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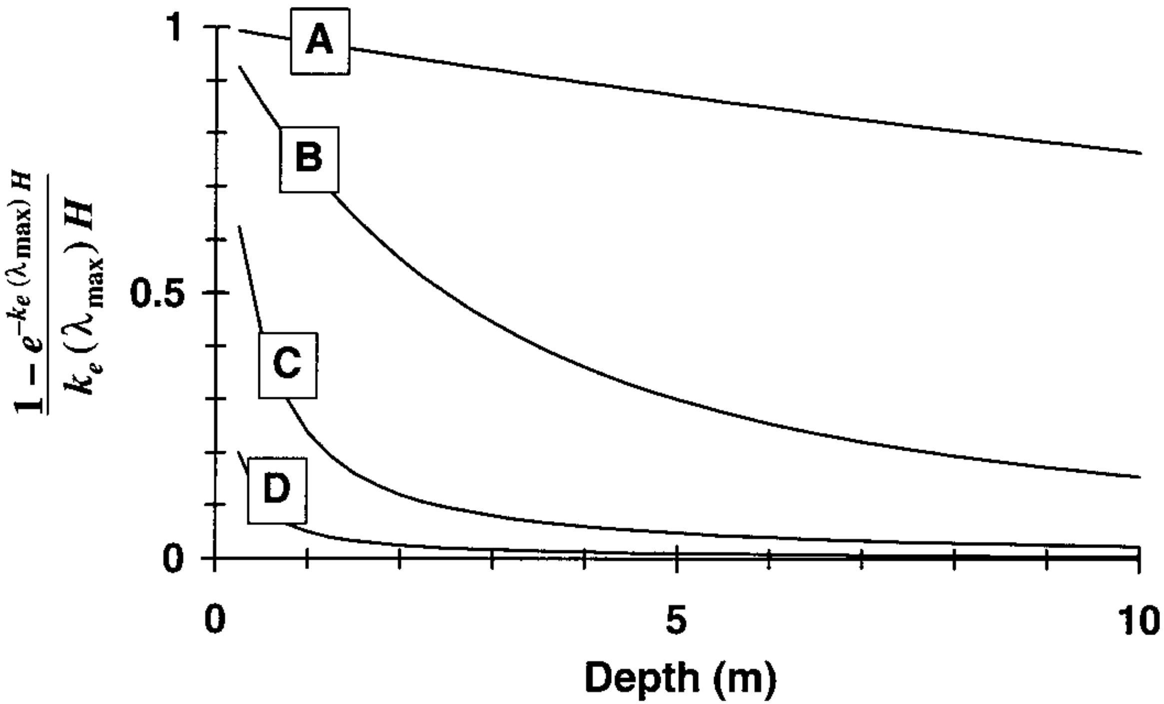
CEE 577: Surface Water Quality Modeling

Lecture #34

Toxics: Hydrolysis and Biodegradation: Recapitulation and Simplified Forms

(Chapra, L42, L43 & L44)

	Water type	Chl*a* (mg L⁻¹)	DOC (mg L⁻¹)	ss (mg L⁻¹)
A	Pure water	0	0	0
B	Lake Tahoe	0.001	0.1	0.5
C	Eutrophic	0.01	0.5	5
D	Hypereutrophic	0.1	2	20



Biotransformation

- Microbially mediated transformation of organic and inorganic contaminants
- Biochemical processes:
  - Metabolism: toxicant is used for synthesis or energy
  - Cometabolism: not "used", but transformed anyway
- Chemical Effects:
  - Detoxication: Toxic to Non-toxic
    - mineralization
  - Activation: Non-toxic to Toxic

Bio kinetics

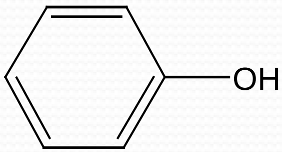
- Michaelis-Menten equation:
  - μ_{max}= maximum growth rate (yr^{-1})
  - X=microbial biomass (#cells/m^3)
  - Y= yield coefficient (cells produced per mass toxicant removed, #cells/µg)
  - k_s= half-saturation constant (µg/m^3)
  - k_b= rate of biotransformation (yr^{-1})
- If $c<<k_s$, then:

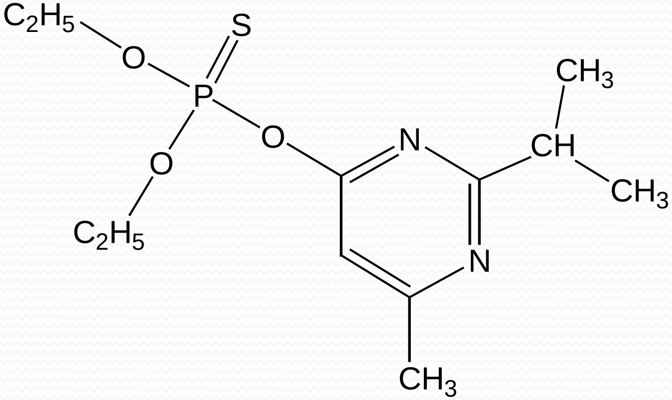
$$k_b = \frac{\mu_{\max} X}{Y(k_s + c)}$$

$$k_b = \frac{\mu_{\max} X}{Y k_s} = k_{b2} X$$

Bio kinetics (cont.)

- Wide environmental range
  - phenol: k_b=4.0 d^{-1}
  - diazinon: k_b=0.016 d^{-1}





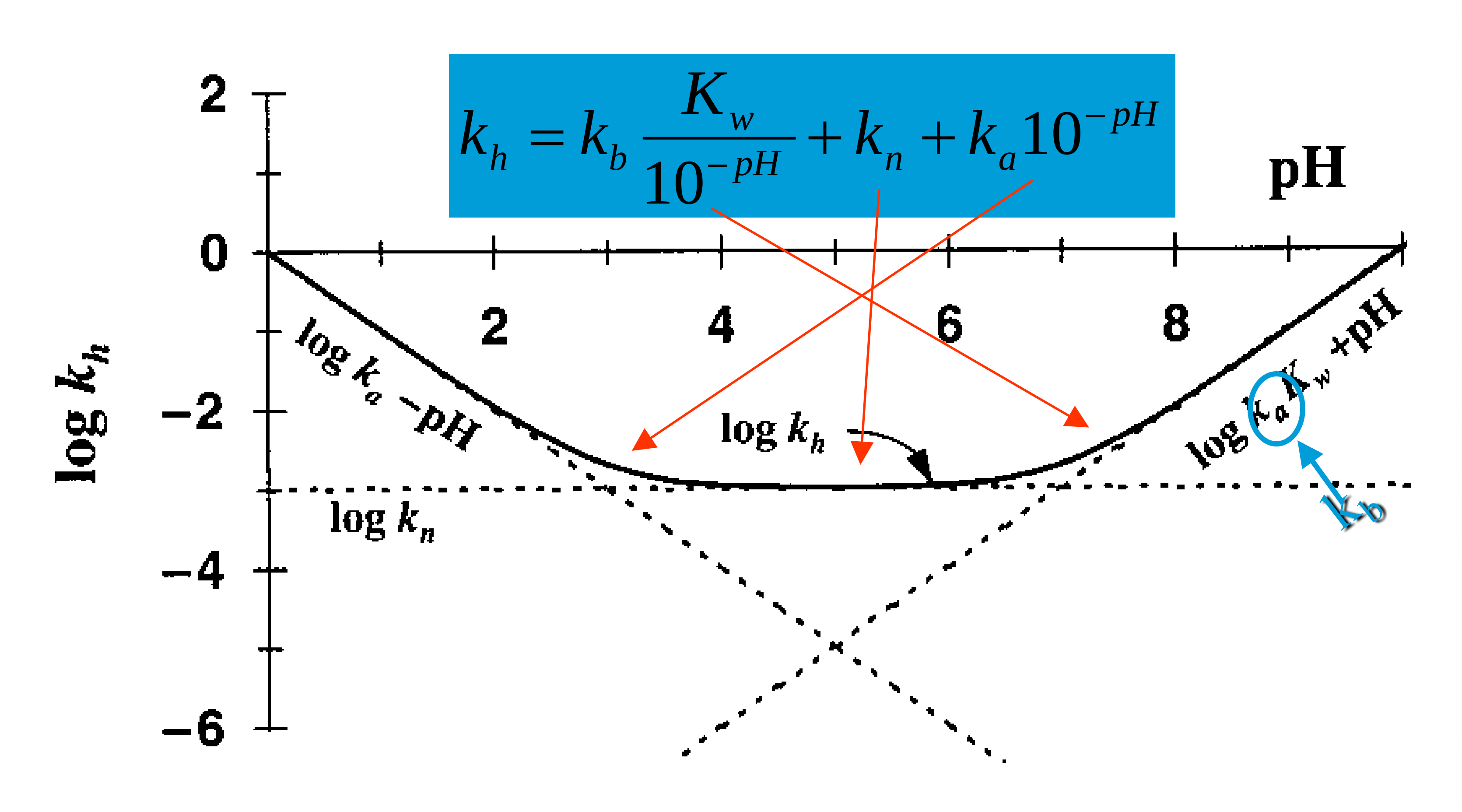
- Temperature correction
  - θ=1.04-1.095

$$(k_b)_T = (k_b)_{20}\theta^{T-20}$$

Hydrolysis

- Reaction with water and its constituents
  - H_2O $$k_h = k_n$$
  - OH^- $$k_h = k_b\left[OH^-\right]$$
  - H^+ $$k_h = k_a\left[H^+\right]$$
- Autodissociation $$K_w = \left[OH^-\right]\left[H^+\right]$$
- Combining: $$k_h = k_b\left[OH^-\right] + k_n + k_a\left[H^+\right]$$
  - or: $$k_h = k_b \frac{K_w}{10^{-pH}} + k_n + k_a 10^{-pH}$$

Graphic Representation



Special Considerations for Metals

- In general they are not subject to decomposition
  - e.g., biodegradation, hydrolysis, photolysis
  - exception: radionuclides undergo radioactive decay
- Most do not volatilize (Hg is an exception)
- They speciate into may forms which differ in toxicity and behavior
- Natural background and non-point loadings may be quite high

- To next lecture