Spatially-explicit bioaccumulation modeling to support human health and ecological risk assessments in a decision analytic context

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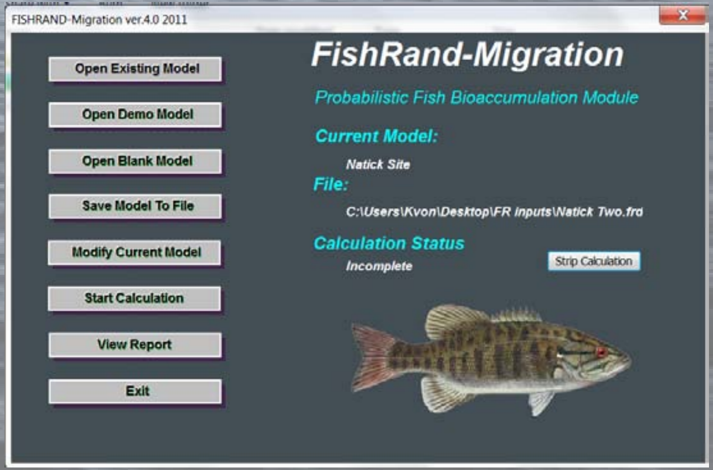


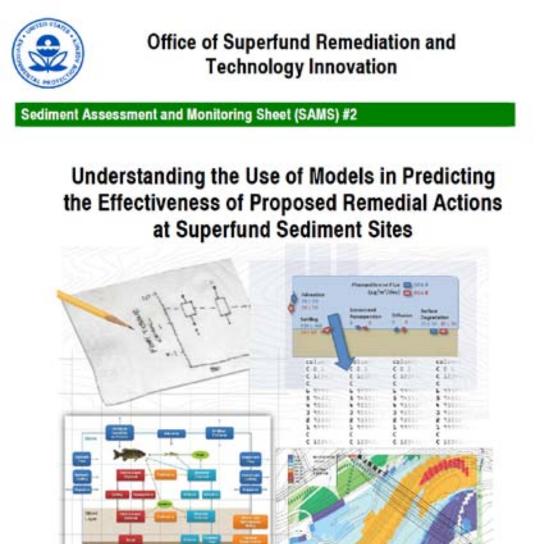
Current Model:
Natick Site

File:
C:\Users\Kvon\Desktop\FR inputs\Natick Two.frd

Calculation Status
Incomplete

Bioaccumulation Models

- Used to predict concentrations in aquatic organisms exposed to sediment-associated contaminants
- Used to evaluate changes in predicted organism concentrations (and resulting human health and ecological risks) as a result of different management alternatives
- Most, if not all, applications based on static exposures (e.g., SWAC, average, etc.)



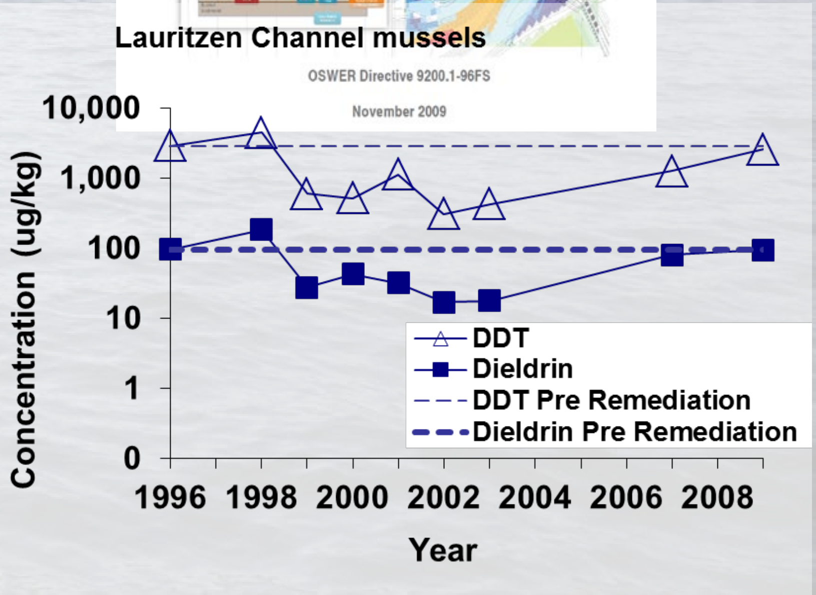
Office of Superfund Remediation and Technology Innovation

Sediment Assessment and Monitoring Sheet (SAMS) #2

Understanding the Use of Models in Predicting the Effectiveness of Proposed Remedial Actions at Superfund Sediment Sites

OSWER Directive 9200.1-96FS

November 2009



Characterizing Exposures

0 mg/kg outside modeling domain

66.7 mg/kg in sediment within modeling domain

- External processing of static exposures represented by one value (average, SWAC, etc.)
- Bioaccumulation models do not represent fish behavior, foraging strategy, life history, habitat preferences
- Either exposed or not – doesn’t capture dynamics of fish behavior
- Don’t typically capture changes over time
- Doesn’t capture uncertainty and variability

ERDC TN-DOER-R17
August 2011

Bioaccumulation Models: State of the Application at Large Superfund Sites

by Karl Gustavson, Katherine von Stackelberg, Igor Linkov, and Todd Bridges

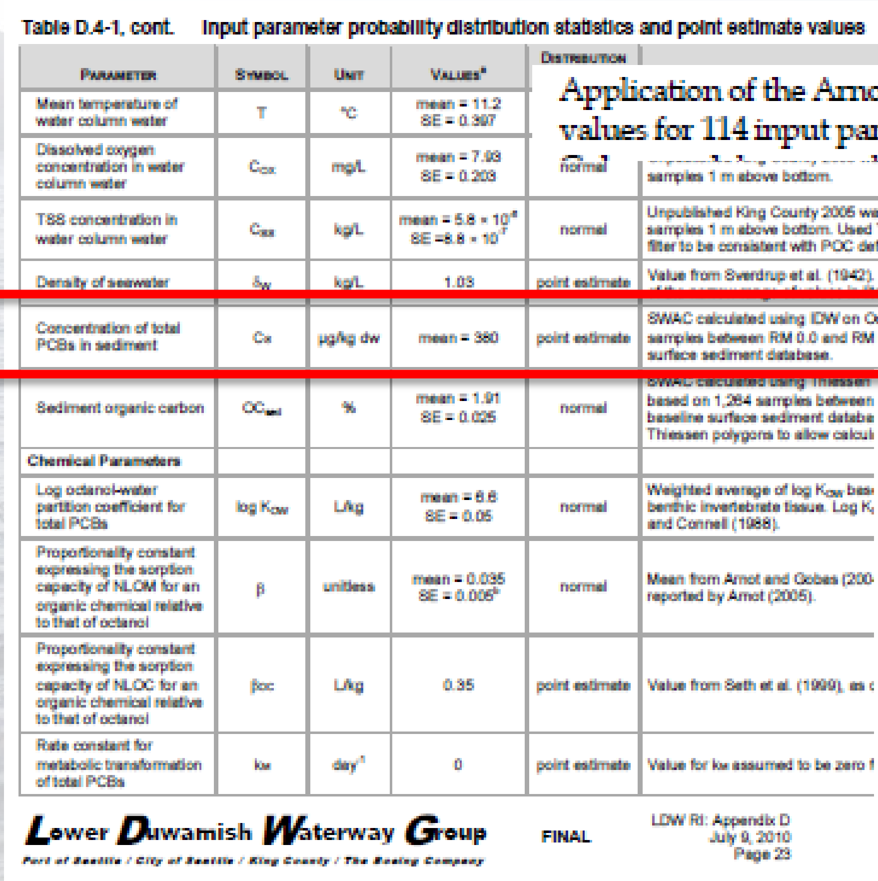


Table D.4-1, cont. Input parameter probability distribution statistics and point estimate values

Parameter	Symbol	Unit	Values[a]	Distribution	
Mean temperature of water column water	T	°C	mean = 11.2 SE = 0.397		
Dissolved oxygen concentration in water column water	C_{OX}	mg/L	mean = 7.93 SE = 0.203	normal	samples 1 m above bottom.
TSS concentration in water column water	C_{SS}	kg/L	mean = 5.8×10^{-6} SE = 6.8×10^{-7}	normal	Unpublished King County 2005 water data (Mickelson 2006) from samples 1 m above bottom. Used TSS samples filtered with a 45-µm filter to be consistent with POC definition (> 45 µm).
Density of seawater	δ_W	kg/L	1.03	point estimate	Value from Sverdrup et al. (1942). Point estimate assumed because
Concentration of total PCBs in sediment	C_S	µg/kg dw	mean = 380	point estimate	SWAC calculated using IDW on October 20, 2006, based on 1,264 samples between RM 0.0 and RM 5.25 from the LDW baseline surface sediment database.
Sediment organic carbon	OC_{sed}	%	mean = 1.91 SE = 0.025	normal	SWAC calculated using Thiessen based on 1,264 samples between baseline surface sediment databa Thiessen polygons to allow calcul
Chemical Parameters					
Log octanol-water partition coefficient for total PCBs	log K_{OW}	L/kg	mean = 6.8 SE = 0.05	normal	Weighted average of log K_{OW} bas benthic invertebrate tissue. Log K and Connell (1988).
Proportionality constant expressing the sorption capacity of NLOM for an organic chemical relative to that of octanol	β	unitless	mean = 0.035 SE = 0.005[b]	normal	Mean from Arnot and Gobas (200 reported by Arnot (2005).
Proportionality constant expressing the sorption capacity of NLOC for an organic chemical relative to that of octanol	β_{OC}	L/kg	0.35	point estimate	Value from Seth et al. (1999), as
Rate constant for metabolic transformation of total PCBs	k_M	day^{-1}	0	point estimate	Value for k_M assumed to be zero f

Lower Duwamish Waterway Group
Port of Seattle / City of Seattle / King County / The Boeing Company

FINAL

LDW RI: Appendix D
July 9, 2010
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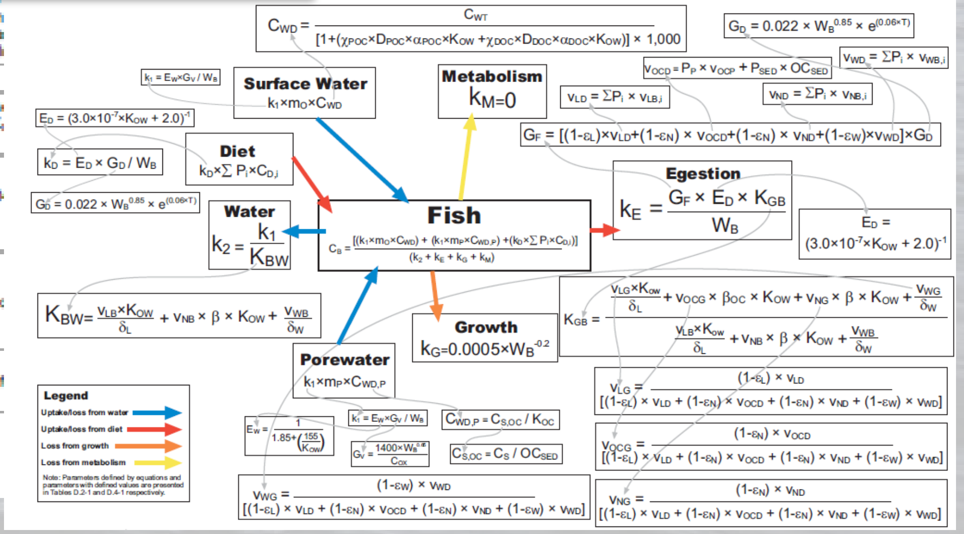
Application of the Arnot and Gobas (2004a) FWM to the LDW required the selection of values for 114 input parameters (including dietary fractions). Because the Arnot and



$$C_{WD} = \frac{C_{WT}}{[1+(\chi_{POC}\times D_{POC}\times\alpha_{POC}\times K_{OW}+\chi_{DOC}\times D_{DOC}\times\alpha_{DOC}\times K_{OW})]\times 1{,}000}$$

$G_D = 0.022 \times W_B^{0.85} \times e^{(0.06\times T)}$

$v_{WD} = \Sigma P_i \times v_{WB,i}$

$v_{OCD} = P_P \times v_{OCP} + P_{SED} \times OC_{SED}$

$k_1 = E_W \times G_V / W_B$

Surface Water
$k_1 \times m_O \times C_{WD}$

Metabolism
$k_M = 0$

$v_{LD} = \Sigma P_i \times v_{LB,i}$

$v_{ND} = \Sigma P_i \times v_{NB,i}$

$E_D = (3.0\times10^{-7}\times K_{OW} + 2.0)^{-1}$

$G_F = [(1-\varepsilon_L)\times v_{LD}+(1-\varepsilon_N)\times v_{OCD}+(1-\varepsilon_N)\times v_{ND}+(1-\varepsilon_W)\times v_{WD}]\times G_D$

$k_D = E_D \times G_D / W_B$

Diet
$k_D \times \sum P_i \times C_{D,i}$

Egestion
$$k_E = \frac{G_F \times E_D \times K_{GB}}{W_B}$$

$G_D = 0.022 \times W_B^{0.85} \times e^{(0.06\times T)}$

Water
$$k_2 = \frac{k_1}{K_{BW}}$$

Fish
$$C_B = \frac{[(k_1\times m_O\times C_{WD}) + (k_1\times m_P\times C_{WD,P}) + (k_D\times\sum P_i\times C_{D,i})]}{(k_2 + k_E + k_G + k_M)}$$

$$E_D = (3.0\times10^{-7}\times K_{OW} + 2.0)^{-1}$$

$$K_{BW} = \frac{v_{LB}\times K_{OW}}{\delta_L} + v_{NB}\times\beta\times K_{OW} + \frac{v_{WB}}{\delta_W}$$

$$K_{GB} = \frac{\frac{v_{LG}\times K_{ow}}{\delta_L} + v_{OCG}\times\beta_{OC}\times K_{OW} + v_{NG}\times\beta\times K_{OW} + \frac{v_{WG}}{\delta_W}}{\frac{v_{LB}\times K_{ow}}{\delta_L} + v_{NB}\times\beta\times K_{OW} + \frac{v_{WB}}{\delta_W}}$$

Growth
$k_G = 0.0005 \times W_B^{-0.2}$

Porewater
$k_1 \times m_P \times C_{WD,P}$

Legend
Uptake/loss from water
Uptake/loss from diet
Loss from growth
Loss from metabolism

Note: Parameters defined by equations and parameters with defined values are presented in Tables D.2-1 and D.4-1 respectively.

$$E_W = \frac{1}{1.85 + \left(\frac{155}{K_{OW}}\right)}$$

$k_1 = E_W \times G_V / W_B$

$C_{WD,P} = C_{S,OC} / K_{OC}$

$$G_V = \frac{1400\times W_B^{0.65}}{C_{OX}}$$

$C_{S,OC} = C_S / OC_{SED}$

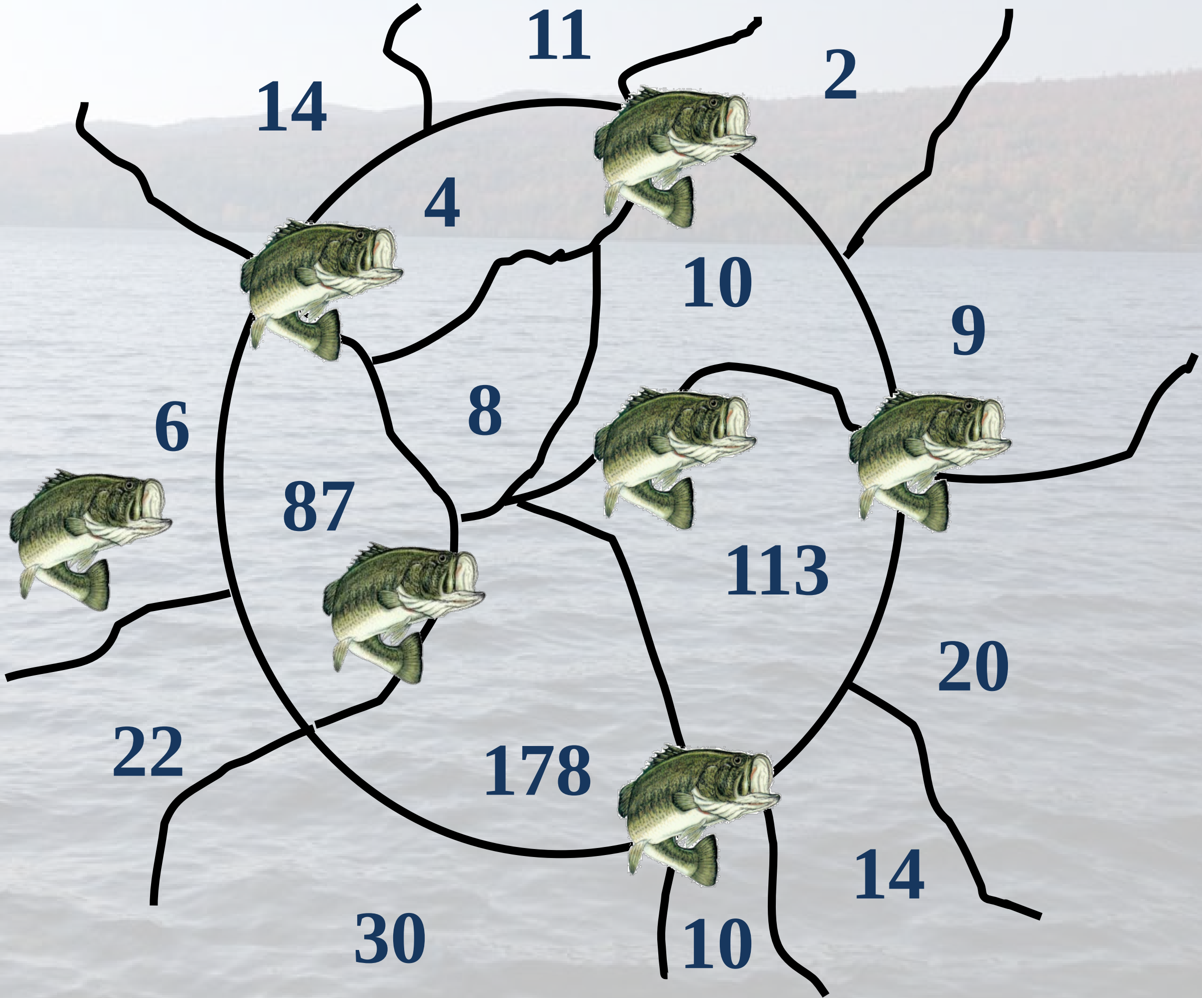
$$v_{LG} = \frac{(1-\varepsilon_L)\times v_{LD}}{[(1-\varepsilon_L)\times v_{LD} + (1-\varepsilon_N)\times v_{OCD} + (1-\varepsilon_N)\times v_{ND} + (1-\varepsilon_W)\times v_{WD}]}$$

$$v_{OCG} = \frac{(1-\varepsilon_N)\times v_{OCD}}{[(1-\varepsilon_L)\times v_{LD} + (1-\varepsilon_N)\times v_{OCD} + (1-\varepsilon_N)\times v_{ND} + (1-\varepsilon_W)\times v_{WD}]}$$

$$v_{WG} = \frac{(1-\varepsilon_W)\times v_{WD}}{[(1-\varepsilon_L)\times v_{LD} + (1-\varepsilon_N)\times v_{OCD} + (1-\varepsilon_N)\times v_{ND} + (1-\varepsilon_W)\times v_{WD}]}$$

$$v_{NG} = \frac{(1-\varepsilon_N)\times v_{ND}}{[(1-\varepsilon_L)\times v_{LD} + (1-\varepsilon_N)\times v_{OCD} + (1-\varepsilon_N)\times v_{ND} + (1-\varepsilon_W)\times v_{WD}]}$$

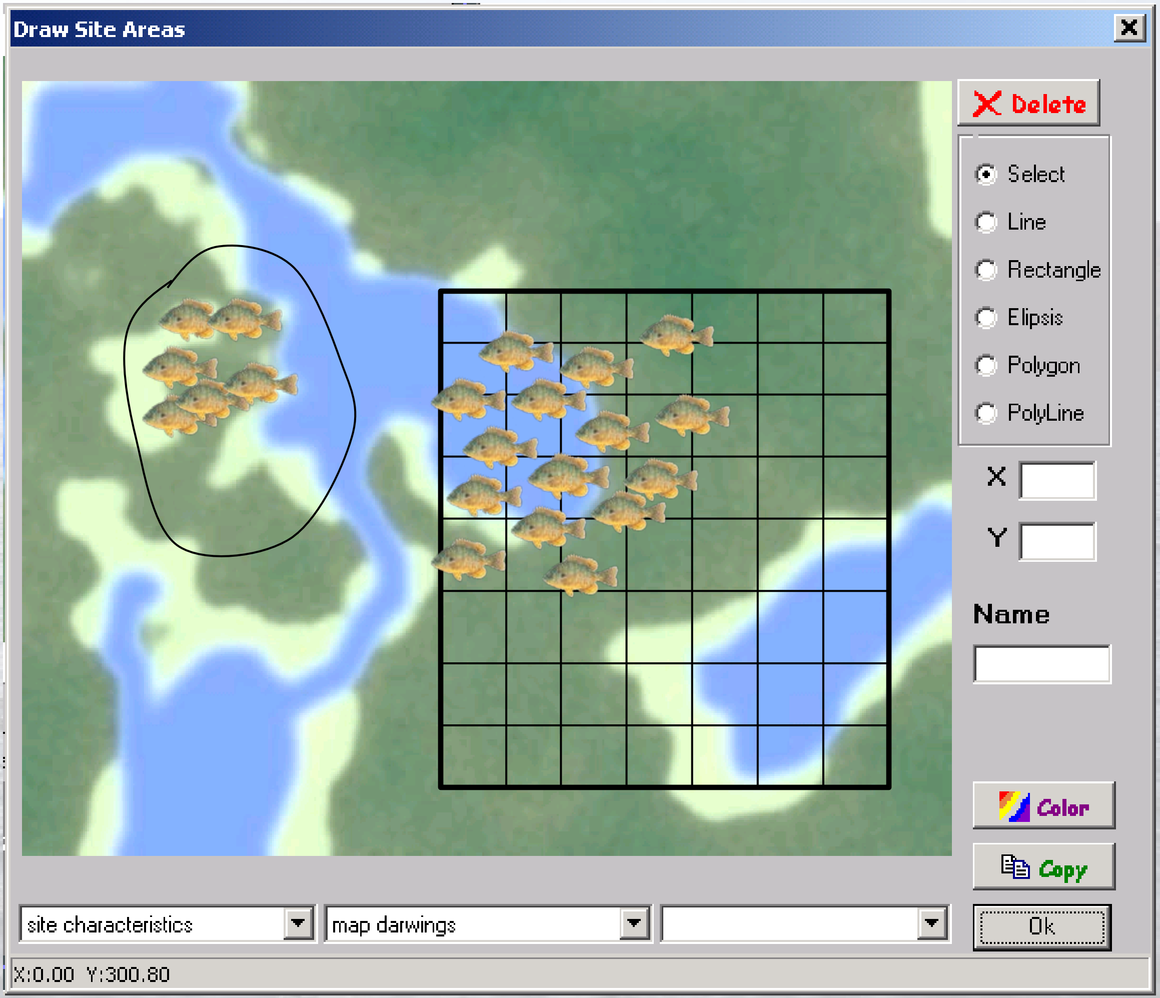
Spatial Heterogeneity in Exposure



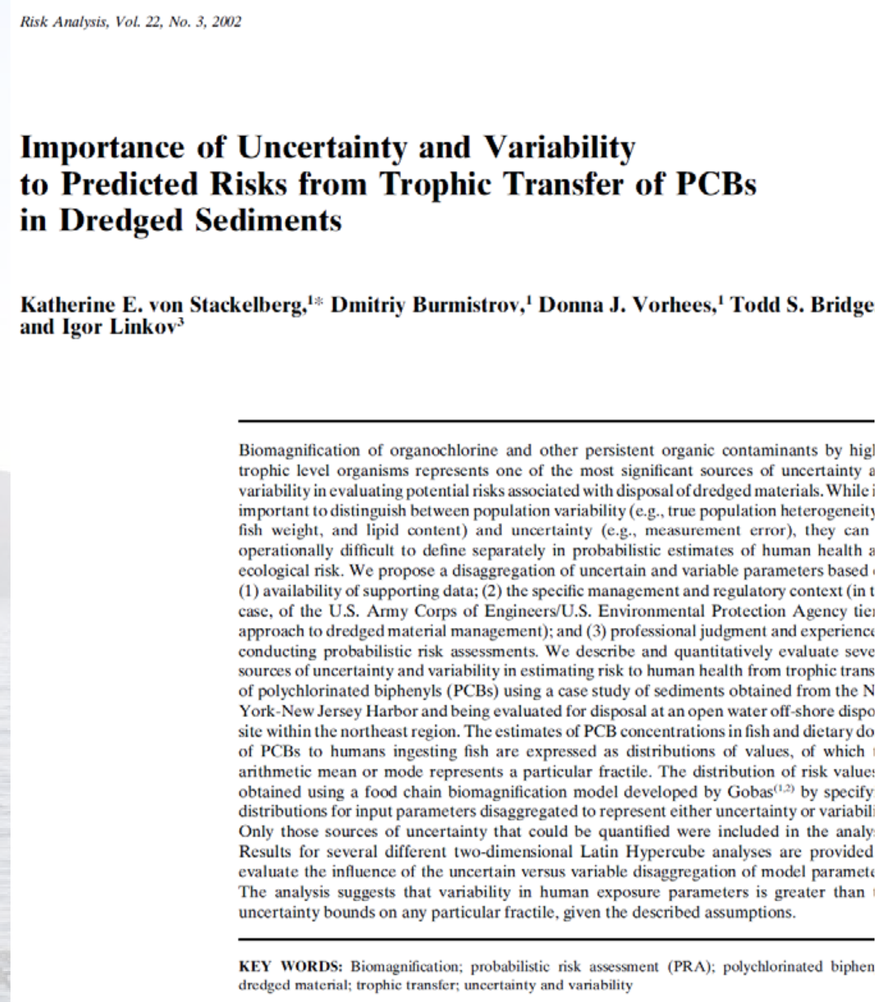
Motivation for Spatially-Explicit Approach

- Spatial and temporal scales associated with ecological receptor exposure
- Fish have localized movements
  - Daily foraging strategies
  - Preferential habitat and foraging areas
- Seasonal habits
  - Migratory status
  - May leave modeling grid for parts of the year
  - Offshore movements

FishRand Approach



- Sampling from a population of fish
- Movements and foraging strategies contribute to the distribution of predicted tissue concentrations
- Takes advantage of GIS-based sediment concentrations
- Probabilistic linkages
    - Decision analytic approaches
    - Integration with economic and other data



Risk Analysis, Vol. 22, No. 3, 2002

Importance of Uncertainty and Variability to Predicted Risks from Trophic Transfer of PCBs in Dredged Sediments

Katherine E. von Stackelberg,[1]* Dmitriy Burmistrov,[1] Donna J. Vorhees,[1] Todd S. Bridges,[2] and Igor Linkov[3]

Biomagnification of organochlorine and other persistent organic contaminants by hig
trophic level organisms represents one of the most significant sources of uncertainty a
variability in evaluating potential risks associated with disposal of dredged materials. While i
important to distinguish between population variability (e.g., true population heterogeneity
fish weight, and lipid content) and uncertainty (e.g., measurement error), they can
operationally difficult to define separately in probabilistic estimates of human health a
ecological risk. We propose a disaggregation of uncertain and variable parameters based
(1) availability of supporting data; (2) the specific management and regulatory context (in t
case, of the U.S. Army Corps of Engineers/U.S. Environmental Protection Agency tie
approach to dredged material management); and (3) professional judgment and experienc
conducting probabilistic risk assessments. We describe and quantitatively evaluate seve
sources of uncertainty and variability in estimating risk to human health from trophic trans
of polychlorinated biphenyls (PCBs) using a case study of sediments obtained from the N
York-New Jersey Harbor and being evaluated for disposal at an open water off-shore dispo
site within the northeast region. The estimates of PCB concentrations in fish and dietary do
of PCBs to humans ingesting fish are expressed as distributions of values, of which
arithmetic mean or mode represents a particular fractile. The distribution of risk value
obtained using a food chain biomagnification model developed by Gobas[1,2] by specify
distributions for input parameters disaggregated to represent either uncertainty or variabili
Only those sources of uncertainty that could be quantified were included in the analy
Results for several different two-dimensional Latin Hypercube analyses are provided
evaluate the influence of the uncertain versus variable disaggregation of model paramet
The analysis suggests that variability in human exposure parameters is greater than
uncertainty bounds on any particular fractile, given the described assumptions.

KEY WORDS: Biomagnification; probabilistic risk assessment (PRA); polychlorinated biphen
dredged material; trophic transfer; uncertainty and variability

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The use of spatial modeling in an aquatic food web to estimate exposure and risk

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Todd S. Bridges[c]

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Abstract

This paper quantitatively evaluates interactions among foraging behavior, habitat preferences, site characteristics and the spatial distribution of contaminants in estimating PCB exposure concentrations for winter flounder at a hypothetical open water dredged material disposal site in the coastal waters of New York and New Jersey (NY–NJ). The models implemented in this study include a spatial submodel to account for spatial and temporal characteristics of fish exposure and a probabilistic adaptation of the Gobas bioaccumulation model to account for temporal variation in concentrations of polychlorinated biphenyls (PCBs) in sediment and water. We estimated the geographic distribution of an offshore winter flounder subpopulation based on species biology, including such variables as foraging area, habitat size, disposal site size and migration characteristics. We incorporated these variables together with an estimate of differential attraction to a management site within a spatially explicit model to assess the range of expected PCB exposures to a winter flounder population. The output of this modeling effort, flounder PCB tissue concentrations, provides exposure point concentrations for estimates of human health risk through ingestion of locally caught flounder. The risks obtained for the spatially non-explicit case are as much as one order of magnitude higher than those obtained after incorporating spatial and temporal characteristics of winter flounder foraging and seasonal migration. Incorporating spatial and temporal variables in food chain models can help support sediment management decisions by providing a quantitative expression of the confidence in risk estimates. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Bioaccumulation; PCBs; Exposure assessment; Spatial; Probabilistic

SERDP Demonstration Project

DEFINE MODELING AREA:

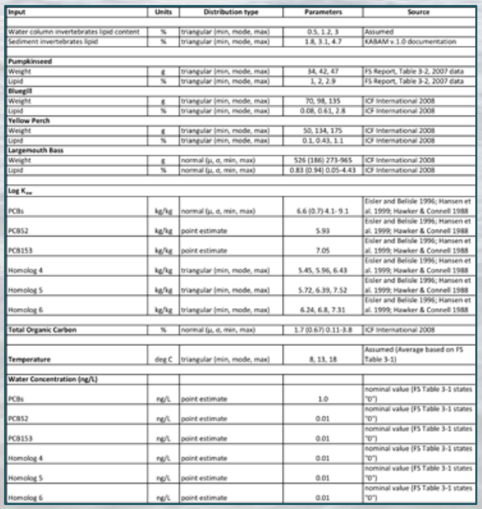
- Base map with GIS-based spatially-defined exposures

SPECIFY INPUTS:

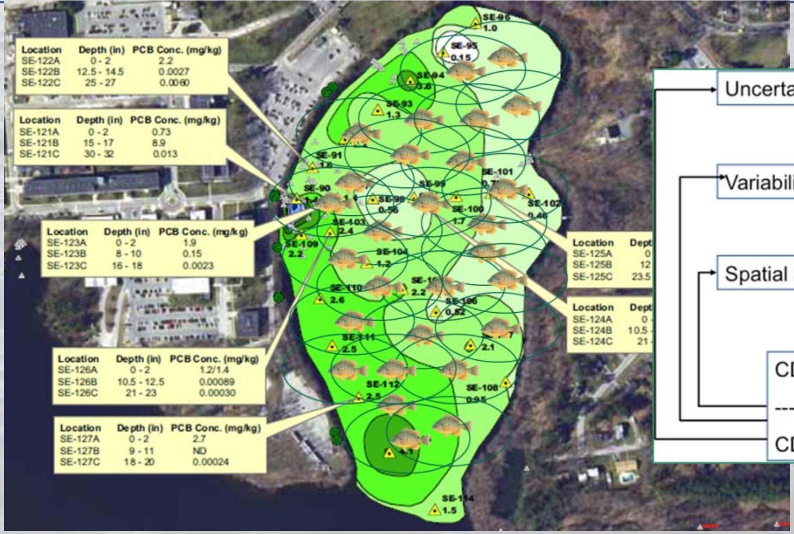
- Simple food web (water column and benthic inverts, pumpkinseed, bluegill, yellow perch, largemouth bass)

THREE MODEL RUNS:

- Inputs to all three runs identical except for sediment concentrations
    - Deterministic (SWAC)
    - Probabilistic (distribution but still averaged)
    - Spatial (in this case, deterministic but spatial; could be distributions)



Input	Units	Distribution type	Parameters	Source
Water column invertebrates lipid content	%	triangular (min, mode, max)	0.5, 1.2, 3	Assumed
Sediment invertebrates lipid	%	triangular (min, mode, max)	1.8, 3.1, 4.7	KABAM v.1.0 documentation
Pumpkinseed				
Weight	g	triangular (min, mode, max)	34, 42, 47	FS Report, Table 3-2, 2007 data
Lipid	%	triangular (min, mode, max)	1, 2, 2.9	FS Report, Table 3-2, 2007 data
Bluegill				
Weight	g	triangular (min, mode, max)	70, 98, 135	ICF International 2008
Lipid	%	triangular (min, mode, max)	0.08, 0.61, 2.8	ICF International 2008
Yellow Perch				
Weight	g	triangular (min, mode, max)	50, 134, 175	ICF International 2008
Lipid	%	triangular (min, mode, max)	0.1, 0.43, 1.1	ICF International 2008
Largemouth Bass				
Weight	g	normal (μ, σ, min, max)	526 (186) 273-965	ICF International 2008
Lipid	%	normal (μ, σ, min, max)	0.83 (0.94) 0.05-4.43	ICF International 2008
Log K_{ow}				
PCBs	kg/kg	normal (μ, σ, min, max)	6.6 (0.7) 4.1- 9.1	Eisler and Belisle 1996; Hansen et al. 1999; Hawker & Connell 1988
PCB52	kg/kg	point estimate	5.93	Eisler and Belisle 1996; Hansen et al. 1999; Hawker & Connell 1988
PCB153	kg/kg	point estimate	7.05	Eisler and Belisle 1996; Hansen et al. 1999; Hawker & Connell 1988
Homolog 4	kg/kg	triangular (min, mode, max)	5.45, 5.96, 6.43	Eisler and Belisle 1996; Hansen et al. 1999; Hawker & Connell 1988
Homolog 5	kg/kg	triangular (min, mode, max)	5.72, 6.39, 7.52	Eisler and Belisle 1996; Hansen et al. 1999; Hawker & Connell 1988
Homolog 6	kg/kg	triangular (min, mode, max)	6.24, 6.8, 7.31	Eisler and Belisle 1996; Hansen et al. 1999; Hawker & Connell 1988
Total Organic Carbon	%	normal (μ, σ, min, max)	1.7 (0.67) 0.11-3.8	ICF International 2008
Temperature	deg C	triangular (min, mode, max)	8, 13, 18	Assumed (Average based on FS Table 3-1)
Water Concentration (ng/L)				
PCBs	ng/L	point estimate	1.0	nominal value (FS Table 3-1 states "0")
PCB52	ng/L	point estimate	0.01	nominal value (FS Table 3-1 states "0")
PCB153	ng/L	point estimate	0.01	nominal value (FS Table 3-1 states "0")
Homolog 4	ng/L	point estimate	0.01	nominal value (FS Table 3-1 states "0")
Homolog 5	ng/L	point estimate	0.01	nominal value (FS Table 3-1 states "0")
Homolog 6	ng/L	point estimate	0.01	nominal value (FS Table 3-1 states "0")



Location	Depth (in)	PCB Conc. (mg/kg)
SE-122A	0 - 2	2.2
SE-122B	12.5 - 14.5	0.0027
SE-122C	25 - 27	0.0060

Location	Depth (in)	PCB Conc. (mg/kg)
SE-121A	0 - 2	0.73
SE-121B	15 - 17	8.9
SE-121C	30 - 32	0.013

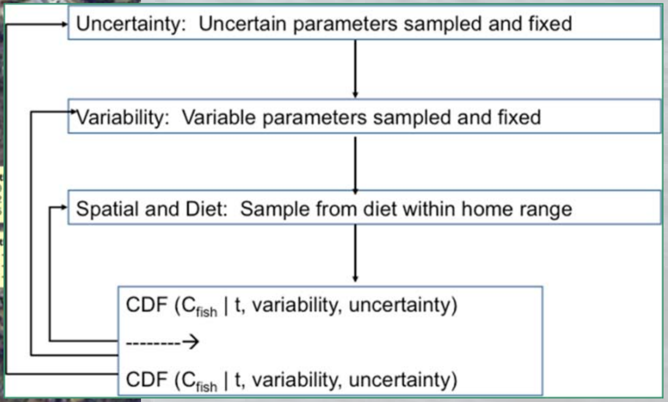
Location	Depth (in)	PCB Conc. (mg/kg)
SE-123A	0 - 2	1.9
SE-123B	8 - 10	0.15
SE-123C	16 - 18	0.0023

Location	Depth (in)	PCB Conc. (mg/kg)
SE-126A	0 - 2	1.2/1.4
SE-126B	10.5 - 12.5	0.00089
SE-126C	21 - 23	0.00030

Location	Depth (in)	PCB Conc. (mg/kg)
SE-127A	0 - 2	2.7
SE-127B	9 - 11	ND
SE-127C	18 - 20	0.00024

Location	Dept
SE-125A	0
SE-125B	12
SE-125C	23.5

Location	Dept
SE-124A	0
SE-124B	10.5
SE-124C	21



Uncertainty: Uncertain parameters sampled and fixed

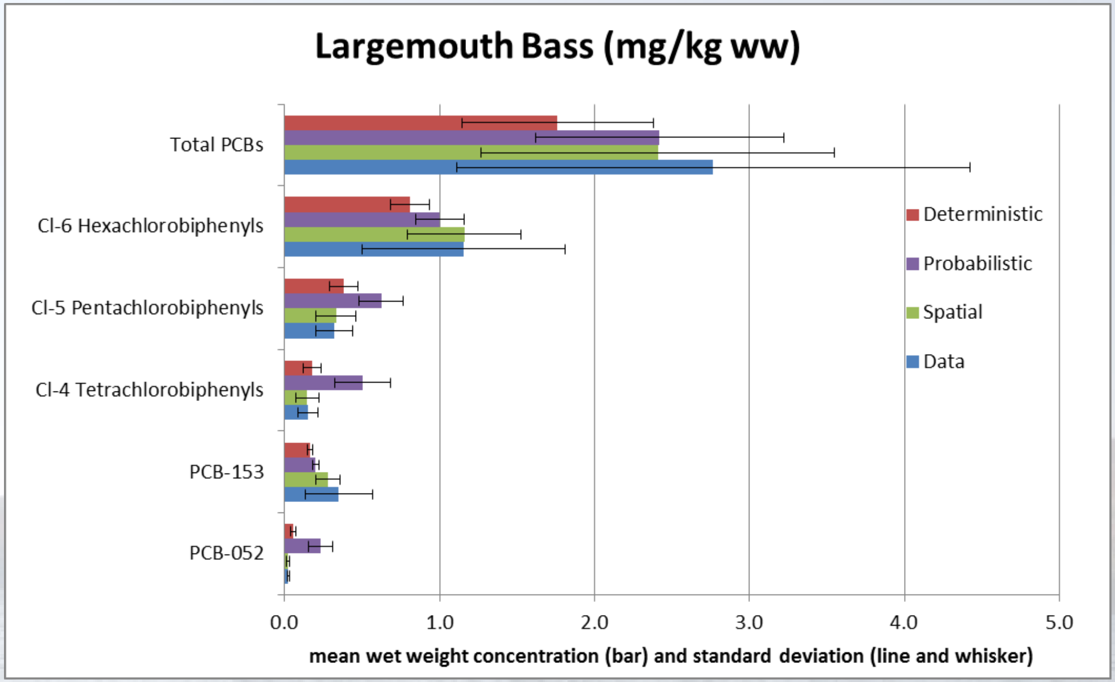
Variability: Variable parameters sampled and fixed

Spatial and Diet: Sample from diet within home range

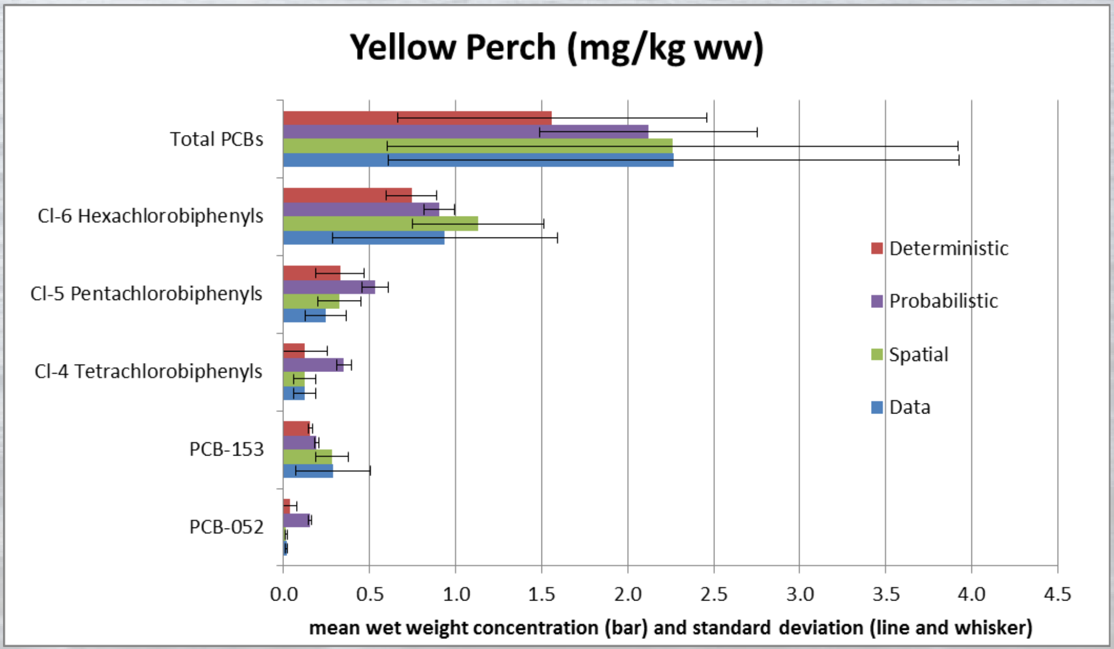
CDF (C_{fish} | t, variability, uncertainty)

--------→

CDF (C_{fish} | t, variability, uncertainty)



Largemouth Bass (mg/kg ww)



Yellow Perch (mg/kg ww)

Species	Observed Mean (mg/kg ww)	Deterministic Case (mg/kg ww)	Probabilistic (No Spatial) (mg/kg ww)	Spatially-Explicit Model Results (mg/kg ww)	RPD Deterministic	RPD Probabilistic	RPD Spatially-Explicit
Yellow Perch							
PCB-052	0.016	0.037	0.155	0.015	78%	162%	-7%
PCB-153	0.289	0.156	0.191	0.281	-60%	-41%	-3%
Cl-4 Tetrachlorobiphenyls	0.124	0.122	0.351	0.122	-1%	96%	-1%
Cl-5 Pentachlorobiphenyls	0.247	0.328	0.53	0.323	28%	73%	27%
Cl-6 Hexachlorobiphenyls	0.938	0.745	0.903	1.130	-23%	-4%	19%
Total PCBs	2.266	1.56	2.12	2.260	-37%	-7%	0%
Bluegill							
PCB-052	0.008	0.016	0.079	0.006	69%	164%	-21%
PCB-153	0.072	0.049	0.043	0.086	-39%	-51%	17%
Cl-4 Tetrachlorobiphenyls	0.045	0.05	0.171	0.049	10%	116%	8%
Cl-5 Pentachlorobiphenyls	0.087	0.111	0.192	0.108	24%	75%	22%
Cl-6 Hexachlorobiphenyls	0.240	0.239	0.283	0.362	0%	16%	41%
Total PCBs	0.582	0.623	0.79	0.848	7%	30%	37%
Largemouth Bass							
PCB-052	0.023	0.054	0.231	0.021	81%	164%	-8%
PCB-153	0.348	0.161	0.198	0.276	-74%	-55%	-23%
Cl-4 Tetrachlorobiphenyls	0.149	0.175	0.502	0.146	16%	109%	-2%
Cl-5 Pentachlorobiphenyls	0.321	0.379	0.622	0.331	16%	64%	3%
Cl-6 Hexachlorobiphenyls	1.154	0.81	1.000	1.160	-35%	-14%	1%
Total PCBs	2.767	1.76	2.420	2.410	-44%	-13%	-14%

RPD = relative percent difference calculated as (predicted-observed)/average(predicted,observed)

green values indicate lowest RPD; blue values indicate within 50% of observed

Example Application and Linkage to Decision Analytic Framework

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Special Series

Decision Analytic Strategies for Integrating Ecosystem Services and Risk Assessment

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(Submitted 22 June 2012; Returned for Revision 7 August 2012; Accepted 28 December 2012)

EDITOR'S NOTE

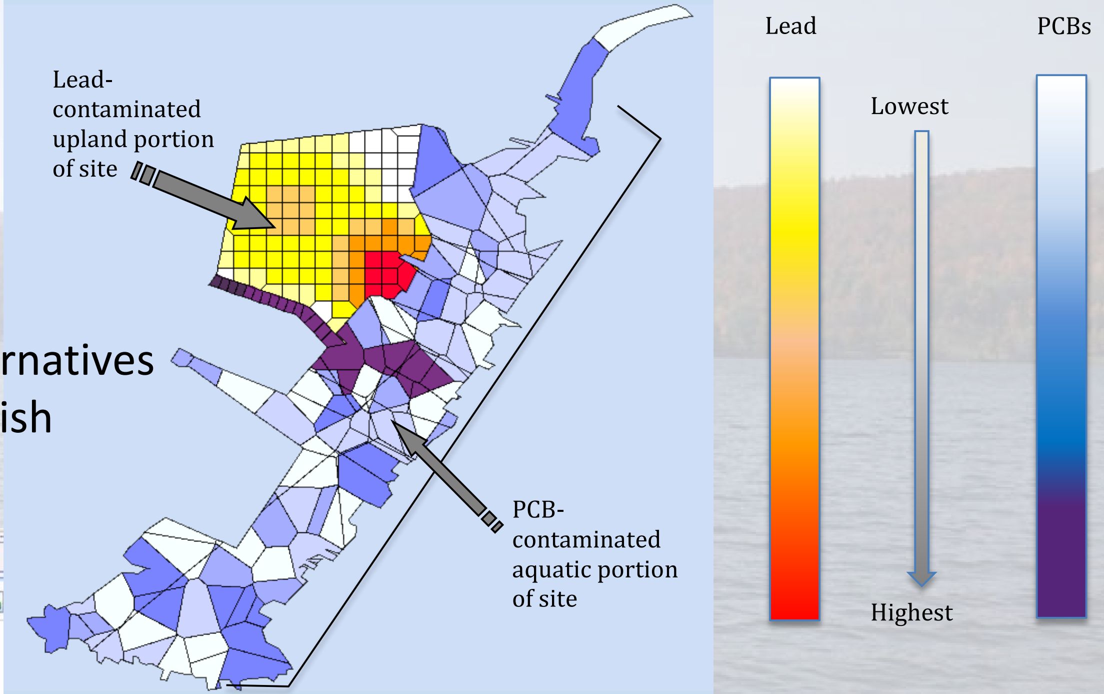
This paper is one of 8 articles generated from the SETAC Special Symposium: Ecosystem Services, from Policy to Practice (15-16 February 2012, Brussels, Belgium). The symposium aimed to give a broad overview of the application of the ecosystem services concept in environmental assessment and management, against the background of the implementation of the European environmental policies such as the biodiversity agenda, agricultural policy, and the water framework directive.

ABSTRACT

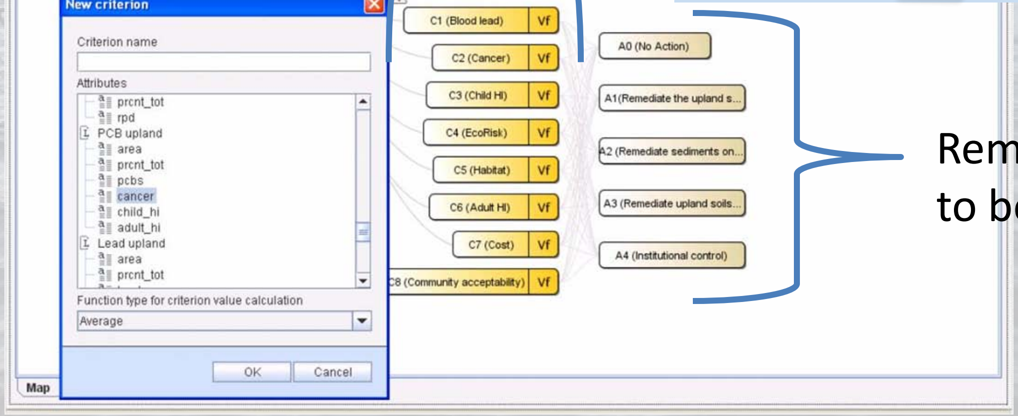
Ecosystem services as a concept and guiding principle are enjoying wide popularity and endorsement from high-level policy thinkers to industry as support for sustainability goals continue to grow. However, explicit incorporation of ecosystem services into decision making still lacks practical implementation at more local scales and faces significant regulatory and technical constraints. Risk assessment represents an example of a regulatory process for which guidance exists that makes it challenging to incorporate ecosystem service endpoints. Technical constraints exist in the quantification of the relationships between ecological functions and services and endpoints valued by humans, and the complexity of those interactions with respect to bundling and stacking. In addition, ecosystem services, by their very definition, represent an anthropogenic construct with no inherent ecological value, which, in practical terms, requires a far more inclusionary decision making process explicitly incorporating a greater diversity of stakeholder values. Despite these constraints, it is possible, given a commitment to sustainable decision making, to simplify the process based on strategic outcomes (e.g., identifying desired end-states in general terms). Decision analytic techniques provide a mechanism for evaluating tradeoffs across key ecosystem services valued by stakeholders and to develop criteria drawn from the entire spectrum of stakeholders in evaluating potential alternatives. This article highlights several examples of ways in which ecosystem service endpoints can be incorporated into the decision-making process. Integr Environ Assess Manag 2013;9:260–268. © 2013 SETAC

Keywords: Ecosystem services Decision analysis MCDA Influence diagrams Sustainability

Evaluation of Remedial Alternatives



Criteria against which alternatives are evaluated (predicted fish tissue concentrations → probabilistic risk results



New criterion

Criterion name

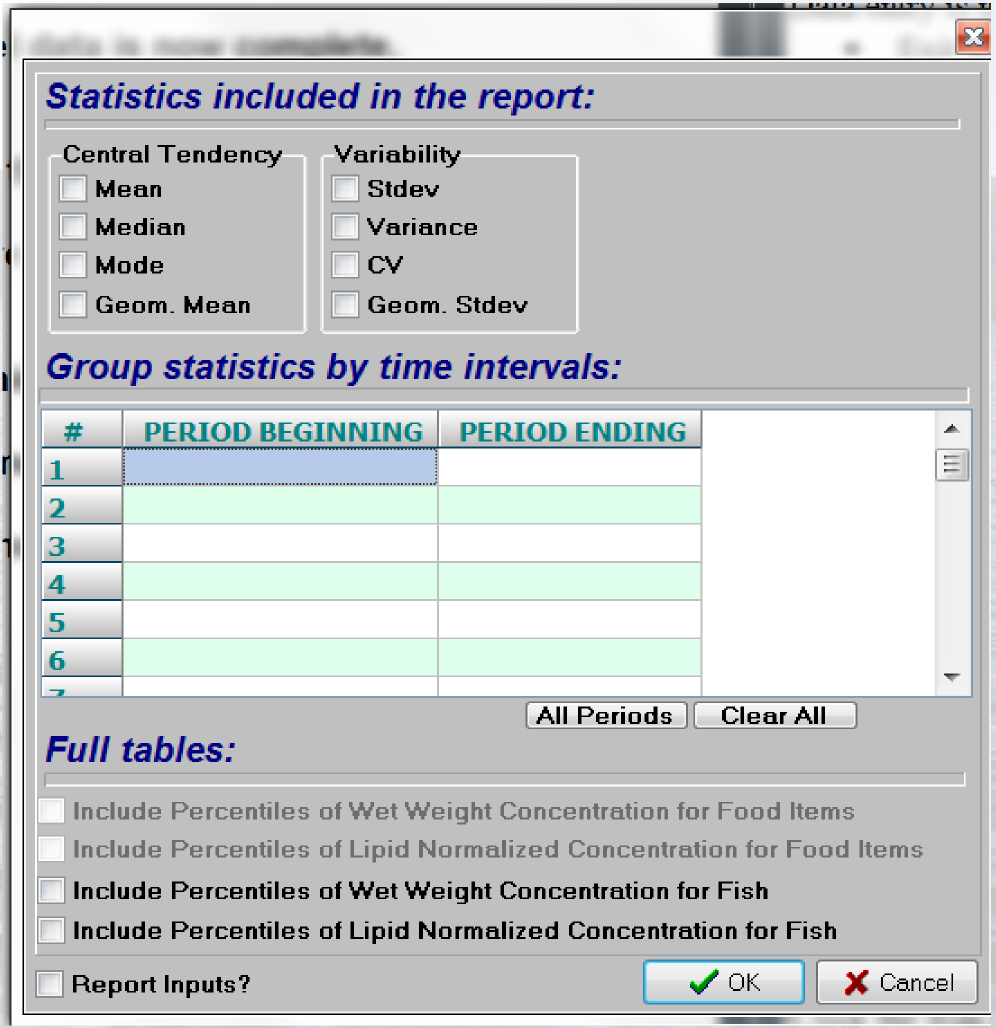
Attributes

- prcnt_tot
- rpd
- PCB upland
  - area
  - prcnt_tot
  - pcbs
  - cancer
  - child_hi
  - adult_hi
- Lead upland
  - area
  - prcnt_tot

Function type for criterion value calculation: Average

Remedial alternatives to be evaluated

Output Statistics from FR Link Directly to Risk Assessment Model to Criteria



Statistics included in the report:

Central Tendency
- ☐ Mean
- ☐ Median
- ☐ Mode
- ☐ Geom. Mean

Variability
- ☐ Stdev
- ☐ Variance
- ☐ CV
- ☐ Geom. Stdev

Group statistics by time intervals:

#	PERIOD BEGINNING	PERIOD ENDING
1		
2		
3		
4		
5		
6		

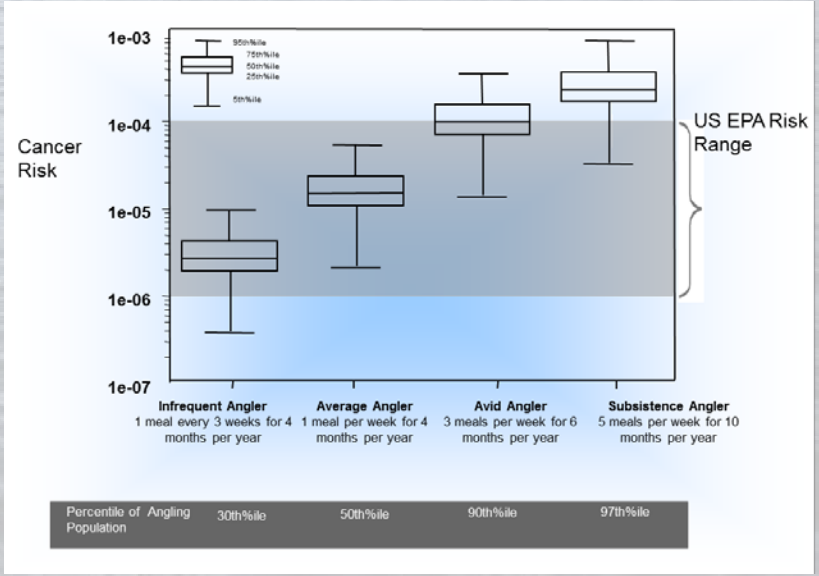
Full tables:

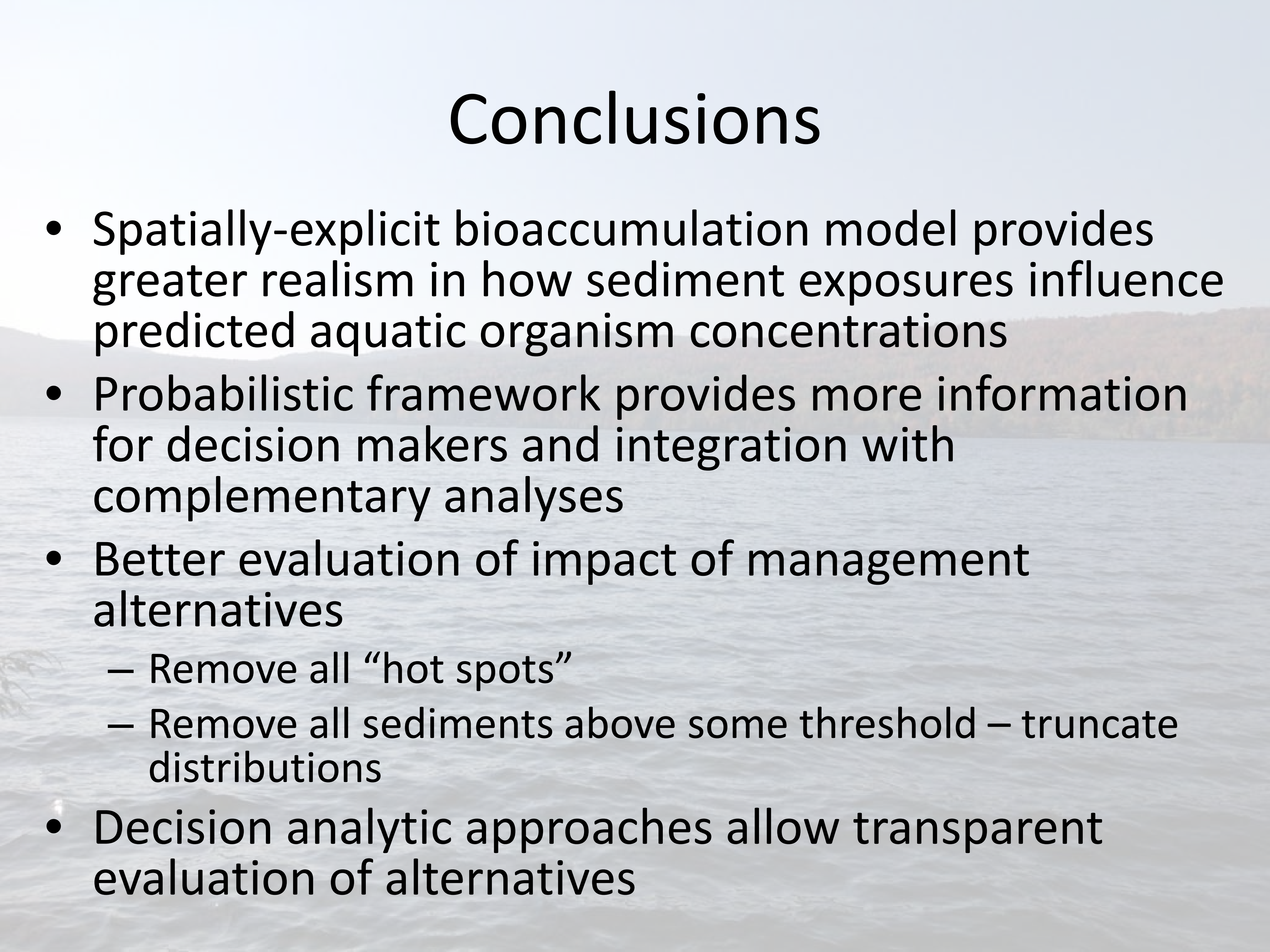
- ☐ Include Percentiles of Wet Weight Concentration for Food Items
- ☐ Include Percentiles of Lipid Normalized Concentration for Food Items
- ☐ Include Percentiles of Wet Weight Concentration for Fish
- ☐ Include Percentiles of Lipid Normalized Concentration for Fish

☐ Report Inputs?

Model can generate different statistics of predicted tissue concentrations for use in risk assessment model

In this example, links directly to risk model within a GIS-based decision analytic framework





Conclusions

- Spatially-explicit bioaccumulation model provides greater realism in how sediment exposures influence predicted aquatic organism concentrations
- Probabilistic framework provides more information for decision makers and integration with complementary analyses
- Better evaluation of impact of management alternatives
  - Remove all “hot spots”
  - Remove all sediments above some threshold – truncate distributions
- Decision analytic approaches allow transparent evaluation of alternatives

Thank You!!

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Acknowledgments

FishRand was developed with funding from the Army Corps of Engineers. Currently, the model is available by request from Dr. von Stackelberg; plans are underway to make it publicly available via web download.