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CEE 577: Surface Water Quality Modeling

Lecture #31

QUAL2E & Toxics: Sorption (Chapra, L41)

The third phase

- Can also consider the DOC phase

$$f_d = \frac{1}{1 + K_d m + K_{DOC} DOC}$$

$K_d \cong 10^{-6} K_{ow} POC/m$

- Which gives us 3 fractions
  - dissolved
  - particulate
  - DOC-bound

$$f_d = \frac{1}{1 + 10^{-6} K_{ow} TOC}$$

$$f_p = \frac{10^{-6} K_{ow} POC}{1 + 10^{-6} K_{ow} TOC}$$

$$f_o = \frac{10^{-6} K_{ow} DOC}{1 + 10^{-6} K_{ow} TOC}$$

Black Carbon

- A pyrolytic form of carbon
  - Diesel soot
  - Other pyrolytic sources
  - Non-pyrolytic
    - e.g., tire wear & urban runoff
- Behaves like GAC
  - Non-linear adsorption
    - Freundlich Isotherm

PtOC & BC model

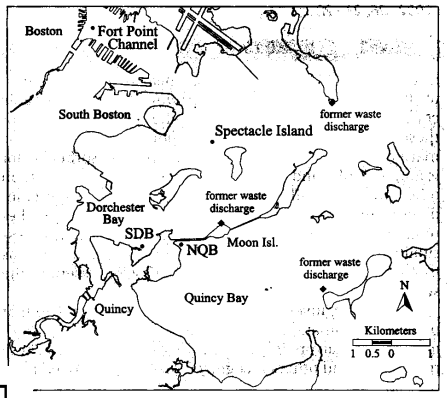
- Two terms $$C_s = f_{oc} K_{oc} C_w + f_{BC} K_{BC} C_w^n$$
  - Simple partitioning for normal PtOC
  - Freundlich isotherm adsorption for BC
- And Re-arranging
  - where $$C_s = K_d C_w$$

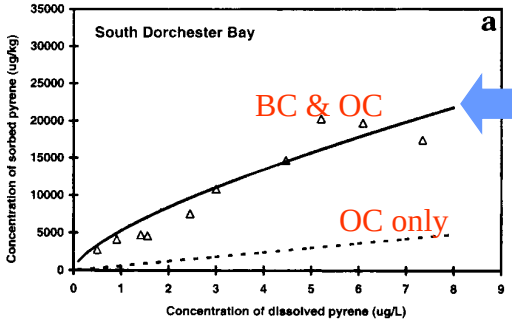
$$K_d = f_{oc} K_{oc} + f_{BC} K_{BC} C_w^{n-1}$$

Accardi-Dey & Gschwend, 2002, Env. Sci. & Technol. 36(1)21-29

Env. Data

- Boston Harbor Study





Freundlich exponent
n = 0.62 ±0.12

Accardi-Dey & Gschwend, 2002, Env. Sci. & Technol. 36(1)21-29

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Simple Dual Mode Model

- Simple DMM
  - Developed to accommodate
    - "dissolution" behavior
      - Linear partitioning
    - competitive adsorptive behavior
      - Langmuir-type isotherm
        - Affinity coeff, $b \equiv K_{ad} / K_{de}$

$$v = \frac{v_m c_d}{\left(k_{de}/k_{ad}\right) + c_d}$$

$$v = \frac{v_m \left(k_{ad}/k_{de}\right) c_d}{1 + \left(k_{ad}/k_{de}\right) c_d}$$

$$v = \frac{v_m b c_d}{1 + b c_d}$$

$$v = K_D c_d + \frac{v_m b c_d}{1 + b c_d}$$

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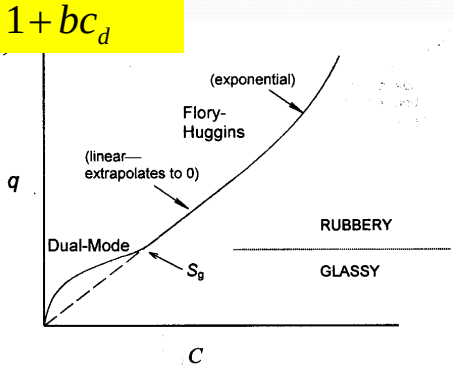
Extended DMM

- Accounts for plasticization by the sorbate

$$v = K_D e^{\sigma v^*} c_d + \frac{v_m \left(1 - {}^{v^*}\!/_{v_g}\right) b c_d}{1 + b c_d}$$



Xia & Pignatello, 2001, Env. Sci. Technol., 35(1)84-94

- To next lecture