Carnegie Mellon University
Department of Civil and Environmental Engineering

12-725: Fate, Transport, and Physicochemical Processes of Organic Contaminants in Aquatic Systems

Presentation Assignment:
Partitioning Behavior of Organic Contaminants in the Environment
Note: We will NOT be doing presentations this year due to COVID-19. This will instead be a 2-part individual assignment
Assignment Due Dates: 3/31/20-part 1 due
4/7/20-part 2 due (uses whole class part 1)

Each person is asked to do the following:

Part 1

Obtain the input chemical properties needed to predict the partitioning in the environment for the compound assigned to you. This includes vapor pressure, aqueous solubility, and K_{ow}. Get reported *measured* properties from **at least two sources**. Estimate the same properties using **at least two** of the methods described in the course. One potential source of information is Appendix C in your *Environmental Organic Chemistry* (EOC) textbook by Schwarzenbach, Gschwend, and Imboden. However, note that many of the properties reported in Appendix C are *calculated* (i.e. estimated) values rather than measured. Other sources include the published literature, Chemical Abstracts SciFinder Scholar (see note below), CRC Handbook of physics and Chemistry, PubChem, Knovel, ChemSpider, or the scientific literature (e.g. Journal of Chemical & Engineering Data or Environmental Science & Technology) (http://www.knovel.com/web/portal/basic_search/display?_EXT_KNOVEL_DISPLAY_bookid=761). Note that these databases can point you to the publications that provided the measurements.

Once the properties are known and estimated, calculate the *concentration* of the compound in each compartment of the **model environment** (page 3) using the appropriate input values. You can assume 25 °C and a release of 1000 moles total of your compound to the environment. Also calculate the *distribution of mass* for your compound between the various compartments. Present a 1-page summary of your inputs and outputs to me (due 3/31/20). Use the following format for your presentations. Use visual aids as appropriate.

Summary format:

(a) Set up a table summarizing the required parameter input **values** for your compound. These include molecular weight, C_w^{sat}, P^{sat}, and K_{ow}. Include the sources of information and the two estimation methods used to get the values.

(b) Briefly **describe the rationale** that you used to select the input values for your model (i.e. averaging, most reliable source, measured, etc.).

(c) Briefly discuss the overall fate (i.e. distribution) of your contaminant in the model environment selected (see last page of this assignment). In what compartment(s) does the compound primarily reside? Is the partitioning behavior, i.e. concentration ratios and calculated mass distributions in line with expectation? Why or why not?

Part 2

Answer the following questions based on the entire set of data from the class:

Using the input and distribution data for each compound, answer the following questions about the partitioning behavior of the set of compounds.

(d) Are there consistent differences among the concentrations of a given compound in the solid compartments: soil, sediment, suspended matter, and biota? Document your conclusion and explain.

(e) Compare the distribution of mass of the various compounds. Explain the differences in partitioning among the six compartments in terms of the chemical's properties and the compartments' properties. Group the compounds based on their partitioning behaviors. Which compound(s) partition(s) most strongly into the air? Which ones(s) into the water? Which one(s) into the sediment? What primarily determines the distribution of the chemicals and their groupings?

(f) If the temperature were to increase by 10 °C, how would this affect the distribution of mass of each of the groups of compounds? Answer this semi-quantitatively, e.g. the concentration in air would increase by ~50% (or whatever is appropriate). Or you can build temperature dependence into your model and calculate it explicitly.

Grades:

The grade for this assignment is equally weighted between the following parts:

1. Documentation. Your written (1 page max) summary of your inputs and partitioning results. Be sure to accurately site all sources of information in an appendix if necessary. (40%)
2. Your discussion regarding the differences in partitioning between the compounds considered (answers (c)-(f)). (60%)

Compound assignments:

1: DDT-Taylor Brown
2: MTBE-Zhaoyang Feng
3: Chloroform-Yushan HuangFu
4: Dimethyl phthalate-Shengbin Jai

5: 2-Chlorophenol-Xu Kang
6: Benzene, 1-Bromo-3-(4-Bromophenoxy)-Rachel Mole
7: Tetrachloroethene -Caity Pietrusza
8: Atrazine-Lohita Rajesh
9: Lindane-Yufei Shao
10: Pentchlorophenol-Simon Stein
11: Arachlor 1242-Harold Wnag
12: Estrone-Shuyuan Wang
13: Malathion-Tessa Weiden
14: 2,3,7,8-Tetrachlorodibenzo-p-dioxin-Stephanie Wong

Model Environment:

Compartment Properties

	Volume [m^3]	Density [kg/m^3]	Organic Fraction [--]
Air	2.00E+09	1.19E+00	N/A
Water	9.50E+05	1.00E+03	N/A
Soil	1.40E+04	1.50E+03	2.00E-02
Sediment	9.90E+03	1.50E+03	4.00E-02
Susp. aq matr	3.50E+01	1.50E+03	4.00E-02
Biota	3.50E+00	1.00E+03	20% Lipid content