Ecological Considerations: Bioaccumulation Assessment

Focus: Organic Chemicals

Office of Science Policy's
Contaminated Sediments Virtual Workshop
Fall 2019

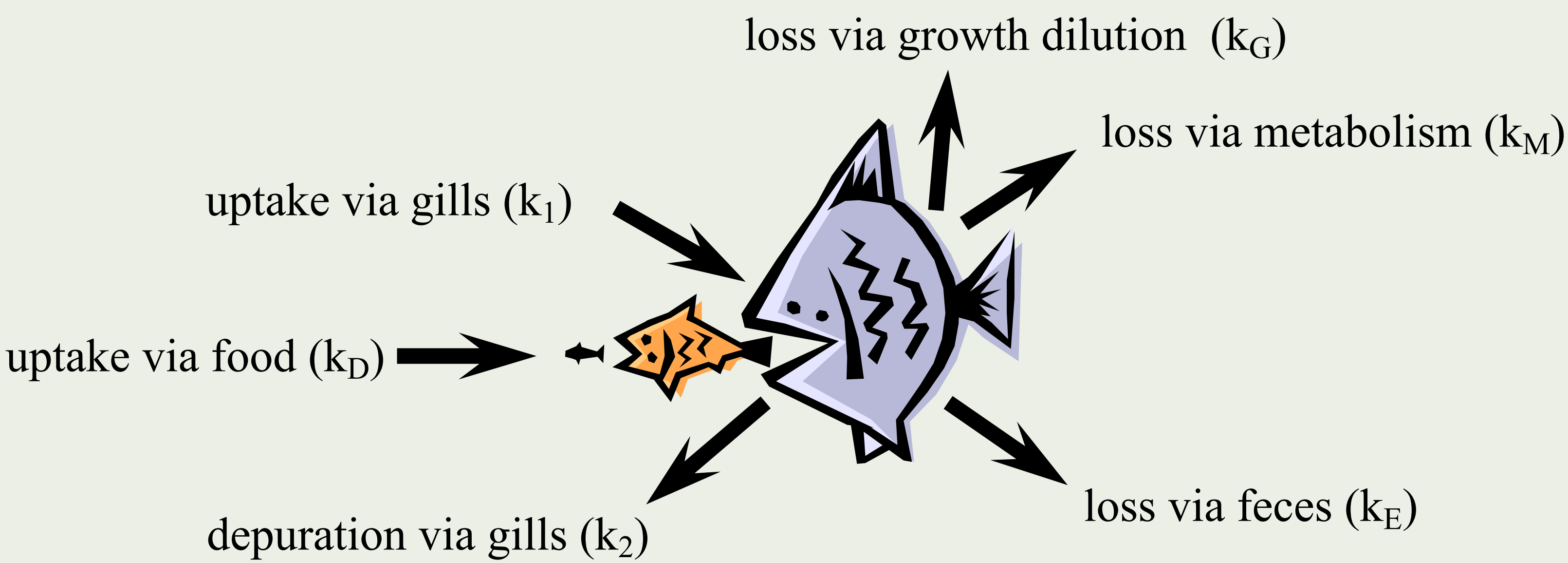
EPA

Yes or No Slide

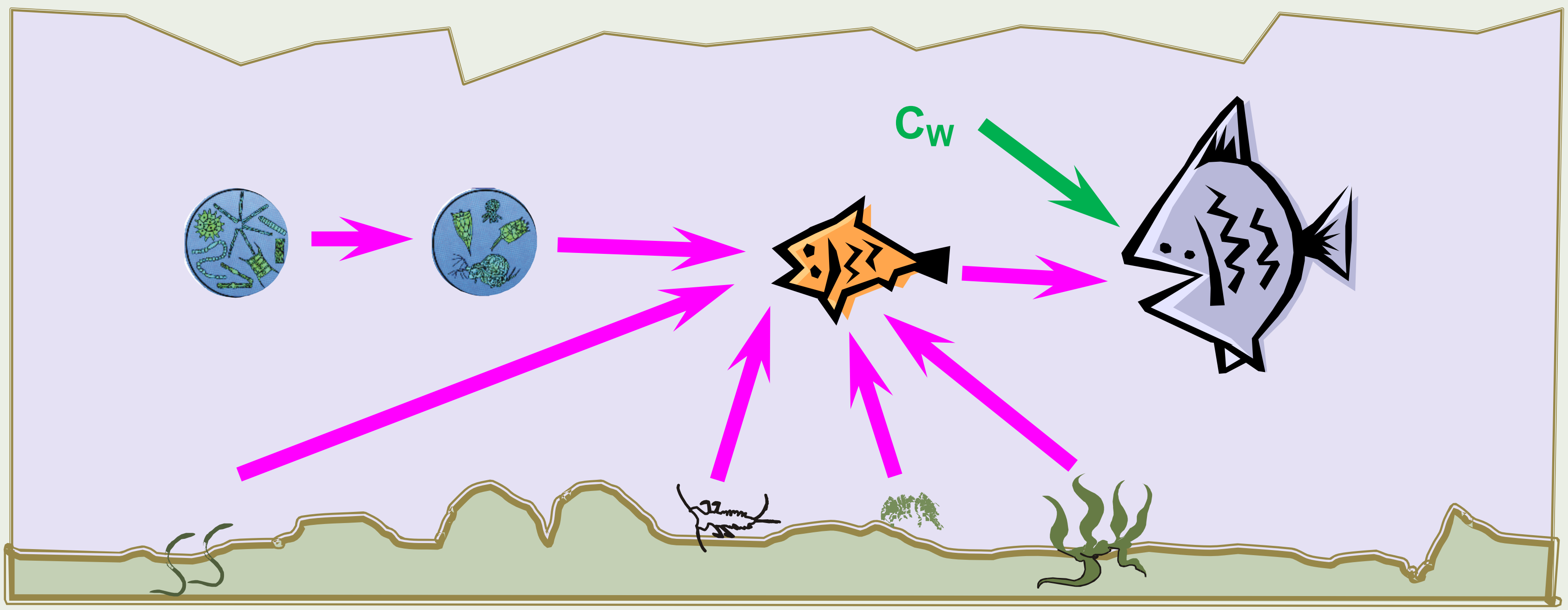
- **How many of you have sites where chemical residues in fish are of concern?**
- **YES OR NO**

Chemical Residues in Fish

- Function of both chemical concentrations in sediment and water.



Fish in simple food web



Approaches to Predicting Chemical Residues in Fish

- **Empirical**
  - » uses field measured BSAFs or BAF^{fd}s
- **Mechanistic**
  - » use food chain models to predict chemical residues in fish
- **Empirical and mechanistic approaches:**
  - » compatible which each other
  - » one can be used to support the other

Empirical: Chemical Residues in Fish

- **Bioaccumulation Expressions**
  - » Sediment basis BSAF = C_{lipid} / C_{soc}
  - » Water basis BAF^{fd} = C_{lipid} / C^{fd}
- **BSAF & BAF^{fd} must be self consistent**
  - » predict the same chemical residue in fish

Empirical Methods

- **Incorporates all bioaccumulation processes**
  - trophic transfer, metabolism, sediment-column water disequilibrium, bioavailability, organism growth, ...
- **Ecosystem specific**
  - incorporates
    - Existing external loading scenarios
    - Fluxes from sediments
    - Contaminant burdens in sediments

Challenges with Empirical Methods

- **Predictive power dependent upon "stable" conditions at the site**
  - Sediment-column water chemical disequilibrium
  - Sources of chemical to the site
  - Food web structure
  - …

- **Analytically**
  - BSAFs easy to measure
    - Assessing predictive power can be difficult
  - BAF^{fd}s more difficult to measure
    - Concentrations in water often very low

Mechanistic Models

- ♦ **For each organism:**

$$ {dC_f}/{dt} = k_1 \times C_w + k_d \sum_{i=1}^{n} \left(f_i \times C_{prey,i} \right) - (k_2 + k_G + k_M + k_E) \times C_f $$

Mechanistic Models: Steady-State Solution

- Steady-state solution: $dC_f/dt = 0$

$$C_f = \frac{\left(k_1 \times C_W + k_d \sum_{i=1}^{n}\left(f_i \times C_{prey,i}\right)\right)}{\left(k_2 + k_G + k_M + k_E\right)}$$

- One equation for each species

Mechanistic Models: Dynamic Solution

- **For each organism:**

$$\frac{dC_f}{dt} = k_1 \times C_w + k_d \sum_{i=1}^{n} \left(f_i \times C_{prey,i}\right) - \left(k_2 + k_G + k_M + k_E\right) \times C_f$$

- **One differential equation for each species**
  - Use numerical integration techniques

Mechanistic Methods

- **Many food chain models**

» Thomann	steady-state
» Gobas	steady-state
» Arnot & Gobas	steady-state
» Mackay (fugacity models)	steady-state
» FishRand-Migration	dynamic & probabilistic
» Aquatox	dynamic
» QEA-Anchor	dynamic & steady-state
» Bass	dynamic
» ...	

Mechanistic Methods at Superfund Sites

- **Many food chain models**

» Thomann	steady-state
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Mechanistic Methods

- **Models require:**
  - Ecosystem conditions
    - Chemical concentrations in water & sediment
    - Temperature
    - DOC, POC, SOC
  - Food chain structure
  - Organism specific parameters
    - weights, lipid contents, growth rates, *in vivo* metabolism rates, diets, migration/movement, ...
  - Chemical specific parameters: K_{ow}

Challenges in Developing Mechanistic Models

- ♦ **Inadequate site-specific data**
  - » Concentrations in water often limited or non-existent
  - » Never enough data for fish
  - » Data for forage fish, invertebrates & phytoplankton lacking
- ♦ **Poorly understood inputs**
  - » Dietary preferences
  - » Migration/movement & foraging behavior
- ♦ **Dynamic Solutions**
  - » Require time varying inputs
    - › Complex modeling for inputs: EFDC and SEDZLJ →→ Concentrations in sediment & water
    - › Environmental conditions: temperature, SS, DOC …
    - › Biota behavior

Challenges in Developing Mechanistic Models

- **Implications**
  - Models highly calibrated to the available data.
  - Non-unique calibrations
    - Different combinations of inputs may lead to the same predicted residues but with very different implications for remedial options.
    - Lower Duwamish River Superfund Site
      - Probabilistic version of Arnot-Gobas model with 114 individual model inputs
        - Virtually all defined by probability distributions and optimized using Monto Carlo methods

Some cautions and thoughts

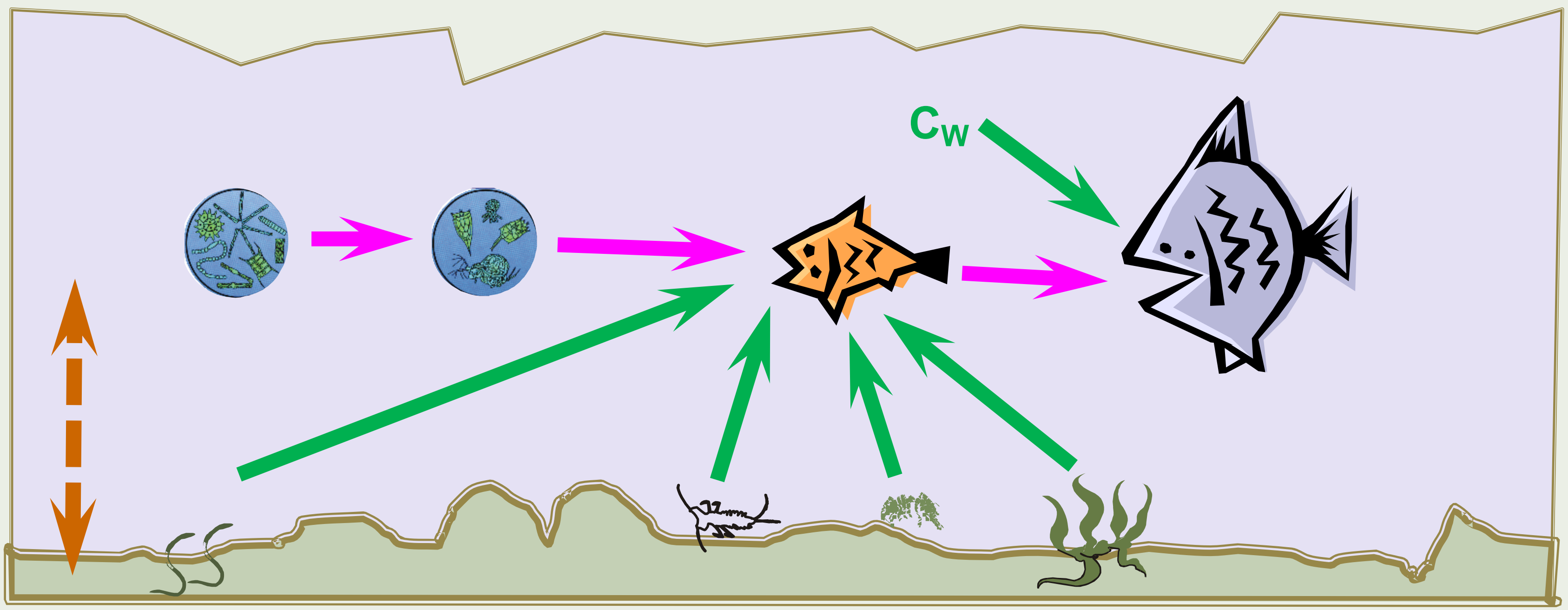
- ♦ **Before launching into developing model**
  - » Understand the need for developing food chain model
    - › What level of complexity is needed for answering your site's question
      - – Simple empirical data?
      - – Simple steady-state model?
      - – Dynamic (time variant model)?
  - » Costs increase with complexity
  - » Time to complete increases with complexity
- ♦ **Measured residues in the fish are the truth!**

PFAS Class
Per- and Polyfluorinated Alkyl Substances

- Models discussed don’t apply
- Lots of research on models for PFAS

For discussion in the extra 30 minutes

Remedial action: Add Activated Carbon to Sediment
What processes are impacted?
What are the effect on residues in the purple fish?



Question and Answer Time

- **Time for Q&A on Bioaccumulation**