitioning for PCB homologs and congeners (L/kg OC)

*How can we interpret BSAF and BAF data?*

*By using food web bioaccumulation models.*

Models provide this capability because:

- They describe the process of bioaccumulation and can account for water & sediment exposure, time variability and food web structure
- They are credible: capable of reproducing field data using parameterizations that are supported by experimental data and are consistent within and across food webs
- Their uncertainty is not overwhelming

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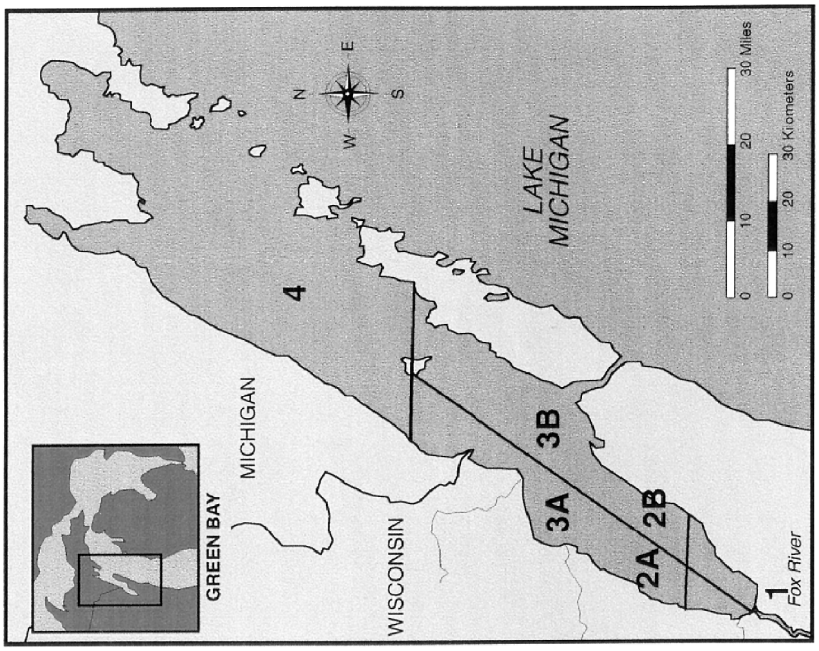
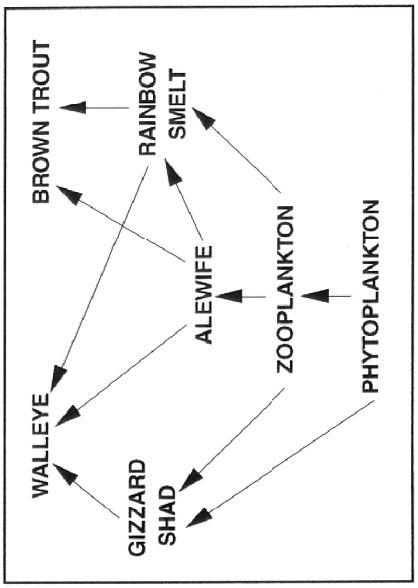
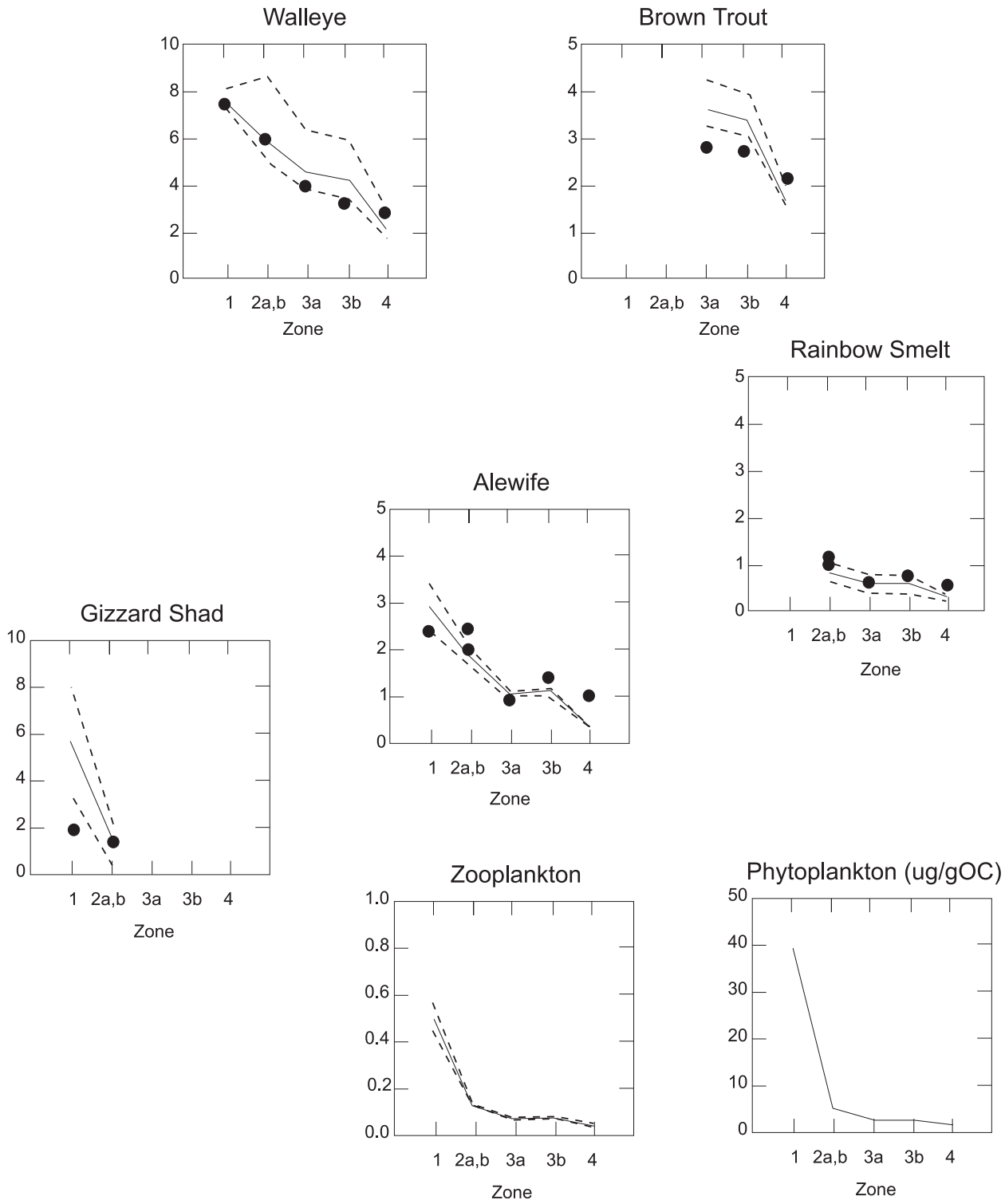


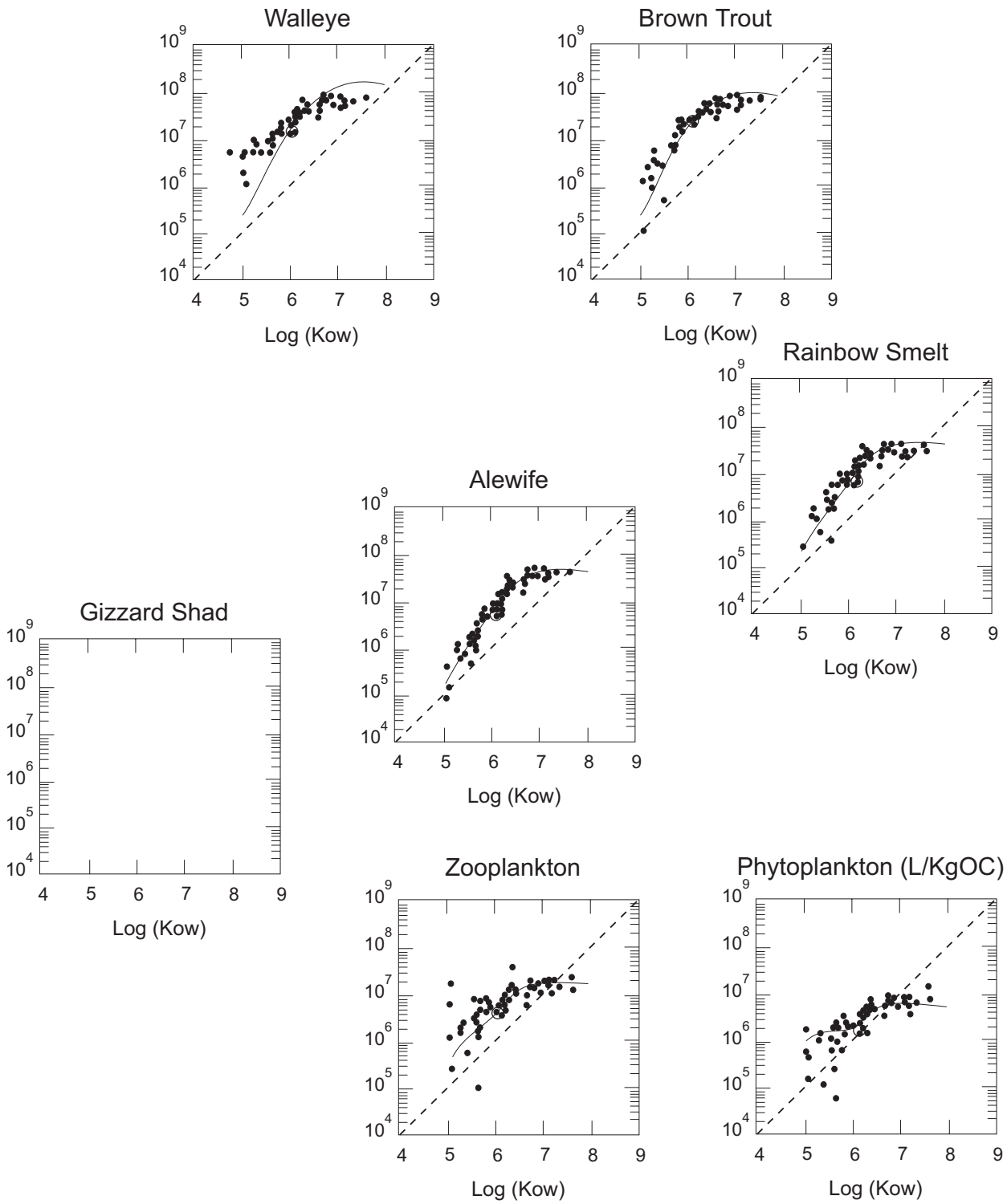



# GREEN BAY WET WEIGHT-BASED CONCENTRATION TOTAL PCBs

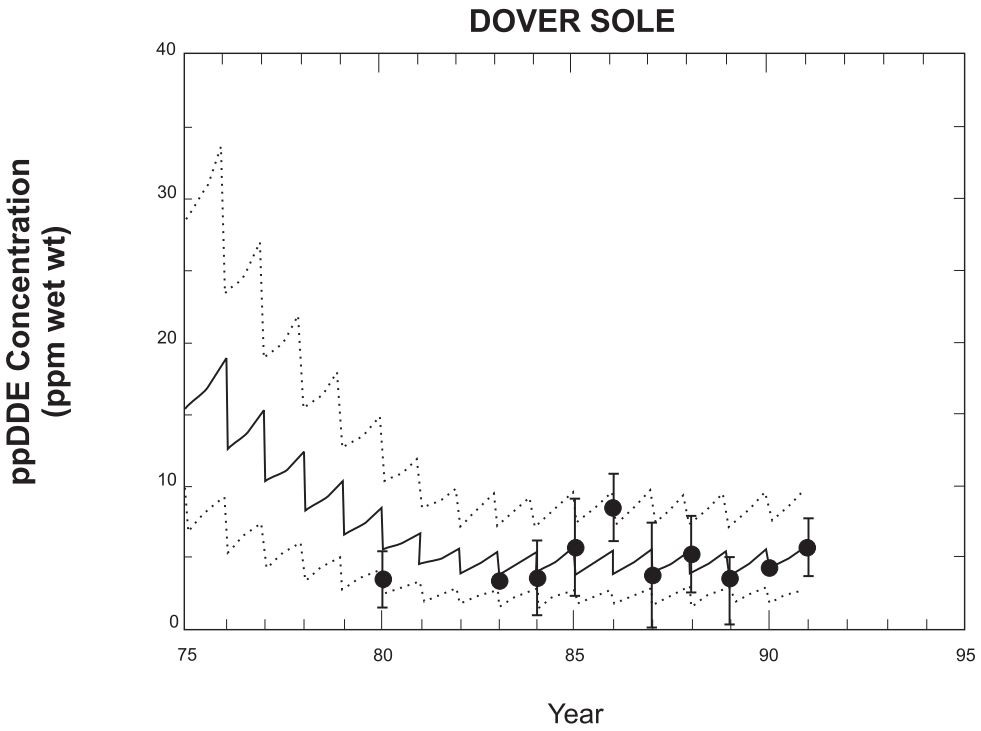



**Food Web Model Calibration. Computed and observed total PCB concentrations, µg/g whole body wet weight, for all spatial zones. Lines: model calculations. Filled circles: data.**

# GREEN BAY LIPID-BASED BAFs



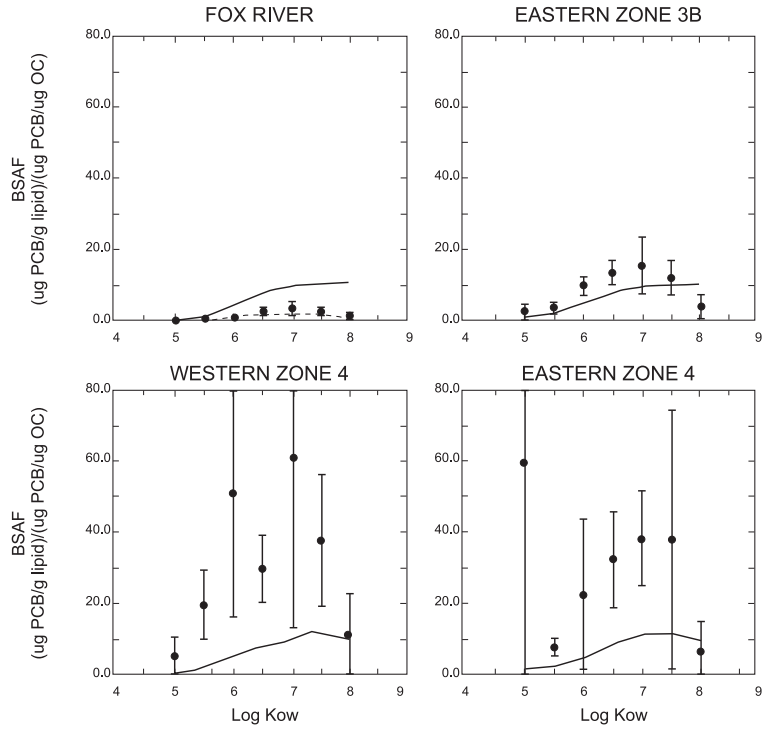

**Food Web Model Calibration. Computed and observed lipid-based bioaccumulation factors for zone 3A. L/Kg lipid.**




Comparison of Predicted and Observed ppDDE Concentrations in Dover Sole
Solid Lines are Model Results
Dashed Lines are 95% Confidence Intervals around the Mean (Monte Carlo)
Data are Arithmetic Means and 95% Confidence Intervals around the Mean

Using a model to examine the Green Bay carp data we conclude the BSAF values in the Fox River and zone 4 represent non-steady state between the fish and the sampled sediment

- Differences in toxicokinetics and bioenergetics do not account for the spatially variable BSAFs
- Differences in food web structure do not account for the spatially variable BSAFs

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Next