Issue Paper on Using Bioaccumulation Information to Develop Risk-based Sediment Remediation Goals for Superfund Sites

Prepared by Larry Burkhard - ORD/NHEERL-MED, Steve Ells - OSRTI, and Marc Greenberg - OSRTI/ERT for use at EPA Sediment Risk Meeting in Dallas, March 15 - 18, 2004.

I Background

Historically, bioaccumulative contaminants such as PCBs, DDT, and mercury in sediment have presented unacceptable human health and/or ecological risks at many Superfund sites. The risks have usually been due to ingestion of contaminated fish by humans or fish-eating mammals and birds. At most of these sites, especially the bigger ones, fish bioaccumulation models or food chain models, such as the Gobas model (or variations of this model), have been used to back- calculate acceptable sediment concentrations from acceptable fish tissue residues. These same models can also be used to estimate the potential ecological and/or human health baseline risks. At these bigger sites, food chain models are often coupled in some fashion to both hydrodynamic models and fate and transport models that provide the input parameters to the food chain models. It is these same computer models, after undergoing site-specific calibration, that are also then used to compare how well or how soon remedial alternatives such as MNR, capping, and dredging, (including different capping designs and dredging scenarios) will achieve protective risk-based fish tissue levels.

Many of the computer models that have been used have required a lot of site data and a lot of computer time and expertise to run the models, and have cost hundreds of thousands of dollars (and sometimes millions) to develop, calibrate, and validate using site specific data. Despite the great cost, there is still a lot of uncertainty (although not always expressed) concerning the model outputs. In light of the resulting uncertainty, and the high costs and long time it takes to run computer models, should we encourage the use of other tools and simple models using mostly empirical data to estimate risk-based sediment cleanup goals? One way to do this, might be to develop a site-specific BSAF (biota-sediment accumulation factor) for each COC that presents an unacceptable risk via fish ingestion.

II Issues

The overarching issue is how to decide when to use a computer-driven food chain model vs. a BSAF approach, or a hybrid approach to develop protective sediment cleanup goals for risks posed by consumption/ingestion of contaminated fish (*i.e.*, risks to humans and higher level ecological receptors). To get to this decision point, the following issues need to be addressed:

1 What are the key factors to consider in making this site-specific determination?
   - Do we need to use a model to estimate baseline risks? If so, can it be the same model?

- Do we also need to use hydrodynamic and fate and transport models to select a remedy?
- If so, can the food chain model be linked to these models?
- Based upon site characteristics, background contaminant levels and other sources, how likely is it that an active remedy will be able to achieve typical low/very low cleanup levels?
- Do we have the time and money and expertise to build and use the models?
- What level of uncertainty and precision is needed to make a remedy decision for the site?
- Do we know enough about fish diets, the dynamics of remediated sediment beds, and the recolonization of remediated areas to predict the time-course and magnitudes of fish tissue responses to remediation?
- Do we need to use a model to determine the relative contributions of various sources of bioaccumulative contaminants (e.g., sediment source, groundwater flux, flood plain erosion, upstream water column, atmospheric input)?

2 If we decide to use a food-chain model, which model should be used?

- Can a simpler fish bioaccumulation model vs. food-chain model be used?
- Can we identify a "best" model for freshwater/marine, lotic/lentic environments? For different food-chains? For different contaminants?
- What are the minimum data requirements for the model? Can they all be collected reliably?
- What are the most sensitive parameters; e.g., lipid content, % OC, AVS, grain size, number of tropic levels, prey ingested, dissolved water conc., sediment to water ratio?

3 If we decide to use a BSAF approach, what/how much site-specific data should be used?

- Are contaminant concentrations in the fish more responsive to water or sediment concentrations? Or are they changing depending upon age and micro habitat?
- Do we have or can we collect adequate sediment and fish tissue data?
- Are selected tissue data (i.e., filets, livers) better than whole-body data for estimating BSAFs?
- If the site has changed in sediment quality or is actively changing, are the fish collected at the site representative of long-term, steady-state bioaccumulation? If not, can steady- state BSAF values be derived or intuited from the available data?
- Do we need fish dietary information or is any available?
- Do we understand the fish life-history and home range and the COC bioconcentration with fish size or age well enough to accurately interpret BSAF results?
- How important is it to understand the relation between site-specific results and BSAF theory?
- How certain are we that we understand what the new steady-state conditions that will exist after dredging or capping?
- Should we always do a bounding analysis to estimate worst case future conditions?
- How do use the data if the correlation is non-linear?

4 Which approaches might be more appropriate for dealing with more than one contaminant?

- Can BSAF results (or modeled bioaccumulation values) for one COC be extrapolated to closely-related chemicals?

Assumptions

1 There is an unacceptable baseline risk to humans and/or ecological receptors due to ingestion of contaminated fish or other biota.

2 A remedy will be selected, *i.e*., MNR, capping, or dredging, or a combination.

3 Existing baseline data demonstrate elevated levels of at least one bioaccumulative contaminant in co-located sediment and biota tissue.

4 Existing fish consumption advisories will be needed for some length of time to ensure protection of human health until remedial action objectives are met.

5 A BSAF approach is less expensive, is more transparent (and therefore easier to explain to the public), and more is known about it's level of uncertainty, *i.e*., statistical uncertainty can be directly estimated for the BSAF ratios or regressions.

6 There will be both short-term and long-term monitoring of sediment and fish after remedy implementation to validate the model or BSAF approach and to evaluate risk reduction.

III Technical Background Information on Models

Short Description of BSAF Approach

The biota-sediment accumulation factor (BSAF) is defined as

$$\mathrm{BSAF} = (C_\mathrm{b} / f_\ell) / (C_\mathrm{s} / f_\mathrm{oc}) \qquad (1)$$

where C_b is the organism chemical concentration (ug/kg wet weight), f_ℓ is the lipid fraction of the organism, C_s is the surficial sediment chemical concentration (ug/kg dry weight) and f_oc is the organic carbon fraction of the sediments, respectively.

The BSAF is a simple ratio! The BSAF definition does not include any statement about ecosystem conditions or relationships between the concentrations of chemicals in the organism and sediment (see Ankley et al. 1992, Thomann et al. 1992). Some have mistakenly assumed that BSAFs are only appropriate for equilibrium conditions (see for example, Wong et al. 2001), and that BSAFs determined for non-equilibrium conditions are somehow incorrect. These assumptions are simply not true.

BSAFs, when properly measured (see below), provide a very meaningful measure of the thermodynamic relationship between the organism and the sediment for the chemical, and aquatic organisms can, for a variety of reasons, have relationships with the sediments which depart significantly from equilibrium conditions. Some of these reasons include biomagnification of chemical between trophic levels within the food web, metabolism of the chemical within the organism and/or in its prey, bioavailability issues, and the disequilibrium[1] of the chemical between sediment and water column in the ecosystem. For organisms closely coupled to the sediments, e.g., oligochaetes and amphipods, one generally measures BSAFs in the range of 1-2 for chemicals not metabolizable by the organisms. BSAFs of 1-2 are what one would expect if the organism was at equilibrium with the sediment.

To use a BSAF to predict a chemical residue in a fish (or other aquatic organisms), the concentration of the chemical in the sediment (on an organic carbon basis) spanning the immediate home range of the organism is required. Sediment samples grabbed randomly without consideration of the organism's home range will, in high likelihood, have poor predictive ability for chemical residues in fish because the sediment data will not be representative of the fish's actual exposure. The prediction of the chemical residue in the fish is done by calculating the product of the BSAF and concentration of the chemical in the sediment (on an organic carbon basis). At Superfund sites, concentrations of chemicals are expressed, evaluated, and discussed on a wet weight basis for aquatic organisms and on a dry weight basis for sediments. Because the BSAF is expressed using concentrations of chemical on a lipid and organic carbon normalized bases, assuming a 6% lipid content in the wet fish tissue, and 2% organic carbon content in dry sediment, and a BSAF of 2 would translate into a fish to sediment ratio of 6 on a wet weight-tissue and dry weight-sediment basis (6 = 2×6%/2%).

To measure BSAFs, the sediments samples must be representative of the fish's actual exposure history (or its immediate home range). For resident species, the collection of samples with proper spatial and temporal coordination should be fairly straight forwards provided one does the work to determine the home range of the species. For Superfund sites, the home range of species might or might not be confined to the site. Thus, sediment sampling, depending upon the immediate home range of the species, might be required beyond the Superfund site. Programatically, sediment sampling beyond the Superfund site is often very difficult, and thus, it is recommend that resident/localized species be selected, if at all possible, for the site. In cases where the home range of the species exceeds the Superfund site and collection of sediment samples beyond the Superfund site are not possible, the potential for measuring BSAFs which are not reflective of the bioaccumulation at the site and with poor predictive ability can be large. These cases will need to be evaluated on a site by site basis to determine the potential and size of possible errors associated with the measured BSAFs. If possible, collection of sediment samples beyond the Superfund site for species with home ranges beyond the site would aid greatly in reducing the uncertainties with the measured BSAFs.

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[1] The disequilibrium of the chemical is determined by dividing the sediment-water column chemical concentration ratio (Π_{socw}) by the chemical's *n*-octanol/water partition coefficient (K_{ow}). When Π_{socw}/K_{ow} equals 1, the sediment and water column are at equilibrium. In general, Π_{socw}/K_{ow} is generally greater than 1, and typically, ranges from 3 to 30 in most ecosystems. For Superfund sites where sediments are highly contaminated, disequilibriums can become very large.

Migratory species, when present at Superfund sites, present special challenges. For migratory species, the same requirements listed above exist, i.e., collection of sediment samples across the home range. Additionally, timing of the collection of the fish relative to their arrival into the area must be accounted for in the sampling design. Clearly, collection of the fish when they have just moved into the area will not provide BSAFs of useful value because the residues in the fish and sediments have no relationship to each other. Depending upon the chemical, times required for the chemical residues in the fish come to some type of meaningful relationships with sediments can vary widely. In general, it is suggested that migratory species be collected just before the species migrates out of the area.

Advice on sampling designs for measurements of BSAFs in field situations as been provided by Burkhard (2003). In general, chlorinated chemicals such PCBs, PCDD/Fs, and DDTs which have large K_{ow}s and low metabolism rates, BSAFs can be determined with one simultaneous (i.e., closely spaced in time) collection of fish and sediment samples. For chemicals with higher rates of metabolism and large K_{ow}s, possibly the PAHs in fish, measurement of BSAFs becomes more difficult because appropriate sampling designs will require additional sample collections to account for temporal variability of the concentrations of chemicals in the water. The importance of temporal variability of concentrations of chemicals in water increases with increasing rate of metabolism because the rate of chemical uptake from water (which is independent of the rate of chemical metabolism) becomes more important in controlling the total chemical residue in the fish with increasing rate of metabolism. Measurement of BSAFs for chemicals with log K_{ow}s less than ≈ 4 can be especially difficult because the water exposure route totally controls the residue in the fish due to the high uptake and loss rates of the chemicals across the gills of the fish. For further details, the reader is referred to Burkhard (2003).

References

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Short Description of Hybrid Empirical/Modeling Approach

The hybrid empirical/modeling approach consists of taking high quality field measured BSAFs and then, extrapolating these values to different ecosystems and species, and to different time periods within an ecosystem. The extrapolated BSAFs would then be used to predict chemical residues in fish (or other aquatic organisms) based upon the concentration of chemicals in the sediment; just like the BSAF approach above.

The actual process of taking high quality field measured BSAFs in one ecosystem and applying them to different ecosystems and species, and to different time periods within an ecosystem would be accomplished using simple food web models. With simple food web models, relative differences in bioaccumulation will be forecasted using the conditions and parameters of the two ecosystems. To illustrate the hybrid approach, BSAFs were predicted for 5-year old walleyes (a trophic level four fish) using the BSAFs measured for adult alewife (a trophic level three fish) in the Zone 4 of the Green Bay, Lake Michigan ecosystem and relative differences between trophic levels three and four fishes, predicted using a simple food web model (see table). There is a slight negative bias in agreement; predicted BSAFs being larger than the measured BSAFs for the 5-year old walleyes. However, for many of the PCB congeners, the agreement between measured and predicted BSAFs are within 10%.

Across Species Extrapolation of BSAFs using the Hybrid Modeling Approach Between Adult Alewife and 5-year old walleye in Zone 4 of the Green Bay, Lake Michigan Ecosystem (Burkhard et al. 2003).

			Hybrid Modeling Approach				
PCB	log K_{ow}	Field measured adult alewife BSAFs	Predicted relative differences	Predicted trophic level four BSAFs	Measured 5-yr old walleye BSAFs	Difference between measured and predicted BSAFs	
47+48	5.82	24.926	1.996	49.764	35.982	-13.782	-38%
49	5.85	14.500	2.040	29.579	27.856	-1.723	-6%
52	5.84	18.328	2.026	37.125	34.529	-2.596	-8%
110	6.48	9.618	2.644	25.427	21.553	-3.874	-18%
118	6.74	7.467	2.711	20.242	19.995	-0.247	-1%
149	6.67	15.020	2.703	40.592	38.146	-2.446	-6%
180	7.36	18.021	2.468	44.474	49.971	5.497	11%

Relative differences predicted using 5% lipid contents in all species, weights of 10 g and 1 kg in forage and piscivorus fishes, respectively, no metabolism, 50:50 pelagic:benthic diet for the forage fish, piscivorus fish eating only forage fish, and a disequilibrium of 25.

Currently, the hybrid empirical/modeling approach is under research and development by ORD's NHEERL Mid-Continent-Ecological Division, and this effort is a tracked effort under ORD's Goal 3: Contaminated Sites Multi-Year Plan research plan. The research effort will determine the data quality requirements for the field measured BSAFs, the level of complexity required in forecasting the relative differences in bioaccumulation by the food web models, and how to account for metabolism when differences in metabolic abilities exist among the species. The effort will result in software, methods, and tools for making the BSAF predictions and provide validation results for the approach.

References

Burkhard, L.P., D.D. Endicott, P.M. Cook, K.G. Sappington, and E.L. Winchester. 2003. Evaluation of two methods for prediction of bioaccumulation factors. *Environ. Sci. Technol.* 37:4626-4634.

Short Description of the Gobas Food Web Model

Citation:

Gobas, F.A.P.C. 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario. *Ecol. Model.* 69:1-17.

Gobas, F.A.P.C.; Z'Graggen, M.N.; Zhang, X. 1995. Time Response of the Lake Ontario Ecosystem to Virtual Elimination of PCBs. *Environ. Sci. Technol.* 29:2038-2046.

Code: http://www.rem.sfu.ca/toxicology/models.htm

The Gobas model is a tool for predicting chemical residues, BAFs, and BSAFs for aquatic organisms given the concentrations of chemicals in water and sediment. To predict chemical residues, the model requires information on the individual species and their diets. With the model, concentrations of chemicals in sediment and water resulting in a given residue in the aquatic organism of concern can be determined.

The Gobas (1993) food web model has been used in both steady-state and dynamic applications. Windows based programs for the steady-state application can be downloaded from the above web site (Version 1.0). In 1995, Gobas updated the 1993 model slightly by changing the equation for determining the fecal egestion rate constant. A Windows based program for the updated steady-state application can be downloaded from the above web site, and this version of the code (Version 1.1) includes the benthic invertebrate submodel of Morrison et al. (1996).

Both versions allow the specification of complex food webs, e.g., fish preying on multiple species including smaller fish, and even age classes of fishes. These versions of the models treat the ecosystem as one environment. The models have the following input parameters:

a)	K_{ow} (& standard deviation) of the chemical	
b)	Dissociation constant pK_d (required only for ionizable organics)	
c)	Molecular weight (required only if fugacity calculation is wanted)	
d)	Henry's law constant (required only if fugacity calculation is wanted)	(Pa.m^3/mol)
e)	Total concentration (& standard deviation) of chemical in water	(g/L)
f)	Concentration (& standard deviation) of suspended solids in water	(kg/L)
g)	Organic carbon content (& standard deviation) of suspended solids in water	(g/g)
h)	Total concentration (& standard deviation) in sediment	(g/kg wet weight)
i)	Organic carbon content (& standard deviation) of the sediment	(g/g)
j)	Water temperature (& standard deviation)	(°C)

k)	For plankton and benthos: lipid content (& standard deviation)	(kg/kg)
l)	For fish: weight (& standard deviation)	(kg)
m)	lipid content (& standard deviation)	(kg/kg)
n)	Metabolism rate constant (& standard deviation)	(day^{-1})
o)	Fish feeding preferences upon species in the food web	(%, must sum to 100%)

Note, standard deviations are not required. If Monte Carlo analysis is run, only those input parameters with non-zero standard deviations will be evaluated.

Assumptions used with Gobas 1993 and updated food web models are:

a) Phytoplankton and zooplankton are in equilibrium with the water column. This means that the BAF (based on the lipid normalized concentration of chemical in the organism and freely dissolved concentration of chemical in the water) for plankton equals the chemical's K_{ow}.

b) With the 1993 model, benthic invertebrates are in equilibrium with the sediment. This means that the BSAF for the benthic invertebrates equals 1. Note, BSAF is the ratio of the concentration of chemical in the organisms on a lipid basis to the concentration of chemical in the sediment on an organic carbon basis (ug/kg-lipid)/(ug/kg-organic carbon).

c) With the updated model, residues in benthic invertebrates are calculated for each species by modeling the uptake and loss of the chemical with the Morrison et al. (1996) submodel. The Morrison et al. (1996) submodel uses kinetic rate constants for uptake and elimination of the from the organism to determine the residue in the benthic organism.

Outputs by with the Gobas 1993 and updated food web models are:

a)	Concentration of chemical in each species on a wet weight basis	(g/kg-wet)
b)	Concentration of chemical in each species on a lipid weight basis	(g/kg-lipid)
c)	Fugacity of the chemical in each species	(Pa)
	For all species:	
d)	Bioaccumulation factor on a wet weight basis	(L/kg-wet)
e)	Bioaccumulation factor on a lipid weight basis	(L/kg-lipid)
	For benthos and fishes:	
f)	Wet weight BSAF	(kg-organic carbon/kg-wet)
g)	BSAF	(kg-organic carbon/kg-lipid)
	For fishes:	
h)	Bioconcentration factor (BCF) on a wet weight basis	(L/kg-wet)
i)	Biomagnification factor (BMF)	(kg/kg)
j)	Chemical intake from water	(g/day)
k)	Chemical intake from food	(g/day)
l)	Chemical lost via gill elimination	(g/day)
m)	Chemical lost via fecal elimination	(g/day)
n)	Chemical lost via growth dilution	(g/day)
o)	Chemical lost via metabolic transformation	(g/day)
p)	k_1, gill uptake rate constant	(l/kg/day)

q)	k_2, gill depuration rate constant	(l/kg/day)
r)	k_{diet}, food assimilation rate constant	(day^{-1})
s)	k_e, egestion rate constant	(day^{-1})
t)	k_g, growth dilution rate constant	(day^{-1})
u)	k_m, metabolism rate constant	(day^{-1})
v)	Monte Carlo uncertainty analysis (using standard deviations provided with the input data) for all output values listed above.	

Dynamic solutions of the Gobas models can be computed using the ECOFATE model (Gobas et al. 1998), and this Windows based program is available from the above web site as well.

In addition to the food web model, ECOFATE incorporates "WASP" like fate and transport model, and to run the model additional input information is required. The additional input information includes:

a) Specification of the geographical environment, e.g., size of river segments, flows, segment interconnections, and so forth.
b) Loadings of the chemical to the segments, or to the water body.

The Gobas food web model has been evaluated and validated, and has been used at Superfund sites.

Based upon analyses of uncertainty for the model, the following general statements can be made about the model:

a) Input parameters having the largest impact upon the predicted chemical residues are the K_{ow} of the chemical, lipid contents of fishes and benthic invertebrates, and the sediment-water column concentration quotient (Burkhard 1998).
b) The diets of individual species can also introduce large uncertainties because of the difficulties in measuring these input parameters. For Superfund sites where sediment contaminants are of concern, establishing high quality estimates of the benthic dietary pathway in species are highly desirable.
c) Although not a concern for PCBs and DDTs (because their rates of metabolism are extremely slow, i.e., set equal to zero), metabolism when included in the model will have a fairly large impact upon the predicted chemical residues in fish.

As with any model, Monte Carlo analyses enable the forecasting of the uncertainties associated with prediction of chemical residues and these types of analyses should be done when ever possible.

The Gobas model incorporates corrections for bioavailability in the water column, and the 1993 and updated versions of the model use a two-phase model for estimating the bioavailable fraction of the chemical. These phases are organic carbon (measured as TOC) and the freely dissolved chemical. The fraction of the chemical that is bioavailable is calculated using the equation:

$$\text{fraction bioavailable} = f_{fd} = 1/(1 + \text{TOC} \times K_{ow})$$

where:

TOC = total organic carbon content of the water (kg/L)
K_{ow} = n-octanol/water partition coefficient of the chemical
f_{fd} = fraction of chemical that is bioavailable (freely dissolved) in the water and, the bioavailable
concentration of the chemical in the water is calculated using the equation:

$$C_w^{fd} = C_w^t \times f_{fd}$$

where:

C_w^{fd} = bioavailable concentration of the chemical in the water (ug/L)
C_w^t = total concentration of the chemical in the water (ug/L)

More recently, EPA and others are using a three-phase model for estimating the freely dissolved chemical. The three phases are particulate organic carbon (measured as POC), dissolved organic carbon (measured as DOC), and the freely dissolved chemical, and hydrophobic organic chemicals have a much lower affinity for DOC in comparison to POC. For further information on the three-phase model, the reader is referred to EPA (2003) for further information.

Food web models, in general, are highly uncertain for chemical with K_{ow}s exceeding 7.5 due to the lack of laboratory data to parameterize of submodels for chemical uptake and depuration.

References

Burkhard, L.P. 1998. Comparison of two models for predicting bioaccumulation of hydrophobic organic chemicals in aquatic food webs. *Environ. Toxicol. Chem.* 17:383-393.

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Gobas, F.A.P.C., J.P. Pasternak. K. Lien and R.K. Duncan. 1998. Development & field-validation of a multi-media exposure assessment model for waste load allocation in aquatic ecosystems: application to TCDD and TCDF in the Fraser River Watershed. *Environ. Sci. Technol.* 32:2442-2449

Morrison, H.A., F.A.P.C. Gobas, R. Lazar, D.M. Whittle and G.D. Haffner. 1996. Development and Verification of a Steady-State Model of the Bioaccumulation of Organic Contaminants in Benthic Invertebrates. *Environ. Sci. Technol.* 30:3377-3384).

US-EPA. Methodology for deriving ambient water quality criteria for the protection of human health (2000). Technical support document volume 2: Development of national bioaccumulation factors. EPA-822-R-03-030, Washington, DC, 2003.

Short Description of the QEAFDCHN Food Web Model

Citation:

Quantitative Environmental Analysis. 2001. Documentation: Bioaccumulation Model QEAFDCHN v. 1.0. Pages 21. QEA, LLC, Montvale, NJ. This document is available at http://www.dnr.state.wi.us/org/water/wm/lowerfox/rifs/feasabilitystudy.html see appendix E.

Descriptions and Applications of the Model:

Quantitative Environmental Analysis. 1999. PCBs in the Upper Hudson River. Volume 2: A model of PCB fate, Transport, and Bioaccumulation. Prepared for General Electric, Albany, NY. This document is available from a GE web site: http://www.hudsonvoice.com or at http://www.ge.com/files/usa/en/commitment/ehs/hudson/Volume_2.pdf

Quantitative Environmental Analysis. 2001. A model of PCB bioaccumulation in the Lower Fox River and Green Bay: GBFood. This document is available at http://www.dnr.state.wi.us/org/water/wm/lowerfox/rifs/feasabilitystudy.html see appendix E.

Code: Visual Fortran code is available from QEA, 305 West Grand Avenue, Montvale, NJ 07645

The QEAFDCHN model is a tool for predicting chemical residues for aquatic organisms given the concentrations of chemicals in water and sediment. To predict chemical residues, the model requires information on the individual species (bioenergetic and physiological) and their diets. With the model, concentrations of chemicals in sediment and water resulting in a given residue in the aquatic organism of concern can be determined. The model is designed for solving for chemical residues in aquatic organisms with chemical concentrations in water and sediment varying over time.

The QEAFDCHN model can be used in a steady-state or dynamic application. The model allows the specification of complex food webs, e.g., fish preying on multiple species including smaller fish, and even age classes of fishes. The model treats individual segments of the greater ecosystem as individual ecosystems and the model has a migration feature. The QEAFDCHN model does not include code for modeling fate and transport of the contaminant in the ecosystem. The model allows inputs of concentrations of chemicals in water and sediment over time, and the time course for these two parameters have to be created outside of this program. The model estimates food consumption for fishes by using bioenergetic models with dietary items expressed on a units of energy (kJ) basis; higher lipid content species have higher energy contents per gram of wet tissue.

The model has the following input parameters:

a) Ratio of the efficiency of contaminant transfer across the gills to the efficiency of oxygen transfer across the gills for each chemical. (–)

b)	Resistance factor for transfer of chemical from lipid to blood (c_R)	(–)
c)	Energy density of sediment and water column particulate matter	(kJ/g C) (kJ/g C)
d)	For steady-state species[2], bioenergetic parameters for each species:	
	Respiration rate	(kJ/g wet-day)
	Growth rate	(day^{-1})
	Food assimilation efficiency	(%)
	Fraction protein in species	(g protein/g wet)
	Exponential Coefficient for temperature dependency for respiration, ρ	($1/^{o}\text{C}$)
	Fraction lipid	(g lipid/g wet)
	Toxicant assimilation efficiency	(%)
	Factor used to calculate elimination rate	(–)
	Partition coefficient of chemical in species	(L/kg)
e)	For age-dependent species, bioenergetic parameters for each species:	
	Age class size	(days)
	Respiration coefficient rate (β)	(kJ/g wet-day)
	Respiration weight exponent (γ)	(–)
	Food assimilation efficiency	(%)
	Fraction protein in species	(g protein/g wet)
	Species specific dynamic action	(–)
	Exponential coefficient for temperature dependence for respiration, ρ	($1/^{o}\text{C}$)
	Swimming speed coefficient (ω)	(cm/s)
	Swimming speed weight coefficient (δ)	(–)
	Swimming speed exponential coefficient for temperature dependence (ϕ)	($1/^{o}\text{C}$)
	Swimming speed exponential coefficient	(s/cm)
	Chemical assimilation efficiency from food	(%)
	Time of break M in annual growth pattern for age class L	(days)
	Weight of species at time break M	(g)
	Fraction lipid of species at time break M	(g lipid/g wet)
	Factor used to calculate elimination rate	(–)
	Partition coefficient of chemical in species	(L/kg)
f)	For migrating species, migration pattern among spatial compartments	
g)	Spatial compartments	
	Temperature cycle for compartment (number of days, temperature)	
	Number of species in compartment	
	Predator-prey relationships in compartment	
h)	Exposure concentrations overtime	
	Dissolved concentration of chemical in water	(ug/L)
	Adsorbed concentration of chemical in water	(ug/g carbon)
	Dissolved concentration of chemical in sediment	(ug/L)
	Adsorbed concentration of chemical in sediment	(ug/g carbon)

Outputs for the QEAFDCHN model are:

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[2] Steady-state species are typically zooplankton and benthic invertebrate species.

a) For each step modeled, for each spatial compartment, for each age dependent species, a time history (in days) of

Contaminant concentration	(ug/g wet)
Weight	(g)
Lipid contents	(g lipid/g)
Growth rate	(g wet/g wet-day) and (kJ/g wet-day)
Energy content	(kJ/g wet)
Respiration rate	(kJ/g wet-day)
Food consumption rate	(kJ/g wet-day)
Chemical uptake from water	(L/g wet-day)
Chemical uptake from food	(ug/g wet-day)
Chemical elimination rate	(day^{-1})

In applying the QEAFDCHN model to the Hudson River, assumptions used with the model were:

a) The BSAF for benthic invertebrates was derived using field measurements, performed by EPA on the Hudson River. The average BSAF computed for Tri+ PCBs of 1.55 was used by the model for benthic invertebrates.

b) For phytoplankton and zooplankton, the trophic transfer factor of 3 [(ug PCB/g lipid)/(ug PCB/g organic carbon) was assumed base upon data from the Green Bay ecosystem of Lake Michigan.

c) The resistance factor for transfer of chemical from lipid to blood, and the dietary portions of benthic and pelagic organisms for forage fish were the only parameters optimized during calibration of the model.

The QEAFDCHN model does not contain a Monte Carlo analysis algorithms for establishing uncertainty bounds for the forecasted chemical residues in fish and other aquatic organisms. The following general statements can be made about the model.

i) An analysis of uncertainties performed on the steady-state model of Thomann et al (1992) (predecessor model of the QEAFDCHN model) reveals that input parameters having the largest impact upon the predicted chemical residues are K_{ow} of the chemical, the sediment-water column chemical concentration ratio, and feeding preferences of benthic invertebrates (how much sediment vs phytoplankton in the diet of the benthic invertebrates). Lipid contents and feeding preferences for fish (benthic vs pelagic organisms) had smaller impact (than the three parameters above) upon the predicted chemical residues (Burkhard 1998).

ii) In Green Bay (Connolly et al. 1992), the outputs of the predecessor model of the current version of the QEAFDCHN were most sensitive to 1) PCB uptake parameters (the ratio of the chemical assimilation efficiency to the food assimilation efficiency and the ratio of the efficiency of contaminant transfer across the gills to the efficiency of oxygen transfer across the gills for each chemical), 2) the hydrophobicity of the chemical (K_{ow}) (the partition coefficient of chemical in species in QEAFDCHN), and 3) migration patterns of the fish.

iii) In the Hudson River, the QEAFDCHN model was evaluated for only the feeding preferences of the forage fish, and resistance factor for transfer of chemical from lipid to blood (c_R) by using a bounding calculation. The Hudson River report using the QEAFDCHN model assert or suggest that forecasts with model are within 2x of measured values and that uncertainties on the predictions are similar. However, without a full Monte Carlo uncertainty analysis, confidence levels for the model outputs are not known.

iv) Although not a concern for PCBs and DDTs (because their rates of metabolism are extremely slow, i.e., set equal to zero), metabolism when included in the model will have a fairly large impact upon the predicted chemical residues in fish. Note, the QEAFDCHN model does not incorporate inputs nor code for addressing metabolic losses of chemicals in its current version.

As with any model, Monte Carlo analyses enable the forecasting of the uncertainties associated with prediction of chemical residues and these types of analyses should be done when ever possible.

The QEAFDCHN model does not incorporate any type of bioavailability correction to freely dissolved chemical in the water column. The model (by allowing the specification of the ratio of the efficiency of contaminant transfer across the gills to the efficiency of oxygen transfer across the gills) allows one to account for differences in bioavailability indirectly.

Food web models, in general, are highly uncertain for chemical with K_{ow}s exceeding 7.5 due to the lack of laboratory data to parameterize submodels for chemical uptake and depuration. The QEAFDCHN model requires the input of the chemical assimilation efficiencies, and thus, as more appropriate values become available, they can used in the model.

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General Definitions

Bioaccumulation	The accumulation of contaminants in the tissue of organisms through any route, including respiration, ingestion, or direct contact with contaminated water, sediment, pore water, or dredged material.
Bioconcentration	A process by which there is a net accumulation of a chemical directly from water into aquatic organisms resulting from simultaneous uptake (e.g., by gill or epithelial tissue) and elimination.
Biomagnification	Result of the process of bioconcentration and bioaccumulation by which tissue concentrations of bioaccumulated chemicals increase as the chemical passes up through two or more trophic levels. The term implies an efficient transfer of chemical from food to consumer, so that residue concentrations increase systematically from one trophic level to the next.
Clean up goal	Clean up or remediation goals state the acceptable contaminant concentrations in each medium for remedial actions to meet. The primary sources for determining the acceptable exposure levels used for developing remediation goals are: (a) concentrations found in Federal and State ARARs and, if these are not available or not protective, (b) risk-based concentrations that are determined to be protective of human health and the environment.
Depuration	Elimination that takes place when previously exposed aquatic or terrestrial organisms are held in uncontaminated water or air, respectively
Elimination	The removal of a compound from the body by diffusion, desorption, or excretion.
Equilibrium	Condition when the change in Gibbs free energy (ΔG) of the system under study is equal to zero and the concentrations in the compartments of the system are constant. In a thermodynamic sense, this indicates that both a steady state of flux and an equivalence in chemical activity have been reached in compartments or phases separated by a membrane or a boundary across which the chemical fluxes occur. No energy is required to maintain equilibrium. Chemical equilibrium rarely occurs in nature.
Flux	The rate of movement of a compound across a boundary. Flux terms in bioaccumulation models are mathematically described as the product of the concentration and kinetic rate constant
Food Chain	A series of predator-prey relationships. The transfer of food energy from the source in autotrophs (plants) through a series of organisms that consume and

	are consumed. Thus, the transfer of energy up through the different trophic positions.
Food Web	The interlocking pattern of various food chains within an ecosystem (e.g., the aquatic food chain + the terrestrial food chain)
Fugacity	"Escaping tendency." Technically defined as the tendency of a gas to expand or escape. Commonly, the term is used to describe the tendency for a substance to move from one environmental compartment to another.
Kinetic rate constant	Represents the fractional change in the amount of chemical in a compartment over time. These values are used in modeling to relate the concentration of a compound in a compartment to the flux of the compound across a boundary. They are often termed "conditional rate constants" in that they are dependent on the environmental conditions under which they are measured.
Octanol-Water Partition Coefficient	K_{ow}, often expressed as a log value. Unitless. The ratio of the concentration of a substance in an *n*-octanol phase to its concentration in the aqueous phase in an equilibrated two-phase *n*-octanol-water system. The log K_{ow} of a substance represents its likelihood to complex or sorb to organic carbon. The log K_{ow} of a chemical is directly proportional to its *n*-octanol solubility.
Partitioning	The tendency of a compound to move from one compartment to another by passive diffusion.
Partition Coefficient	The ratio of chemical concentrations in two compartments or phases under steady-state conditions (e.g., K_{ow}, K_{doc}, K_{oc}). Unitless.
Steady-state	The state in which fluxes of material moving bidirectionally across a membrane or boundary between compartments or phases have reached a balance. An equilibrium between phases is not necessarily achieved. A simple conceptualization is the state at which "as much is coming in as is going out". Note, steady-state is where $dC/dt = 0$, concentrations in the compartments are not changing over time.
Trophic Level	A segment of the food chain in which all organisms obtain food and energy in, basically, the same manner (e.g., photosynthesis, herbivory, or carnivory) and in which all organisms are the same number of links from the photosynthetic segment.