

Environmental Water Quality BAE 452/552

Session 11
Specific Pollutants & Interactions in Soils II

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Organic Chemicals

- Use to increase yield of agricultural crops and assist in controlling pests and diseases
- Use became substantial in 1945 when DDT was commercially produced
- Since then rapid growth and environmental concerns increased

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Organic Chemicals

- Pesticides:
 - herbicides for weed control
 - Algicides for algal growth
 - Insecticides for insect control
 - Fungicides for fungus control
- Hydrocarbons, fluorocarbons (in sprays and cooling liquids), polychlorinated bi-phenyls (PCB in paper), volatile organic chemicals, solvents

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Organic Chemicals

Herbicides:

- S-triazine, picloram, 2,4,5-T, 2,4-D, atrazine

Insecticides:

- Organochlorine (DDT, dieldrin, aldrin, heptachlor, lindane; very persistent!), organophosphorus, and carbamate chemicals

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Organic Chemicals

Mobility:

- Atmosphere (drift, volatilization, wind erosion), note that drift losses vary from 25 to 75%!
- Ground water (leaching depending on adsorption)
- Surface water (runoff and erosion)

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Organic Chemicals

- Distribution of total organic chemical in soil:
$$C_T = C_d[\theta_v + \rho_{dry} K_d + (n - \theta_v)/K_H]$$
- $K_d = 6.17 \times 10^{-7} f_{oc} K_{ow}$ (presented in session 9)
- $K_d = K_{oc} (\%OC)/100$ [L kg⁻¹]
where
 $\%OC = 0.59(\%OM)$
 $\text{Log}(K_{oc}) = 1.029 \text{ log}(K_{ow}) - 0.18$ found by Rao and Davidson (1982)
or $K_{oc} = 0.66 K_{ow}^{1.029}$

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Organic Chemicals

Tables by Rao and Davidson (1982) (EPA report #600/3-82-060) for selected pesticides:

- Organic carbon partition coefficients (K_{oc})
- Octanol-water partition coefficients (K_{ow})
- Mean 1st order decay coefficients (k_i)

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Organic Chemicals: Example1

- Find the K_d for atrazine for soil with 2% OC.

Solution:

- From Table by Rao and Davidson (1982), $K_{oc} = 163$
- $K_d = K_{oc} (\%OC)/100 = 163 (2)/100 = 3.26 \text{ L kg}^{-1}$

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Organic Chemicals: Example2

- Determine the fraction of DDT that is contained in pore water of a saturated soil with $\rho_{dry} = 1400 \text{ kg m}^{-3}$, $n = 0.45$, and $\%OM = 4\%$.

Solution:

From Table by Rao and Davidson, $K_{ow} = 3.7 \times 10^5$

$K_{oc} = 0.66K_{ow}^{1.029} = 0.66 \times (3.7 \times 10^5)^{1.029} = 3.54 \times 10^5$
and $\%OC = 0.59(4\%) = 2.36$

$K_d = K_{oc} (\%OC)/100 = 3.54 \times 10^5 \times 2.36/100 = 8,359 \text{ L kg}^{-1}$

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Organic Chemicals: Example2

- $K_d = 8,359 \text{ L kg}^{-1}$, $\rho_{dry} = 1400 \text{ kg m}^{-3}$, $n = 0.45$.

Solution continued:

$$C_T = C_d[\theta_v + \rho_{dry} K_d + (n - \theta_v)/K_H]$$

$$\text{fraction: } C_d/C_T = 1/[\theta_v + \rho_{dry} K_d]$$

$$C_d/C_T =$$

$$1/[0.45 + 1400 \text{ kg m}^{-3} \times 0.001 \text{ m}^3 \text{ L}^{-1} \times 8,359 \text{ L kg}^{-1}] \\ = 0.000085 \text{ indicating almost all DDT is adsorbed}$$

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Toxic Metals

Important metals:

- Arsenic (As)
- Cadmium (Cd)
- Chromium (Cr)
- Copper (Cu)
- Lead (Pb)
- Mercury (Hg)
- Zinc (Zn)

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Toxic Metals

Precipitation and metal complexation:

- Oxidation of reduced iron, manganese, sulfides
- Reduction of higher valency metals by interaction with OM (selenium, silver)
- Reduction of sulfate to sulfide
- Alkaline-type reactions (increased pH)
- Adsorption or coprecipitation of metallic ions with iron or manganese oxides, clays, and OM
- Ion exchange reactions with clays

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Toxic Metals

Methylation of metals:

Mercury and Arsenic undergo biological methylation in anaerobic sediments. Bacteria transform inorganic Hg or As into organic methyl or dimethyl compounds that are far more toxic than the inorganic form

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Soil Microorganisms

What types?

- Bacteria (single cell)
- Fungi (multi-cellular)
- Algae (eucaryotic)
- Protozoa (single cell eucaryotic, w/out cell wall, sometime in oocyst or cyst)
- Worms
- Viruses (parasitic)

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Soil Microorganisms

- Most microbial population in A-horizon.
- Of concern are pathogenic microorganisms:
 - Pathogenic bacteria
 - Viruses
- Filtration limits movement of bacteria while adsorption limits movement of viruses.
- Best adsorption of viruses is at pH = 7

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Soil Microorganisms

- Factors on survival:

Factor	Type	Comment
pH	bacteria	Shorter survival in acid soil (3-5)
Predation by soil microflora	bacteria	Increased survival in sterile soil
Moisture	both*	Longer survival in moist soil
Temperature	both	Longer survival at lower T
Sunlight	both	Shorter survival near surface
OM	bacteria	Longer survival or regrowth of some when sufficient OM present

* bacteria and viruses

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Soil Microorganisms

- Survival of pathogens and viruses in soils:

Organism	Range in survival time (Days)
<i>Salmonella</i>	15 to > 200
<i>Salmonella typhi</i>	1 - 200
Tubercle bacilli	> 200
Entamoeba cysts	6 - 8
Enteroviruses	8
Hookworm larvae	42
Viruses	7 - 180

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