ENV 6002: Physical and Chemical Principles of Environmental Engineering

Fall 2008 | University of South Florida

Midterm Examination | Civil & Environmental Eng.

Tues., Oct. 14, 2008 | J. A. Cunningham

Instructions:

1. You may read these instructions, but do not turn the page or begin working until instructed to do so.
2. Answer all questions in the exam booklet provided, and write your name conspicuously on the exam booklet.
3. You are allowed one sheet of 8.5-by-11-inch paper (or A4 paper) with hand-written notes. You may write on both sides of that paper. However, mechanical reproductions (photocopying, laser printing, scanning, etc.) are not allowed; all notes must be hand-written.
4. A calculator is recommended, but it may not be pre-programmed with formulae from the class.
5. Time limit: 70 minutes. Stop working when asked. If you continue working after time has been called, you will be penalized at a rate of 1 point per minute.
6. Show all work and state all assumptions in order to receive maximum credit for your work.
7. Make sure your answers include units if appropriate. ***Watch your units!!***
8. This exam contains 4 questions, some with multiple parts. The total point value for the exam is 70 points -- one point per minute. Gauge your time accordingly!
9. Use a reasonable number of significant digits when reporting your answers. *You are likely to be graded down* if you report an excessive number of significant digits. In some cases, the problem may indicate the precision to which you should report your answer.
10. Don't cheat. Cheating will result in appropriate disciplinary action according to university policy.
11. Page 2 of this exam (the back of this page) contains data, constants, and conversion factors that might be helpful to you as you complete the exam.

Properties of ethylbenzene (EB):

This exam contains two questions dealing with the contaminant ethylbenzene (EB), which is an aromatic hydrocarbon found in petroleum. It is a relatively common environmental contaminant. Below is information on the physical-chemical properties of EB at 25 °C.

	Ethylbenzene
Atomic formula	C_8H_{10}
Molecular weight (g/mol)	106.17
Liquid density, ρ (g/cm^3)	0.86
Aqueous solubility, C^{SL} (mg/L)	168. (note the units, mg/L)
Octanol-water coefficient, K_{ow}	
Vapor pressure, P^{sat} (Pa)	
Aqueous diffusivity, D (m^2/sec)	1.0×10^{-9}

Some other potentially useful constants:

Ideal gas constant, R: 8.314 Pa•m^3•mol^{-1}•K^{-1} = 82.06×10^{-6} atm•m^3•mol^{-1}•K^{-1}

Molecular weight of water, H_2O: 18.01 g/mole

Density of water at 20°C: 0.998 g/mL

Aqueous diffusivity of oxygen at 20°C, D_{O2}^{L}: 2.0×10^{-9} m^2/sec

Henry's constant for oxygen at 20°C, H_{CC}: 30

Atomic Weights: **C** = 12.011 **Cl** = 35.453 **H** = 1.0079 **N** = 14.007 **O** = 15.999

Potentially useful conversion factors:

Pressure: 1 atm = 760 mm Hg = 760 torr = 101325 Pa

Mass: 1 kg = 1000 g = 1×10^6 mg

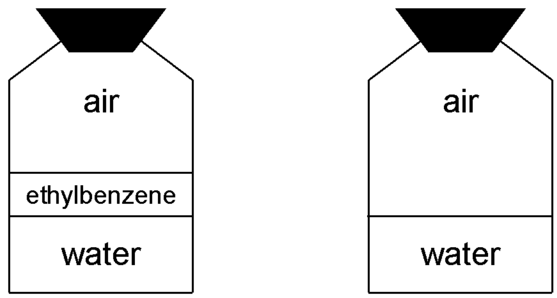
Temperature: 25 °C = 298.15 K

Volume: 1 m^3 = 1000 L = 1×10^6 mL = 1×10^6 cm^3

1. (10 pts) Below are three pairs of terms that we have discussed in this course. Choose ***one*** of these pairs. Define the two terms as they pertain to contaminant fate and transport, water quality, and/or other topics relevant to this course. Also explain how the two terms are related or relevant to each other. Try to include the most salient information. About 3–6 sentences should probably be sufficient. Try not to spend more than 10 minutes on this problem.
   a. water quality criteria, maximum contaminant level
   b. xenobiotic, PBT
   c. CERCLA, "joint, several, and retroactive"

Exam continues →

2. (20 pts) Consider two closed beakers as shown below. Both beakers contain water and air, and are contaminated with ethylbenzene (EB). The temperature of both systems is 25 °C, and you may assume that both systems are at equilibrium.



Beaker #1 has a layer of pure EB floating on top of the water; therefore the aqueous concentration of EB in the water is $C_{EB}^{aq} = C^{SL} = 168$ mg/L. The layer of EB is called a "non-aqueous-phase liquid," or NAPL, and it floats on top of the water because the density of EB is less than the density of water. In beaker #2, the aqueous concentration of EB is lower by a factor of 100: $C_{EB}^{aq} = 1.68$ mg/L.

a. (6 pts) Estimate/calculate the *mole fraction* of EB in the aqueous phase (x_{EB}^{aq}) for beaker #1. Estimate/calculate the mole fraction of EB in the aqueous phase for beaker #2.

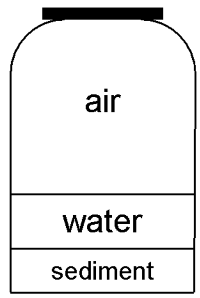
b. (6 pts) Estimate/calculate the *activity coefficient* of EB in the aqueous phase (γ_{EB}^{aq}) for beaker #1. Estimate/calculate the activity coefficient of EB in the aqueous phase for beaker #2.

c. (4 pts) Look at the mole fraction you calculated for EB in beaker #1. What is the significance of this value with regard to the validity of Henry's Law in these systems? Explain briefly (a couple sentences should suffice).

d. (4 pts) Suppose you measured the vapor-phase mole fraction of ethylbenzene, y, in each beaker. Which beaker would have a higher value of y? How much higher would it be? How do you know? Show your calculations and/or explain your reasoning as appropriate.

Exam continues →

3. (25 pts) Consider a closed system as shown in the figure below. A closed bottle contains air, water, and sediment. The system is contaminated with ethylbenzene. The system is at 25 °C, and you may assume that it is at equilibrium.



The volume of water in the bottle is 65 mL. The volume of air in the bottle is 420 mL. The mass of sediment is 24 g, and the sediment has a bulk density $\rho_s = 1.6$ g/cm^3 = 1600 g/L and a fraction of organic carbon f_{oc} = 2.7% = 0.027.

Suppose we know that, in this system, there is 10 times as much ethylbenzene mass on the sediment as there is in the water. Suppose we also know that there is 2 times as much ethylbenzene mass in the air as there is in the water. That is, $M_{EB}^{\mathrm{sed}} : M_{EB}^{\mathrm{air}} : M_{EB}^{\mathrm{water}} = 10:2:1$.

a. (5 pts) Which of the three phases (sediment, air, or water) has the highest *concentration* of ethylbenzene, on a mass/volume basis? Which of the three phases has the lowest concentration of EB on a mass/volume basis? Explain your reasoning and/or show your calculations as appropriate.
b. (10 pts) Based on the information given, show that the *vapor pressure* of ethylbenzene, P^{sat}, is about 1220 Pa. Hint: make use of an appropriate *concentration ratio* that you may have found in part (a).
c. (10 pts) Based on the information given, show that the octanol-water partition coefficient of ethylbenzene, K_{ow}, is about 1590. Hint: make use of an appropriate *concentration ratio* that you may have found in part (a).

Exam continues →

4. (15 pts) Below is a table of chemical properties (at 25 °C) for three chemicals that are sometimes found as environmental contaminants.

- Methyl tert-butyl ether (MTBE) is a gasoline additive
- Fluoranthene is a polycyclic aromatic hydrocarbon (PAH)
- 1,1,1-trichloroethane (TCA) is a solvent

	MTBE	Flouranthene	TCA
Atomic formula	$C_5H_{12}O$	$C_{16}H_{10}$	$C_2H_3Cl_3$
Molecular weight (g/mol)	88.2	202.3	133.4
Liquid density, ρ (g/cm^3)	0.74	1.25	1.34
Aqueous solubility, C^{SL} (mg/L)	40,300	0.22	1,300
$\log_{10}(K_{ow})$	0.94	5.23	2.49
Vapor pressure, P^{sat} (Pa)	32,360	0.0012	16,600

Suppose that all three of these chemicals have been accidentally released into a lake. The lake ecosystem consists of four environmental compartments: water in the lake, air above the lake, sediment at the bottom of the lake, and fish that live in the lake. Suppose that the releases happened long enough ago that the system is starting to approach equilibrium.

a. (8 pts) For each of the three chemicals, indicate where you would expect the chemical to be found, i.e., in which compartment or compartments do you think each chemical "prefers" to reside? Briefly explain your reasoning for each chemical, and/or show any calculations that you deem necessary.

b. (7 pts) To really answer this question well, you would need some other information that is not included here. What other information would you like to have to answer this question in more detail? Be as specific as you can.

END OF EXAMINATION