Contaminant Modeling in San Francisco Bay: Lessons from Other Estuaries

Dr. Joel Baker

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University of Washington Tacoma

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Outline

- *Utility and challenges of modeling chemical contaminants in estuaries*
- *Approaches and common traits of estuarine contaminant models*
- *What is missing?*
- *Final thoughts*

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Utility of Contaminant Models in Estuaries

- *Source apportionment*
  - Relative magnitude of:
    - different current source types
    - specific current sources
    - local *versus* regional *versus* global sources
  - Magnitude of current *versus* historical loadings

Utility of Contaminant Models in Estuaries

- *Evaluation of Management Actions*
  - Permitting and compliance
  - Remediation planning
  - Restoration effectiveness

Utility of Contaminant Models in Estuaries

- *Estimate Ecosystem-level Response Times*
  - Time to recovery
  - ‘curve bending’ by specific management actions

Challenges in Modeling Contaminant Behaviors in Estuaries

- *Spatial heterogeneity*
  - Not well mixed
  - Migratory birds and anadromous fish
- *Proximity to shoreline*
  - Highly altered and rapidly changing landscapes
  - Fringes matter
- *Complex particle dynamics*
  - Sediment-water exchange
  - Flocculation where fresh meets salt

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Modeling Chemical Contaminants in Aquatic Ecosystems:

Seminal Papers in PCB Modeling

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Modeling Chemical Contaminants in Aquatic Ecosystems: Karickhoff *et al.* 1979

SORPTION OF HYDROPHOBIC POLLUTANTS ON NATURAL SEDIMENTS

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(*Received* 4 *September* 1978)

Abstract—The sorption of hydrophobic compounds (aromatic hydrocarbons and chlorinated hydrocarbons) spanning a concentration range in water solubility from 500 parts per trillion (ppt) to 1800 parts per million (ppm) on local (North Georgia) pond and river sediments was investigated. The sorption isotherms were linear over a broad range of aqueous phase pollutant concentrations. The linear partition coefficients (K_p) were relatively independent of sediment concentrations and ionic strength in the suspensions. The K_p's were directly related to organic carbon content for given particle size isolates in the different sediments. On an organic carbon basis ($K_{oc} = K_p$/fraction organic carbon), the sand fraction (>50 μm particle size) was a considerably less effective sorbent (50–90% reduction in K_{oc}) than the fines fraction (>50 μm particles). Differences in sorption within the silt and clay fractions were largely related to differences in organic carbon content. Reasonable estimates of K_{oc}'s can be made from octanol/water distribution coefficients, which are widely catalogued or easily measured in the laboratory.

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Modeling Chemical Contaminants in Aquatic Ecosystems: Karickhoff *et al.* 1979

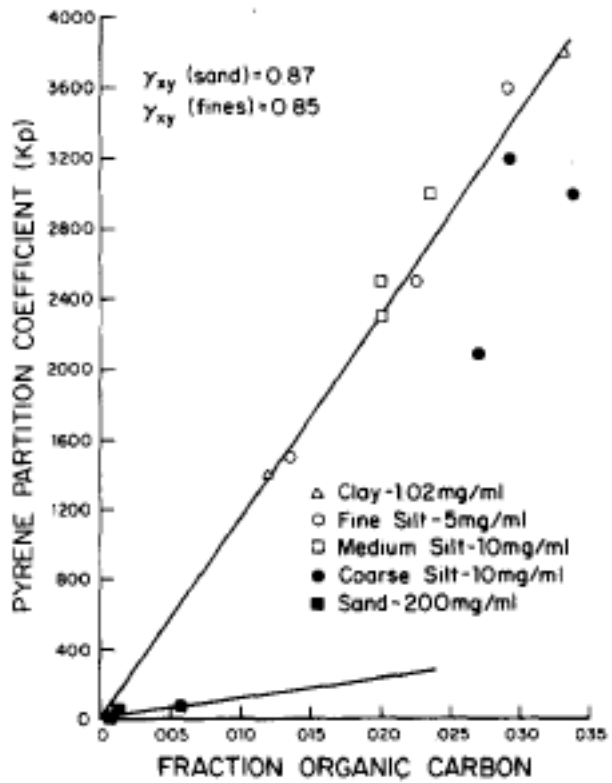

Fig. 3. Pyrene K_p as a function of sediment organic carbon.

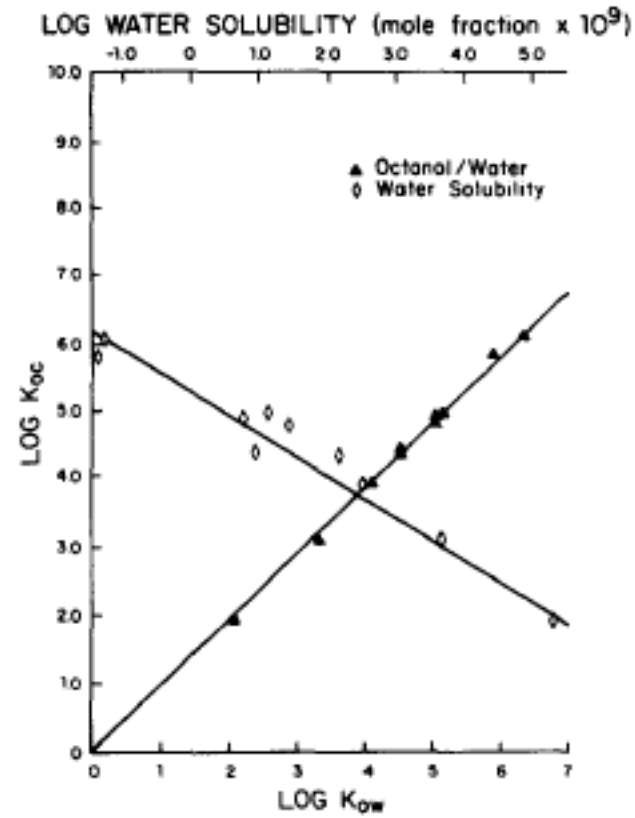

Fig. 5. Sorption K_{oc} as a function of compound water solubility and octanol/water distribution coefficients.

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Modeling Chemical Contaminants in Aquatic Ecosystems: Mackay, 1989

J. Great Lakes Res. 15(2):283–297
Internat. Assoc. Great Lakes Res., 1989

MODELING THE LONG-TERM BEHAVIOR OF AN ORGANIC CONTAMINANT IN A LARGE LAKE: APPLICATION TO PCBs IN LAKE ONTARIO

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Institute for Environmental Studies
University of Toronto
Toronto, Ontario M5S 1A4

ABSTRACT. *A model, based on the fugacity concept, is described and illustrated by application to the time varying fate of a contaminant (PCBs) in Lake Ontario over the period 1940–2000. Expressions are included for loadings and partitioning of the contaminant between the phases of air, aerosols, water, suspended and bottom sediments, various trophic levels of aquatic organisms, and gull eggs. Also included are expressions for transformation rates, and transport rates for diffusion between water and sediment, and water and air, wet and dry atmospheric deposition, sediment deposition, burial and resuspension, and water and suspended matter inflow and outflow. The results obtained by numerical integration and by assuming reasonable loading and air concentrations*

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Modeling Chemical Contaminants in Aquatic Ecosystems: Mackay, 1989

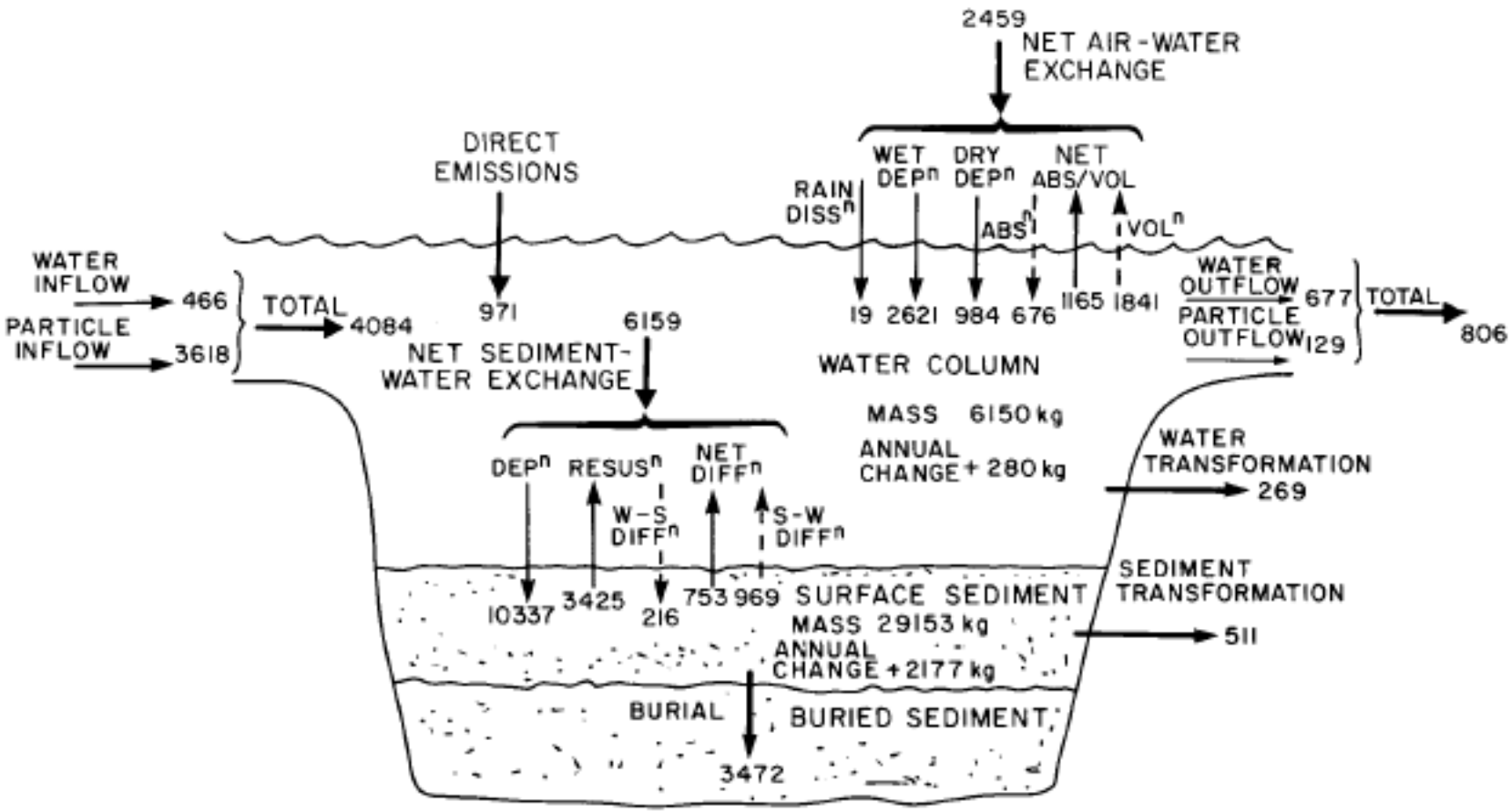

FIG. 5. Estimated PCB flows in 1965 (kg/year).

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Modeling Chemical Contaminants in Aquatic Ecosystems: Gobas and Mackay, 1988

DYNAMICS OF DIETARY BIOACCUMULATION AND FAECAL ELIMINATION OF HYDROPHOBIC ORGANIC CHEMICALS IN FISH

Frank A.P.C. Gobas*, Derek C.G. Muir**, Donald Mackay*

* Institute for Environmental Studies, University of Toronto
Toronto, Ontario, Canada, M5S 1A4

** Department of Fisheries and Oceans, 501 University Crescent
Winnipeg, Manitoba, Canada, R3T 2N6

ABSTRACT

A compilation of available literature data on uptake efficiencies of hydrophobic, organic chemicals from food by fish is presented. It is shown that the uptake efficiency of chemical from food (E_o) follows a relationship with the 1-octanol-water partition coefficient (K_{OW}), i.e., $1/E_o = 5.3.10^{-8}.K_{OW} + 2.3$. A model is derived for chemical uptake from food, which is shown to be consistent with the observed food-uptake data. The equations provide an explanation for the phenomenon of food chain accumulation, which is observed in natural ecosystems for several hydrophobic halogenated aromatic hydrocarbons.

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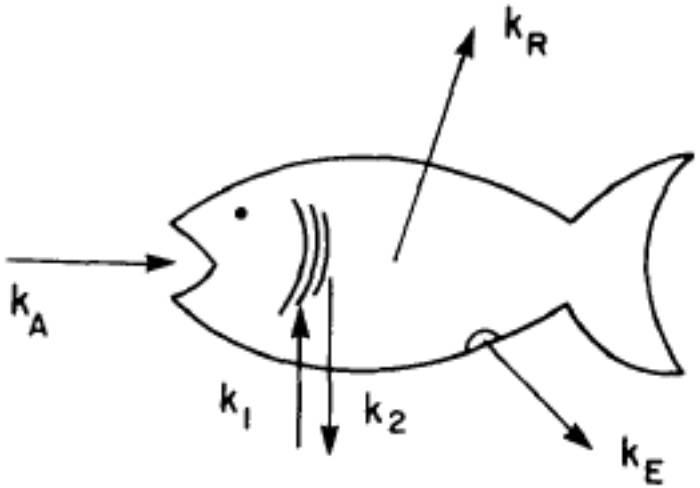
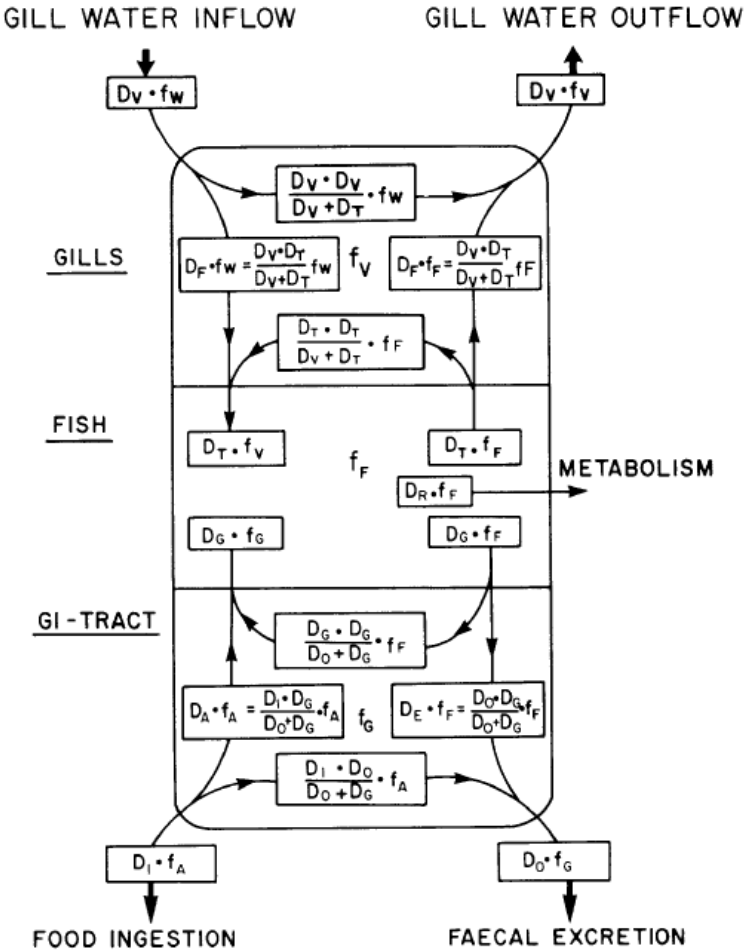
Modeling Chemical Contaminants in Aquatic Ecosystems: Gobas and Mackay, 1988





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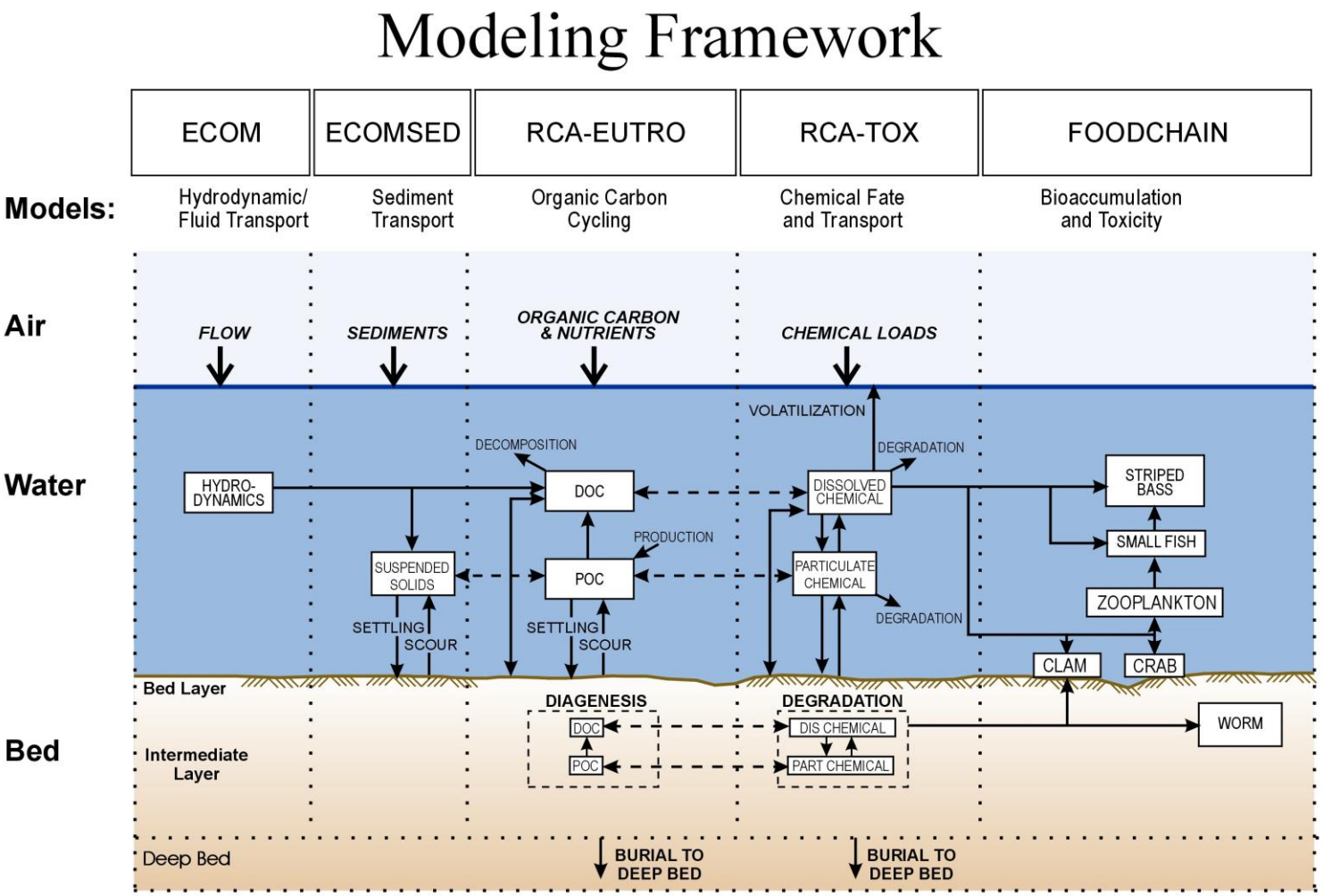
Modeling Contaminants Using a Series of Linked Models

Example: NY/NJ Harbor CARP Model



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Environmental Toxicology and Chemistry, Vol. 23, No. 10, pp. 2396–2409, 2004

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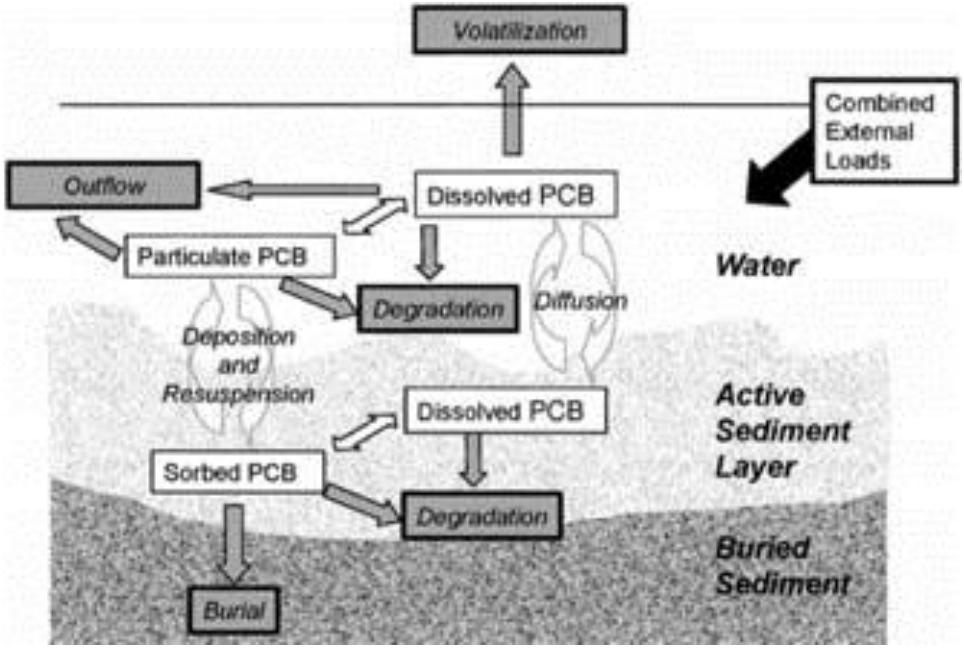
Special Issue Honoring Don Mackay

THE LONG-TERM FATE OF POLYCHLORINATED BIPHENYLS IN SAN FRANCISCO BAY (USA)

JAY A. DAVIS*
San Francisco Estuary Institute, 7770 Pardee Lane, Oakland, California 94621, USA

(*Received* 3 *July* 2003; *Accepted* 20 *February* 2004)

One box!



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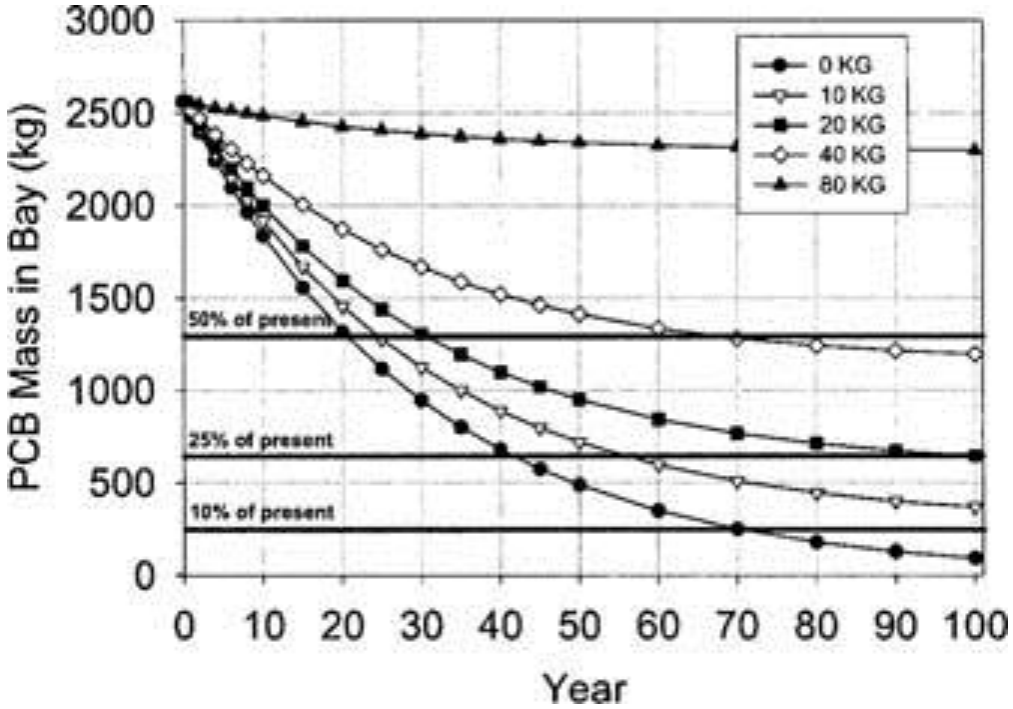

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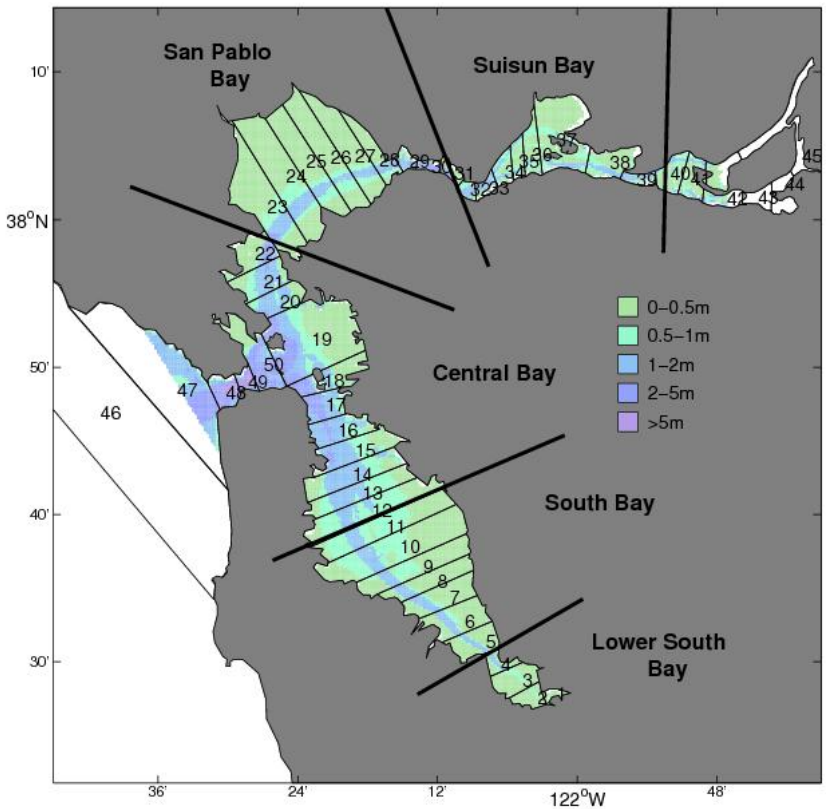
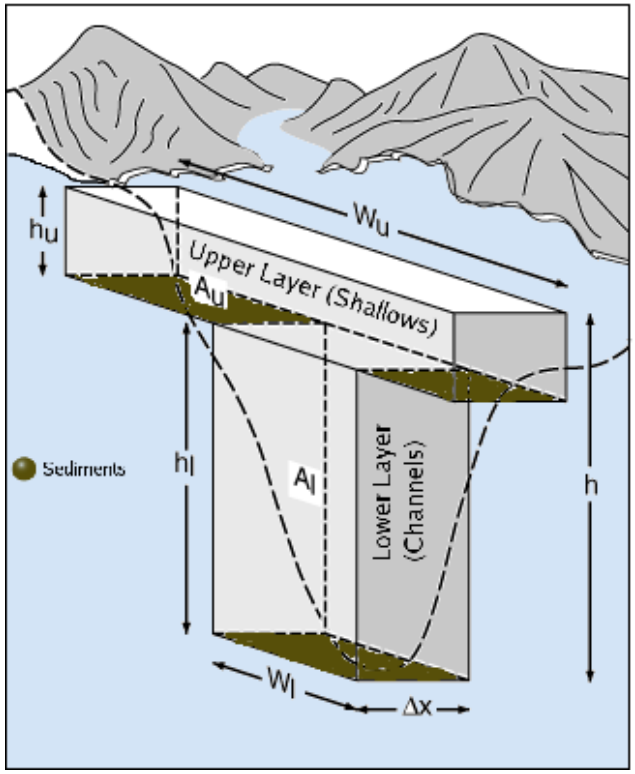
Model Refinement: Multibox Model

(Oram et al., 2008)

100 boxes in the water column





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Modeling Chemical Contaminants in Aquatic Ecosystems: NY/NJ Harbor CARP Model

Management Question

- è Which **sources of contaminants** need to be reduced or eliminated to render future dredged material clean?

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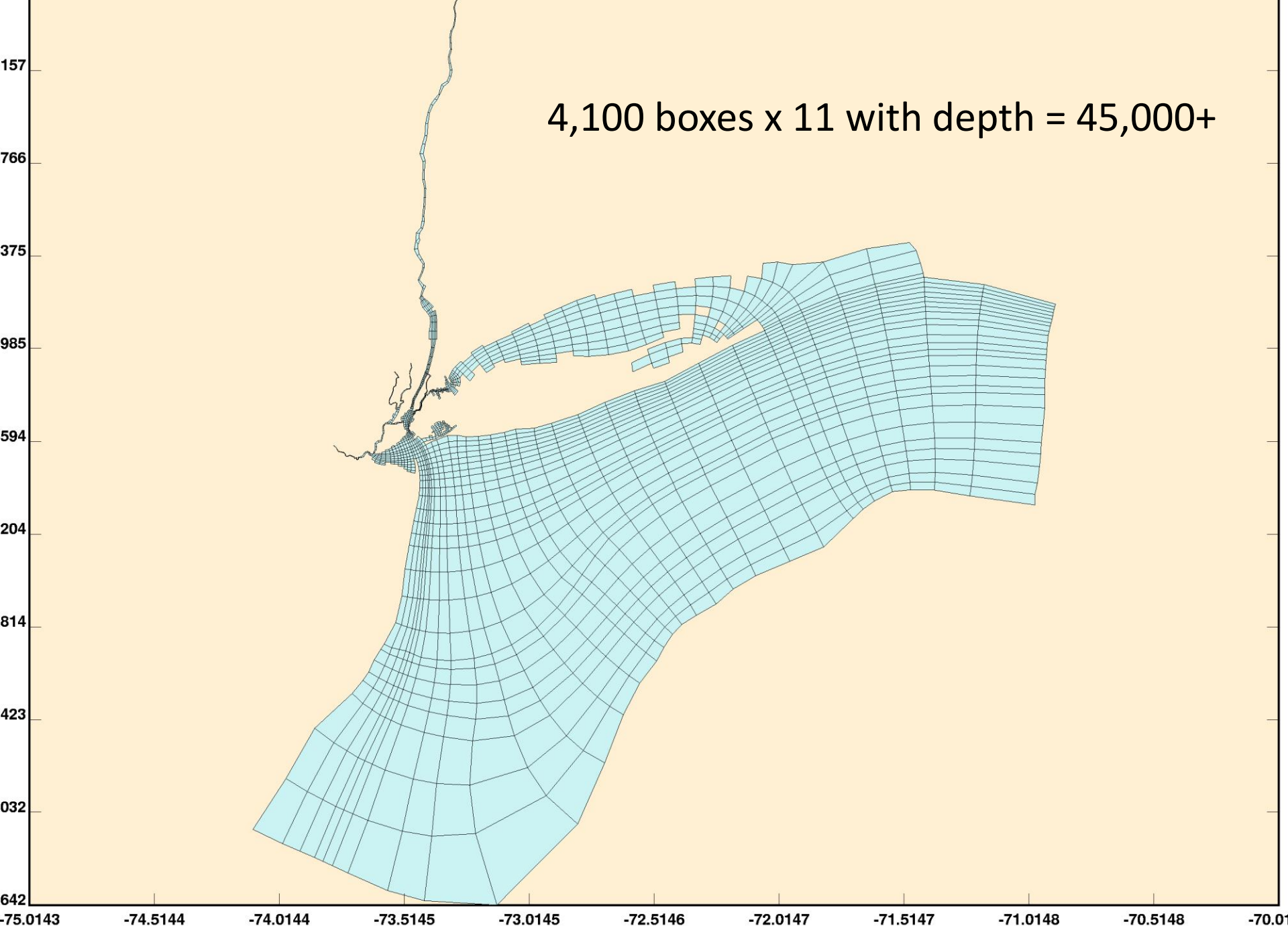
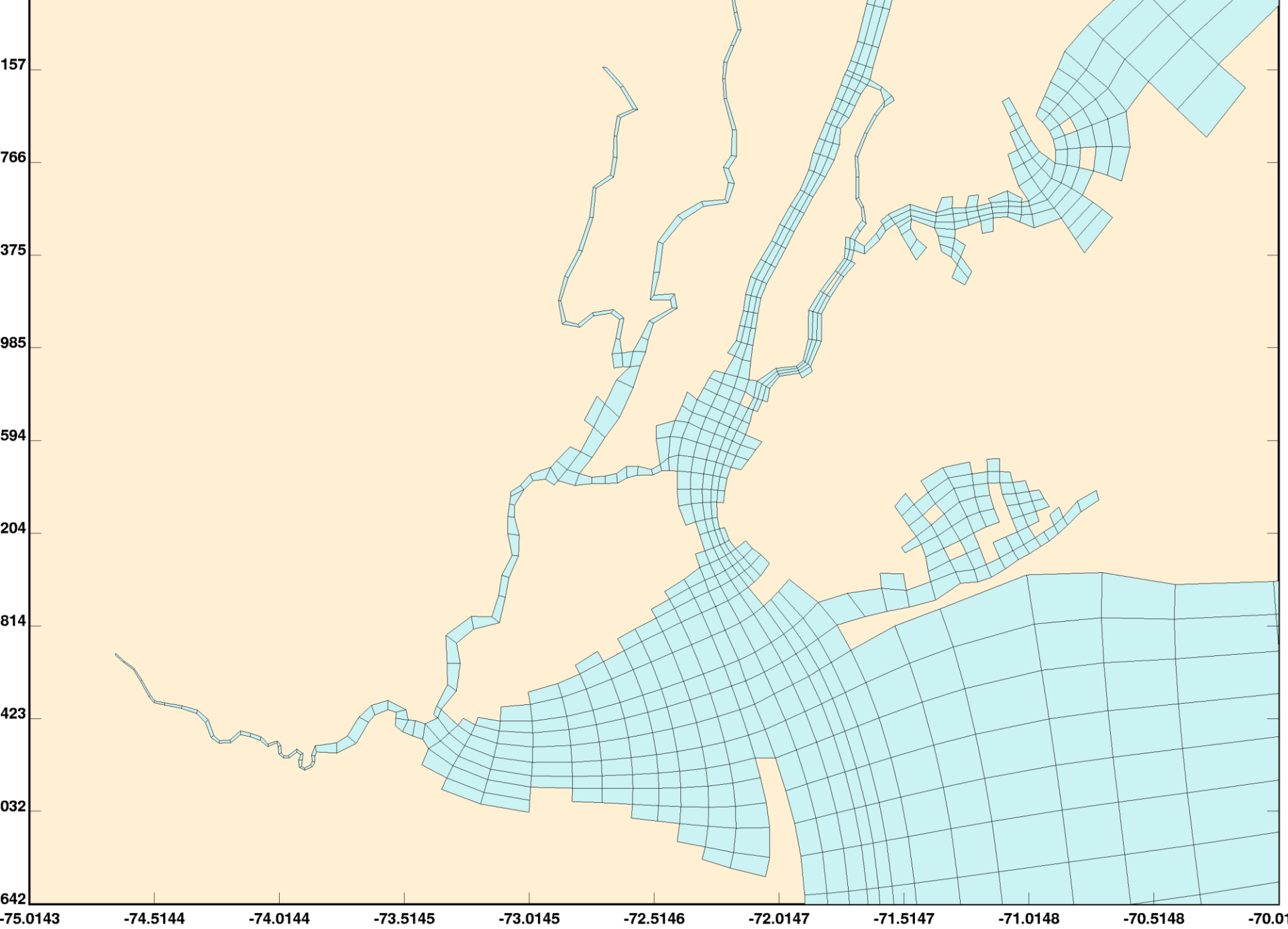
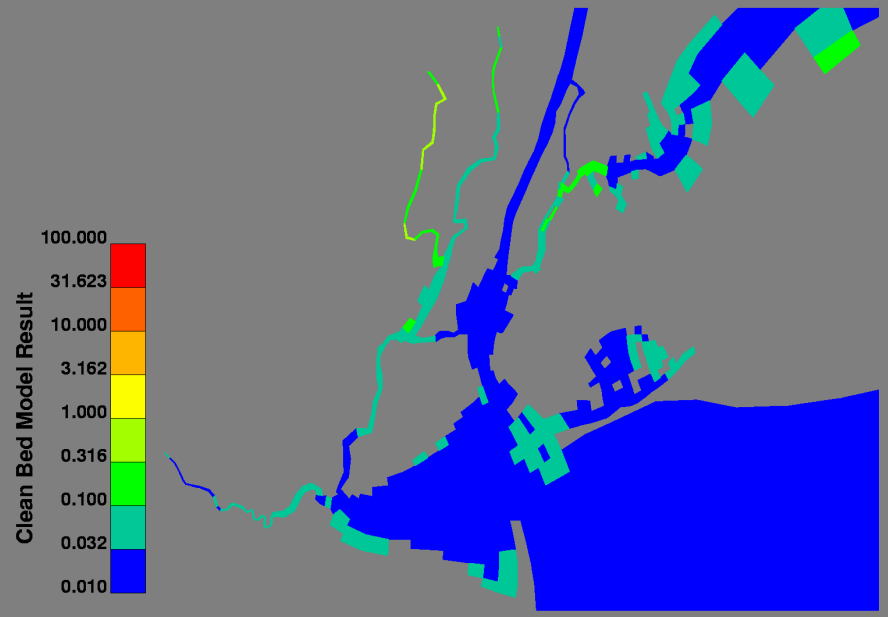
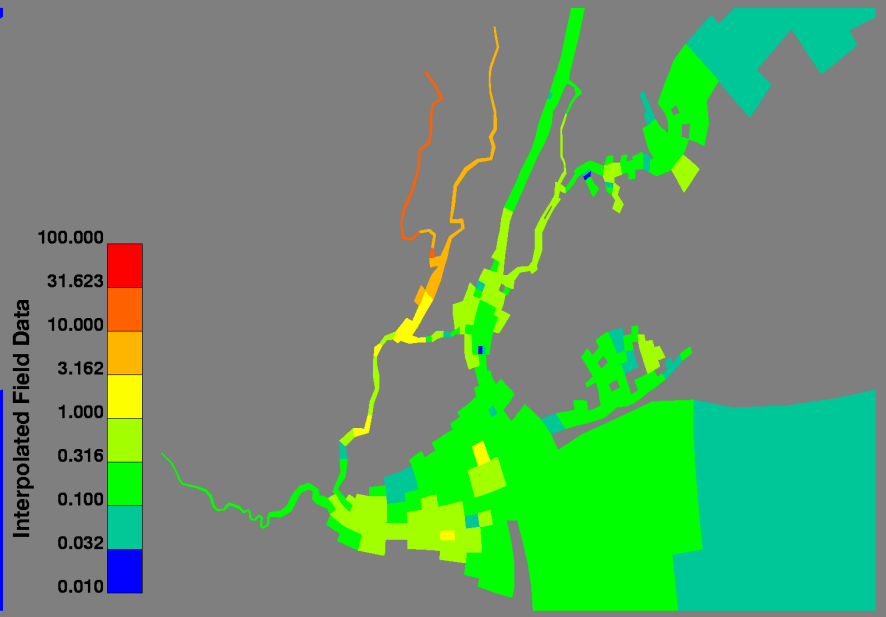


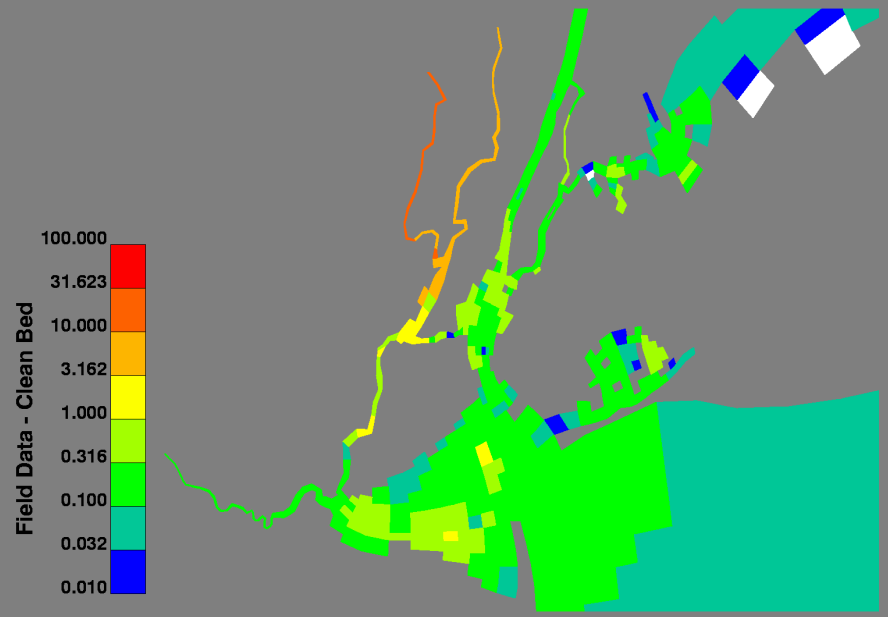
Full CARP Model Grid



CARP Model Grid in The New Jersey Areas







Summary of 2,3,7,8-TCDD interim "clean bed" analysis

2,3,7,8-TCDD DIOXIN (ng/gm-OC) Clean Bed Versus Interpolated Field Data

Common Traits

- *Sediment-water exchange rates control long-term behavior*
- *Loadings drive concentrations*
- *Equilibrium partitioning assumed*
- *Fish and birds are treated simply*

Outline

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- *What is missing?*
- *Final thoughts*

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The bathtub ring effect

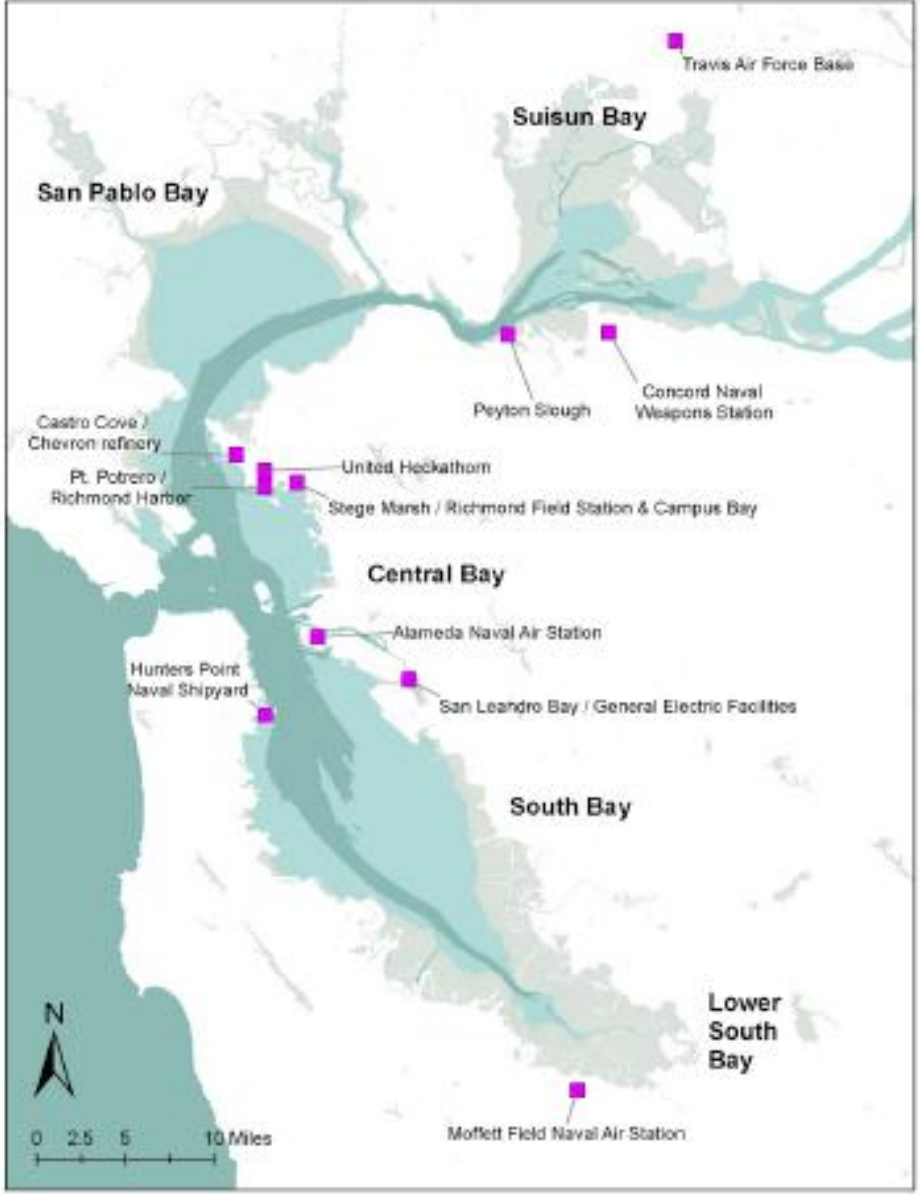
- *Nearshore area are contaminated from:*
  - past activities on the land
  - active trapping of particle-bound pollutants

- *Many estuarine species depend on nearshore habitats*
  - refuge and nesting
  - food resources

The critical question is: Where do the biota get there contaminant burden?

Conceptual Model of Contaminant Fate on the Margins of San Francisco Bay

Draft Report



My proposed approach:

Focus on carbon/energy flows, not on sediment transport

Jones, C., Yee, D., Davis J. A., McKee, L. J., Greenfield, B. K., Melwani, A. R., and Lent, M. A. (2012). Conceptual Model of Contaminant Fate on the Margins of San Francisco Bay. Draft Report. Contribution No. 663. San Francisco Estuary Institute, Richmond, California.

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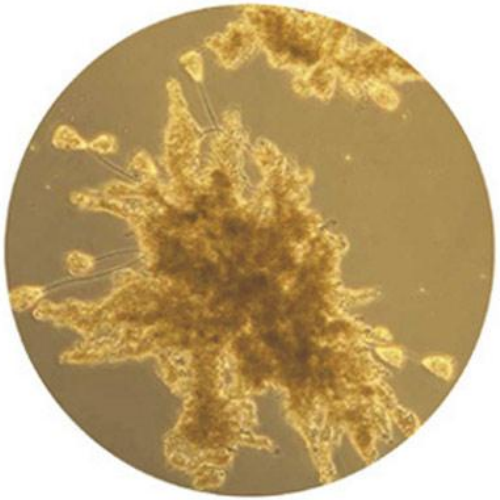
Phase partitioning and particle transport in the water column

- *Different types of particles show substantially different affinities for organic contaminants*

- *Particles interact through well-characterized flocculation mechanisms*



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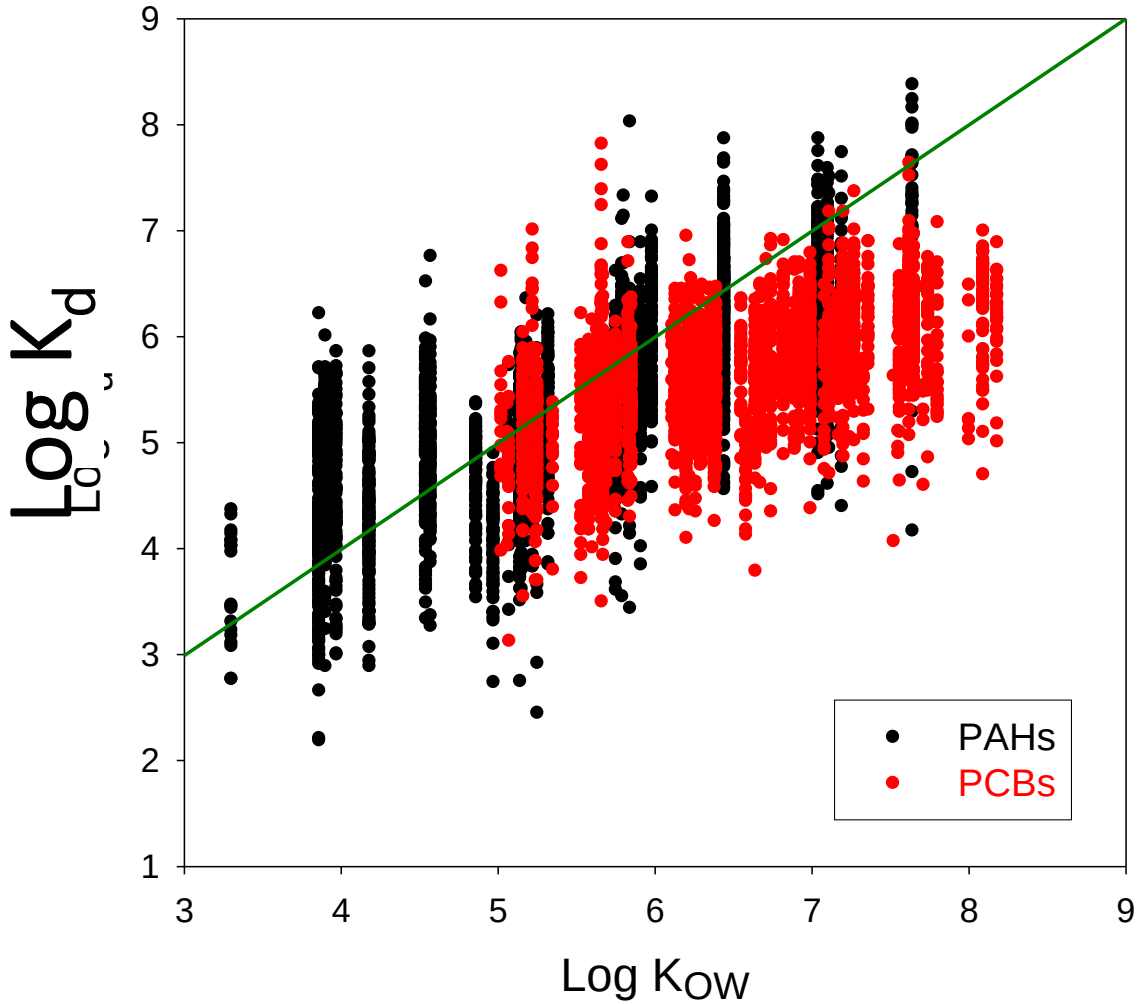
$$K_d = \frac{[\text{Mass on Filter/Volume Filtered}]}{[\text{Mass on XAD/Volume Processed}][\text{TSS}]}$$



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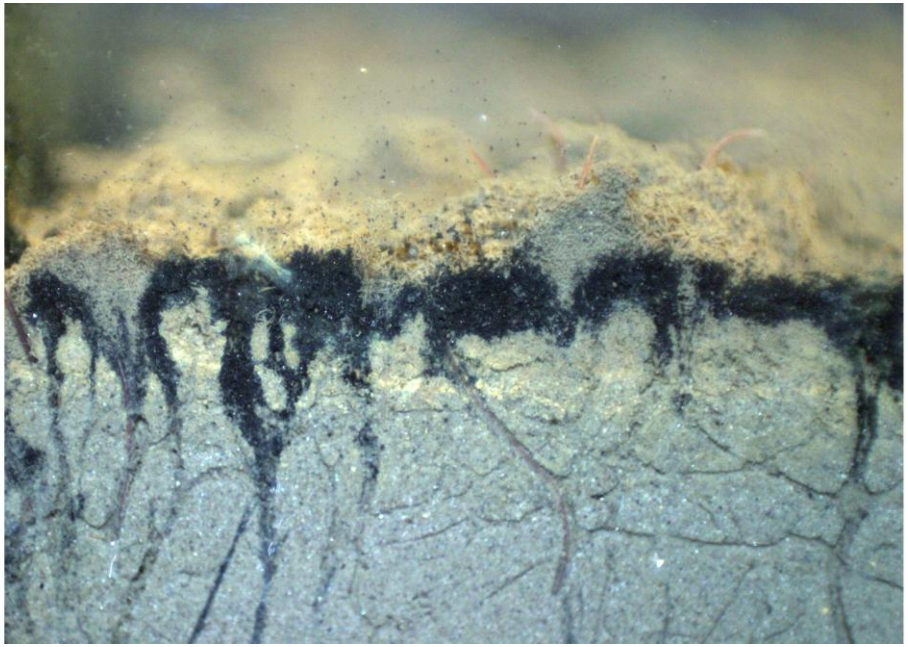
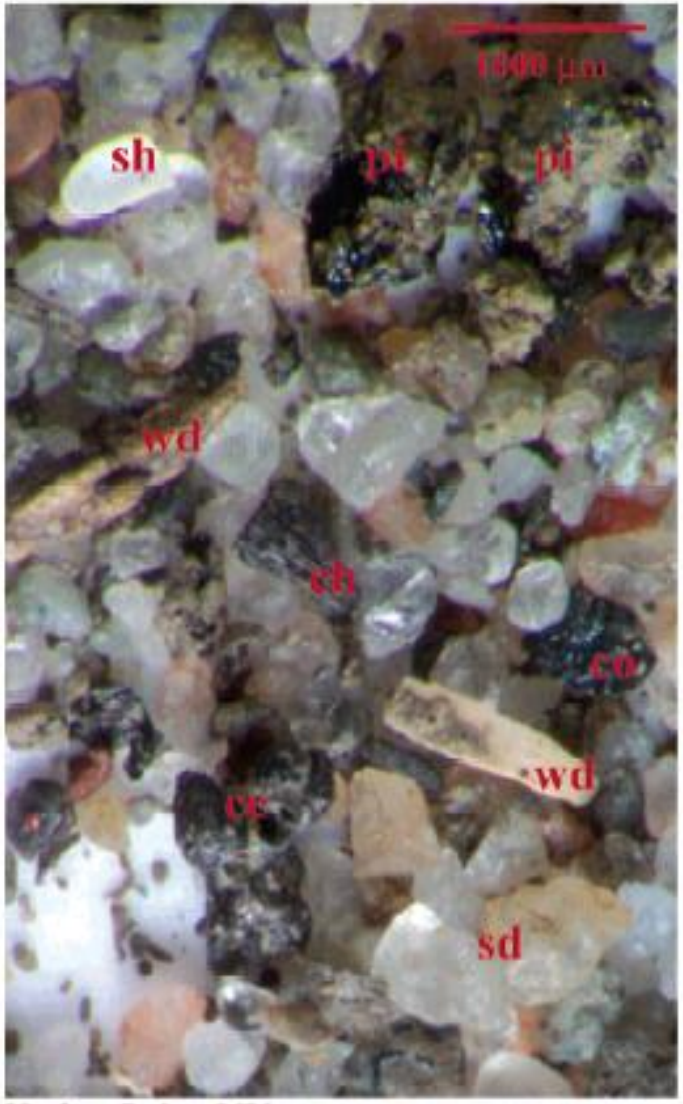
PCB and PAH Speciation among Particle Types in Contaminated Harbor Sediments and Effects on PAH Bioavailability

UPAL GHOSH,*
JOHN R. ZIMMERMAN, AND
RICHARD G. LUTHY
Department of Civil and Environmental Engineering, Stanford University, Stanford, California 94305-4020



Environ. Sci. Technol. **2003**, *37*, 2209–2217

Photo: X. Sun, UMBC



Harbor Point, NY

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Model to Predict the Behavior of PCBs in Carbon-Amended Sediments.

1. **PCBs begin at equilibrium in activated carbon-amended sediment between OC, AC, and porewater**

2. **Particles are eroded by bottom shear stress into clean overlying water**

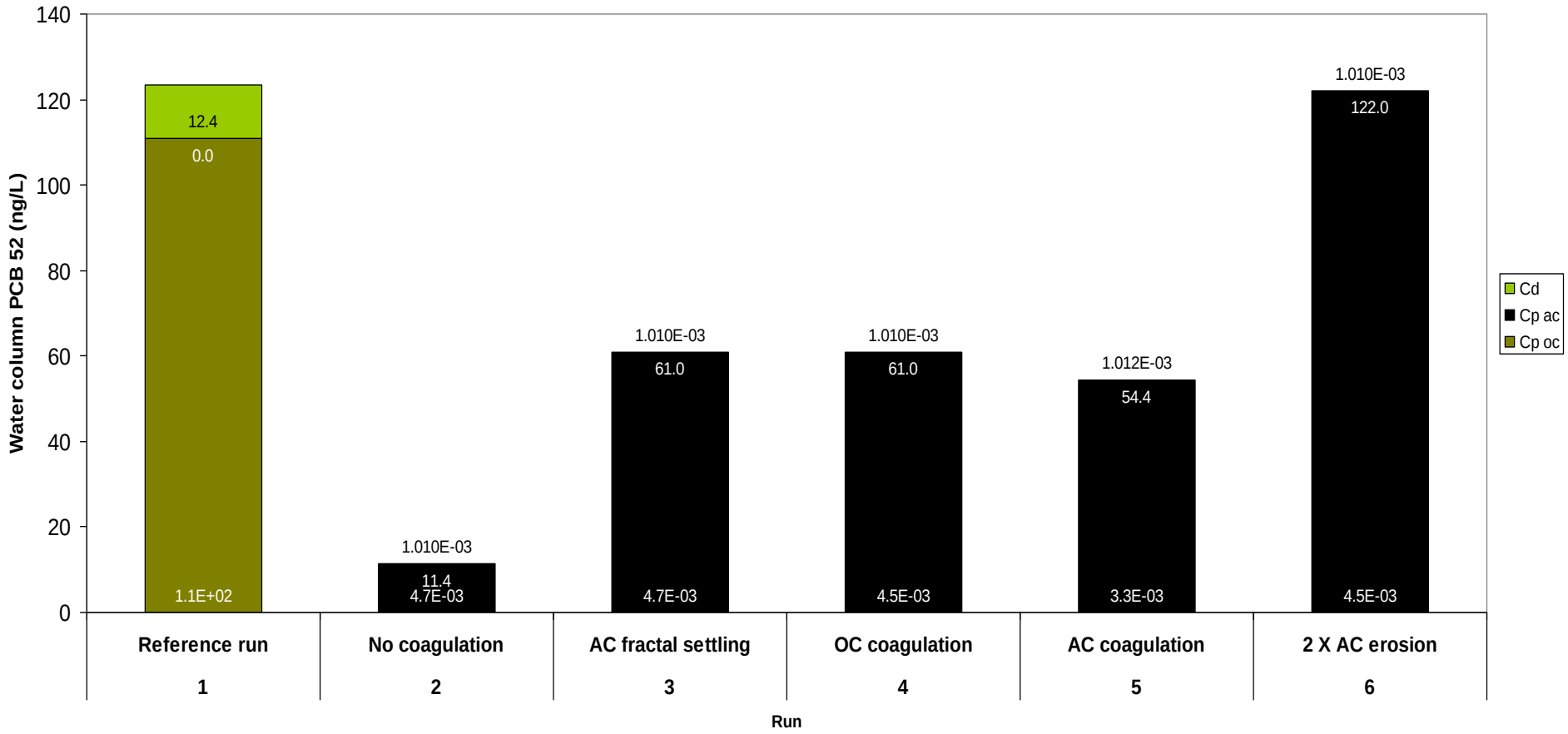
3. **PCBs desorb *via* porous diffusion**

4. **Particles settle by either Stokes settling or fractal model**

5. **Particles coagulate**

6. **Model is run to steady state**

Water Column [PCB] with of Activated Carbon Amendments



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Modeling Variability in Biota-Contaminant Interactions

- *All field data show that contaminant levels in biota is much more variable than predicted by current models.*
  - Are we interested in the mean or the extremes?

- *Bioenergetics and individual-based modeling approaches are becoming more commonplace in fisheries management.*
  - Forage fish example in San Francisco Bay

Outline

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Final Thoughts

Complex models are too expensive to develop and run too slowly to be useful

Moore's Law and Silicon Qubits

You can't calibrate a highly resolved model

Self-learning using real-time observations?

Final Thoughts

Sediment transport is too hard to model

In situ measurements and highly resolved hydrodynamics

Nobody understand complex models

Pixar studios

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