Carnegie Mellon University
Department of Civil and Environmental Engineering

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

Problem Set #5 Spring 2020
Due February 20 by 5pm

1. Given the following information:

Compound	ΔH_{vap} (kJ/mol)	H_w^E (kJ/mol)
Benzene	34	4
Dipropylether	27	-19
Methylbenzene	38	6
1-hexanol	62	-14

   (a) Rank the compounds in order of increasing vapor pressure (lowest to highest). Explain your reason.
   (b) Rank these compounds on order of increasing aqueous solubility (lowest to highest). Explain your reasoning.
   (c) Which compound's air-water partition coefficient should be the <u>most</u> sensitive to changes in temperature? Explain your reasoning.

2. Estimate the aqueous solubility of the following compounds at 25 °C in mg/L using two different estimation methods. Cite sources for the estimation methods, data, and experimental/reported values used. Compare the estimated values with reported values and calculate the error (%). (Note: I have provided a chapter from a book on solubility estimation methods).
   (a) chloroform, (b) anthracene

3.   Q10.2 and Q 10.4 in EOC

4.   P10.5 in EOC

5.   Starting with equation 10-2 in your textbook:

$$K_{i,lw} = \frac{C_{il}}{C_{iw}} = \frac{\gamma_{iw}}{\gamma_{il}} \frac{V_w}{V_l}$$

Derive the expression to calculate the $C_{i,w}$ from an organic mixture containing species i.

$$C_{i,w} = x_{i,mix} \gamma_{i,mix} C_{i,wL}^{sat}$$

Where $x_{i,mix}$ the mole fraction of species i in the organic mixture and $\gamma_{i,mix}$ is the activity coefficient of species i in the organic mixture. Also, derive an expression for the partitioning of species I from an organic mixture and water, $K_{i,mix,w}$.

6. What is the concentration of chloroform and vinyl chloride in groundwater at 15 °C at equilibrium with a large volume of methylene chloride (dichloromethane) containing chloroform and vinyl chloride at 1wt% and 0.01wt%, respectively?