Contaminant Fate and Transport in the Environment EOH 2122, Lecture 10, Aerobic and Anaerobic Biodegradation of Organic Compounds, Modeling Biodegradation and Bioconcentration and Accumulation in Aquatic Organisms

Conrad (Dan) Volz, DrPH, MPH
Bridgeside Point
100 Technology Drive
Suite 564, BRIDG
Pittsburgh, PA 15219-3130
office 412-648-8541 : cell 724-316-5408: Fax 412-624-3040 cdv5@pitt.edu Assistant Professor, Environmental and Occupational Health, University of Pittsburgh, Graduate School of Public Health http://www.pitt.edu/~cdv5/ ; Director-Center for Healthy Environments and Communities http://www.chec.pitt.edu; Director, Environmental Health Risk Assessment Certificate Program http://www.publichealth.pitt.edu/interior.php?pageID=82

Aerobic Biodegradation of Organic Compounds

Biodegradation and BOD Relationship

- BOD is an overall measure of the concentration of biologically degradable material
- BOD gives us no information about the specificity of organic compounds in the mixture or their degradation rates
- In aerobic degradation the most energy comes from oxidation of carbon that is in its most reduced state.

Microbial Oxidation of Anthropogenic Compounds

- Tremendous variety of microorganisms that have the ability to use pollutants such as alcohols, fuels and solvents as well as natural organic detritus as a source of energy.
- Microorganisms can be configured to help humans in the event of fuel spills etc.
- Microbial oxidation of more soluble and low molecular weight hydrocarbons occurs quickly (like alcohols and organic acids).
- The rate of microbial degradation decreases for contaminants with;
  - Increasing molecular weight.
  - Lower solubility in water.
  - Increasing number of aromatic rings.
  - Increasing numbers of branches.
  - The number of halogen atoms in their make-up (chlorine, fluorine, bromide etc.)
- If there were a train derailment on the Allegheny River and equal masses of Cyclohexane, Dichloroethane, Acetic Acid and PCB (Aroclor 1260) were spilled into the river-in what order would you expect aerobic microbial biodegradation to remove the contaminant? What compounds would you expect might only be partially degraded or have no significant degradation?

Anaerobic Microbial Degradation of Anthropogenic Compounds

- As DO is depleted microorganisms shift to using other oxidants such as SO4 (-2 oxidation state) and ecological conditions increasingly become reducing.
- The degradation of some organic contaminants occurs more readily in reducing environments. These contaminants -

-Have more oxidized carbon (remember this does not refer to oxygen but the oxidation state of the key carbon atoms).

-Are reduced meaning that they go from a more positive oxidation number to lower oxidation number.

- See figure 2-25 on page 146 of text.

Modeling Biodegradation

Kinetic Model

- Assumptions
  - Microorganisms are in contact with the water at all times.
  - Water contains a dissolved organic compound that serves as an energy source.
  - Biodegradation rate is same as uptake rate, so there is sufficient enzyme to continually catalyze the reaction.

Michaelis-Menten Enzyme Kinetics

- V=Vmax C/C + Ks -Where V is the rate of chemical uptake per cell in mass per cell-Time, Vmax is the maximum chemical uptake per cell. C is the concentration of the contaminant in water in mass per cubic Liter, and Ks is the half saturation constant also in mass per cubic Liter
- Rate of Uptake vs. Chemical Concentration is plotted in Figure 2-26.
- When C = Ks than V is ½ of Vmax also when Ks is much greater than C than uptake is proportional to concentration and obeys first order kinetics-Formula 2-71b.
- If C is far greater than Ks than uptake approaches independence of C-zero order kinetics so that V is approximately equal to V max.
- Rate of uptake of a contaminant from water is proportional to both the rate of chemical uptake per cell and the cell density.

Bioconcentration and Accumulation in Aquatic Organisms

- Bioconcentration – The process of aquatic organisms accumulating chemicals from water only.
- Bioaccumulation - The process of aquatic organisms accumulating chemicals from both water and food.

Bioconcentration Factor- (BCF)

- **Bioconcentration Factor- (BCF) –** The ratio of the concentration of a chemical in an organism to the concentration of that chemical in seawater, freshwater or brackish water.
- Therefore-

$$\frac{\text{mg of chemical/kg of organism}}{\text{mg of chemical in solution/Liter}} = \text{Liter/kg}$$

- BCF can be an observed ratio or be the prediction of a partitioning model.

Partitioning Models

<u>Assumptions</u>

- Pollutant chemicals partition in passive way between water and the organism.
- Chemical equilibrium exists between chemicals concentrations in the water and the organism.

These assumptions are most valid for lipophilic (hydrophobic) chemicals- they are more rapidly exchanged between the water and organism than they are excreted or biodegradated by the organism.

<u>Fish Model- Fish is a bag of oil and tissue water.</u>

- Chemical partitions between the bag and surrounding water according to:

-Kow which is the reciprocal of the chemicals water solubility.

-The lipid content of the fish.

- Table 2.9 in Hemond and Fechner-Levy presents a number of formulas for determining BCF.

- Such as---- log BCF = 2.791 – 0.564 log S where S is Water Solubility of chemical in ppm. This formula has been determined using Brook and Rainbow Trout, Sunfish, Flathead Minnow and Carp
- Review Figure 2-28----BCF- remember that the log BCF are highly correlated with log K_{ow} but that a single prediction can be off by a factor of three so averages using a number of formulas for each species provides more accuracy.
- Kinetic Models that depend on the dynamics of intake, storage, metabolic transformation and excretion of specific chemicals in specific organisms can be used to estimate **bioaccumulation.**

Depuration

- Use a first order kinetic model to estimate the depuration (cleansing) or partial removal of a contaminant from a fish given a specific contaminant concentration so
- C = Co e-kt Where C is the concentration at any time t, Co is the initial concentration, k is the first order rate constant (depuration-essentially analogous to decay) and t is the time.