Water Contaminants

- Office: 35-307 (discussion by appointment welcomed!)
- Email: ychoi81@snu.ac.kr
- Course material/textbook:
  1. Lecture notes
  2. Schwarzenbach, Gschwend, Imboden, Environmental Organic Chemistry, 2nd ed., John Wiley & Sons, 2003

Water Contaminants

- Study different types of water contaminants and their fate in various settings of water environment
- Some background on environmental organic chemistry
- Focus on organic contaminants and the physicochemical mechanisms involved in their fate

Student presentation & paper discussion

- Only one exam for this class? But…
- One of the student leads the class
- Topic & paper selection & posting
  - Select a topic & a paper (relevant to the class!) and submit a brief presentation plan at least **3 business days prior to the class assigned**

    (Tue class → Thu; Thu class → Mon)
  - Post the paper link to eTL at least **2 business days prior to the class assigned**

    (Tue class → Fri; Thu class → Tue)

Student presentation & paper discussion

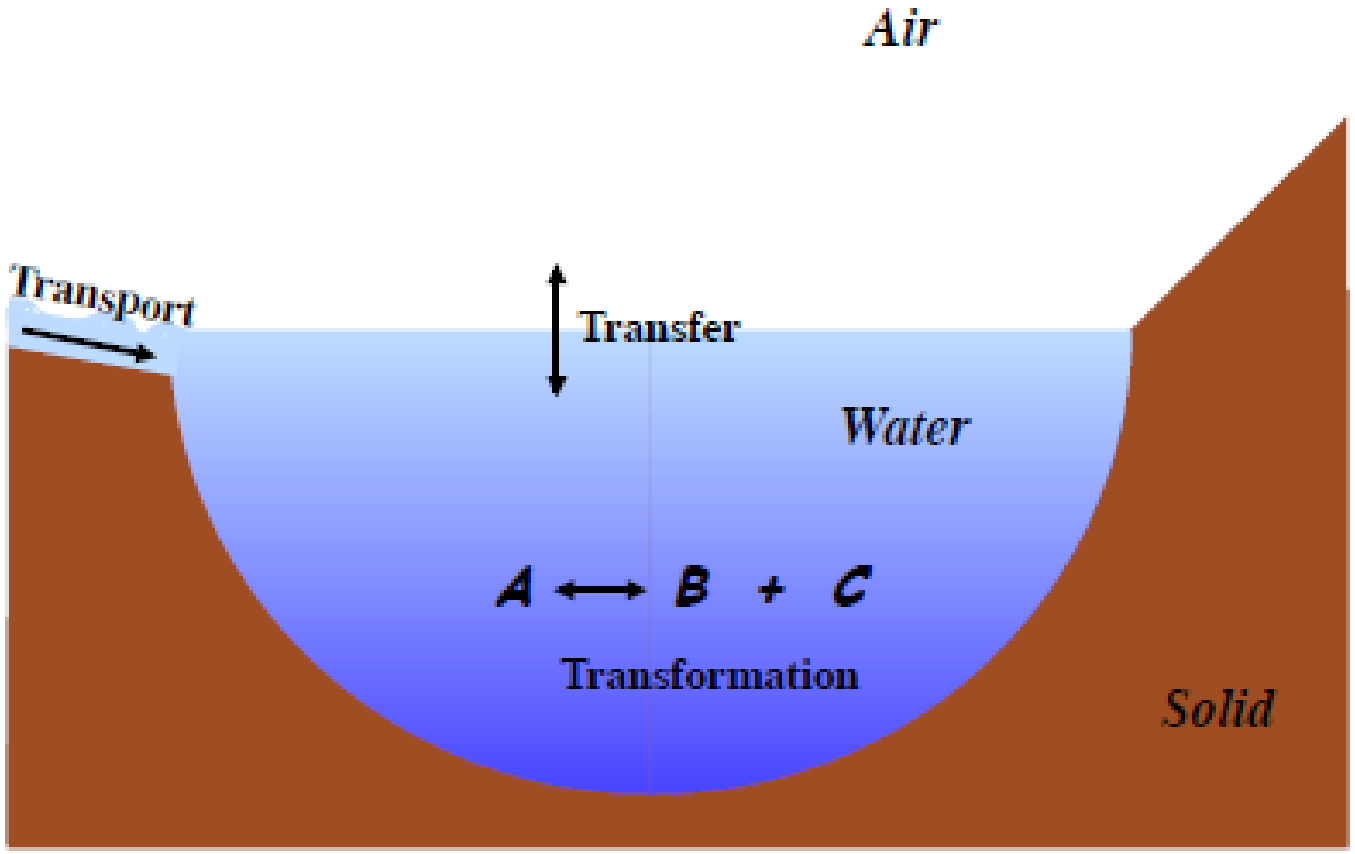
- Contents
  - General background on the selected topic
  - Critical review of the selected paper
  - Provide ≥3 discussion points to facilitate student discussion
  - Presentation (20 min) + Discussion (30 min)

Contaminant fate and transport?

http://www.virginmedia.com/science-nature/wildlife

http://www.heraldsun.com.au

Transport, phases, interphases



Contaminant fate & transport?

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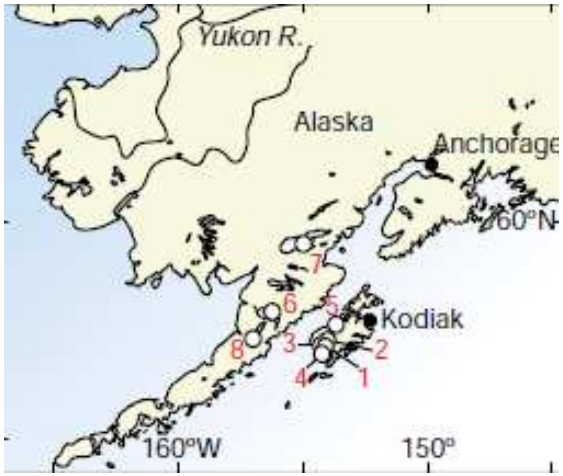
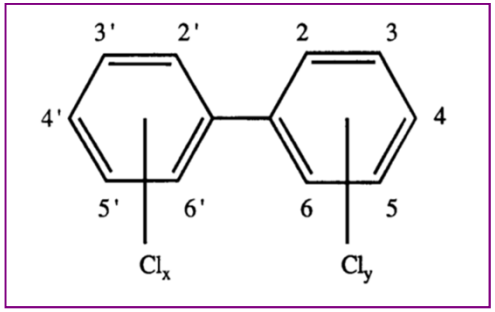


- Sediment PCB conc. proportional to # salmon spawning/km^2
- PCB congener distribution in salmon lakes' sediments similar to distribution in salmon; different from distribution in no-salmon lakes' sediments
- Pacific salmon
  - Amadramous: move from salt to freshwater to breed or spawn
  - Semelparous: die after spawning

Krummel et al., 2003, Nature, 425:255-256

Transport against hydraulic gradient

- Salmons concentrate PCBs (biovectors)



PCB molecular structure

Bioconcentration of PCBs in Lake Ontario

PCB congener	microgram PCB per * 52	66	153
MW	291.97	291.97	360.71
dissolved	6.3E-0.5	3.1E-0.5	5.0E-0.5
bottom sediment	25	46	25
suspended sediment	15	27	23
plankton	2.4	1.6	2.2
mysids	3.5	15	30
amphipods	22	30	45
oligochaetes	6.3	8.3	7.5
small smelt	7.6	2.7	64
large smelt	18	72	130
trout/salmon	62	160	430

*liter for dissolved; kg dry wt. for sediments; kg wet wt. for organisms

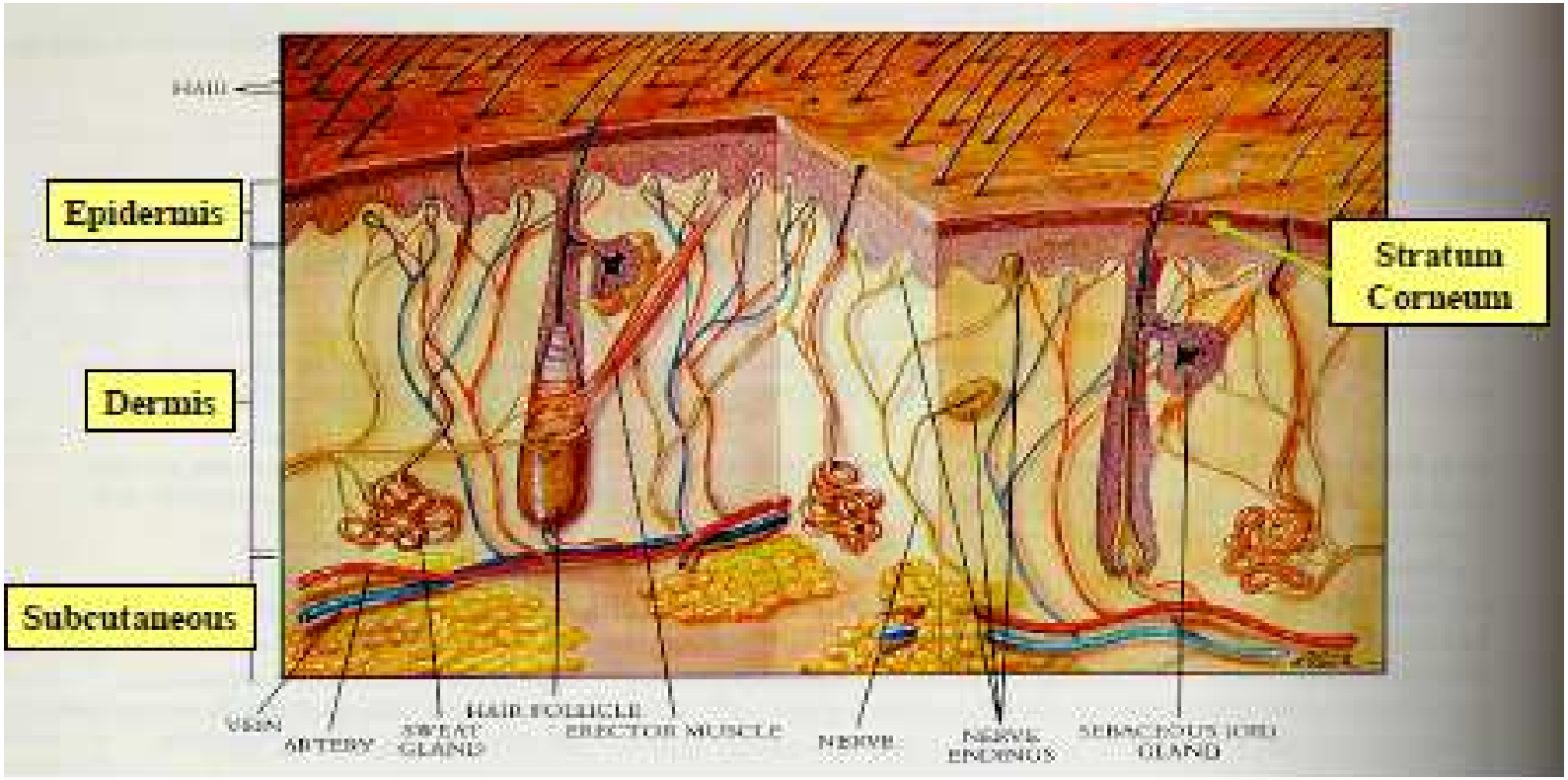
Oliver & Nilmi, 1988, ES&T, 22:388-397

Dermal uptake of soil and sed. bound contam.

http://www.heraldsun.com.au

http://news.naver.com/main/read.nhn?mode=LSD&mid=sec&sid1=106&oid=144&aid=0000273454

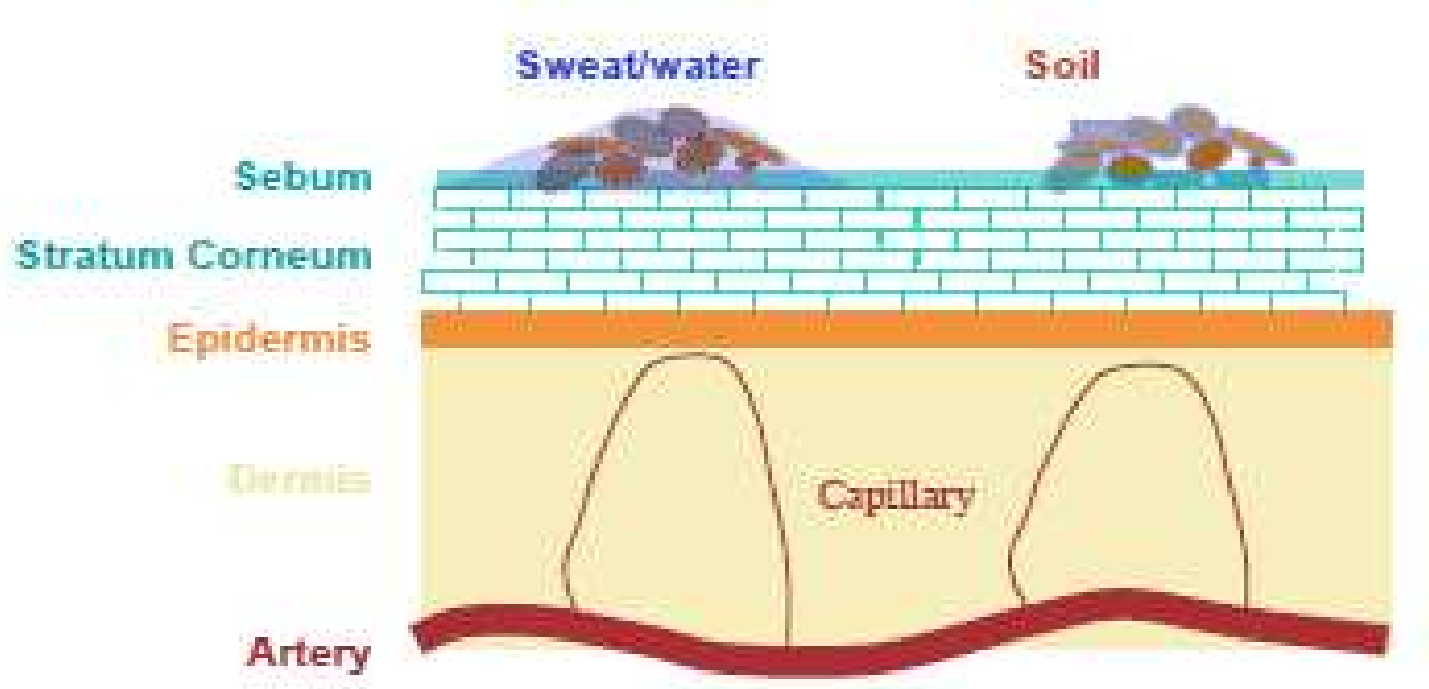
Human skin



Functions

metabolism, sensory organ, prevent water loss or uptake, regulate temperature, breakdown drugs, resist damage, insulate, exchange air & fluids

Dermal exposure to soil & sed. bound contam.



Sebum – oily secretion of the sebaceous gland

Stratum corneum – dead cells; hydrophobic

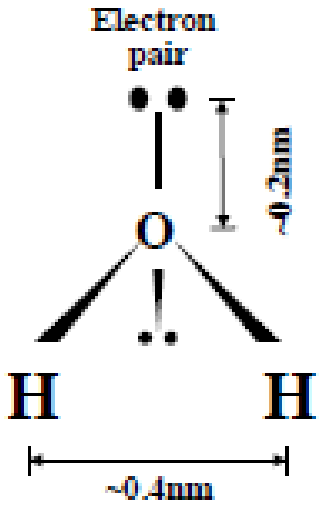
Epidermis, dermis - hydrophilic

Dermal exposure - considerations

- **Mass transfer/equilibria between**
  - Soil & sweat/sebum
  - Sweat/sebum & *stratum corneum*
  - *Stratum corneum* & epidermis
  - Epidermis & dermis
  - Dermis & blood
- **Transport in:**
  - *Stratum corneum*
  - Epidermis
  - Dermis
- **Soil coverage, residence time on skin**
- **Air to skin; water to skin; …**

Water – a unique solvent

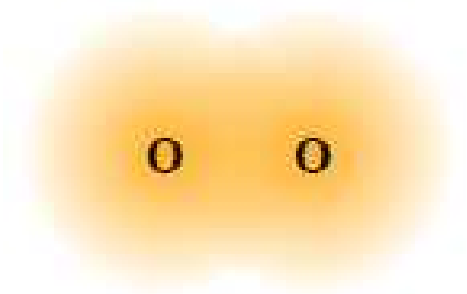
Property	H_2O	H_2S	CH_4	CH_3OH
Molecular weight	18	34	16	32
Dipole moment (Debyes)	2.0	0.9	0.0	1.7
Boiling point (°C)	100	-60	-161	65
Enthalpy of vaporization (kJ/g)	2.30	0.55	0.88	1.10
Melting point (°C)	0	-85	-181	-94
Enthalpy of fusion (kJ/g)	0.33	0.07	0.06	0.10



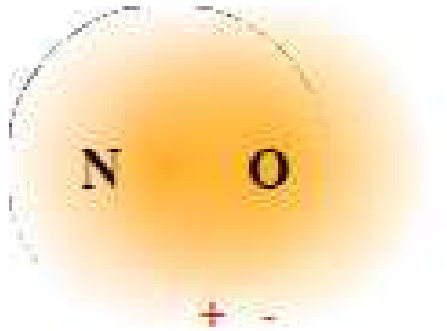
Dipole moment

A molecule has a dipole moment if the center of the molecule's positive charges is not at the same spot as the molecule's negative charges

O_2 – no dipole moment

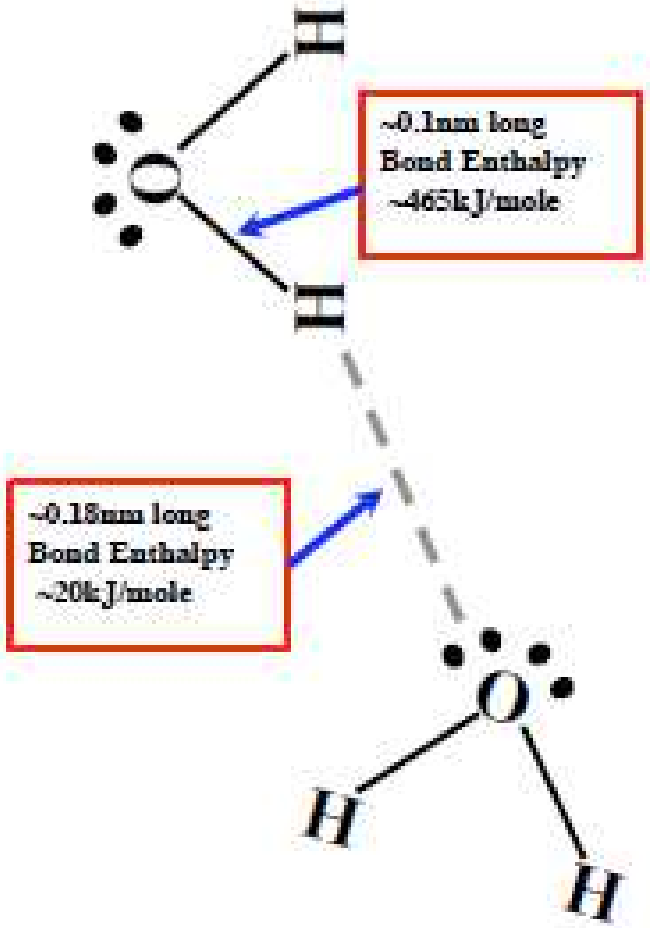


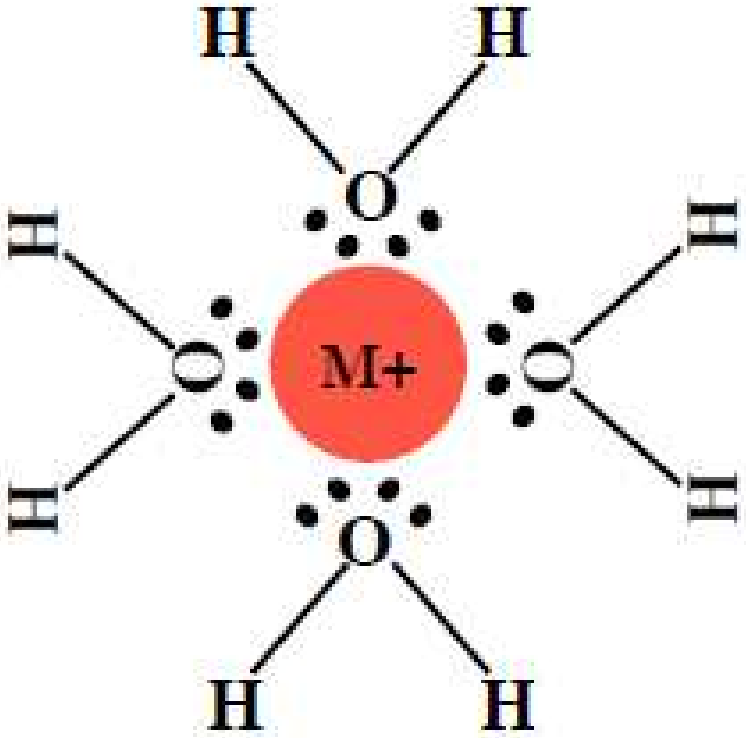
NO – dipole moment



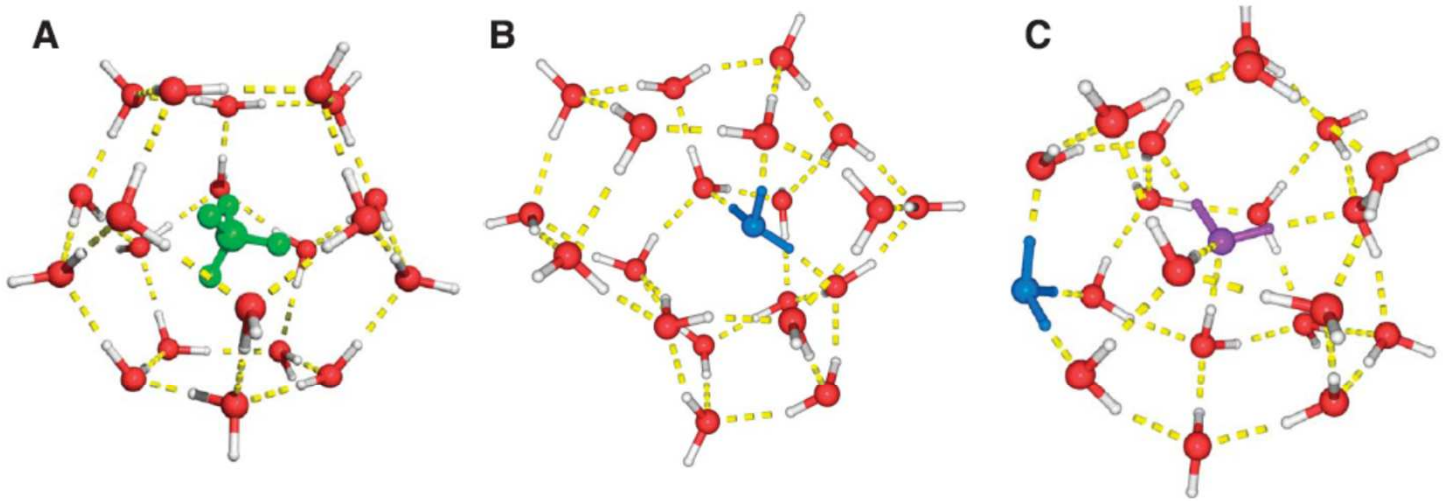
Electron density shifted to oxygen

Water – hydrogen bonding & dipole moment





Hydrogen bonding



Stable water clusters. (**A**) Methane clathrate consists of a dodecahedral water cage surrounding a methane molecule (green). The $n = 21$ protonated water cluster suggested by analogy has the H_3O^+ ion (blue) taking up a position inside the clathrate cage (**B**) or on its surface (**C**), displacing a neutral water molecule (purple) to the cage interior. The hydrogen bonds are indicated by the dashed lines in yellow.

Zweir, 2004, Science, 21:1119

- H_2O structure promotes incorporation of hydrogen bonding, polar, ionic entities
- Non-hydrogen bonding, non-polar, non-ionic entities disrupt water's structure