

ENV 6519: Physical & Chemical Processes in Environmental Engineering

Spring 2012

Homework #2

Due Thurs., Jan. 26, 2012

University of South Florida

Civil & Environmental Eng.

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Assignment for 2012: problems 1–5; skip problem 6

(1) (25 pts)

- (a) (5 pts) Complete problem 7-1 in the Water Treatment text book. You can either follow the procedure from the text book, or from the notes given in class, whichever you prefer. (You should get the same answer either way.)

Problem 7-1 asks you to compute the energy required to separate PERC from water at a constant concentration (either 5 mg/L or 10  $\mu\text{g/L}$ ). The issue with this is as follows: when you separate out some of the PERC, then the concentration changes, and then the assumption of constant concentration is no longer valid. So the way you did part (a) is nice as an exercise, but isn't very useful in reality. Let's try to take it a step farther.

- (b) (5 pts) Assume that you have a volume  $V$  of water, and it contains a concentration  $C$  of some contaminant (where  $C$  has units of mass per volume). You perform a separation and you remove a very small amount of the contaminant from the water. The change in the contaminant concentration is  $\Delta C$ , and the mass of contaminant that you removed is  $V \Delta C$ . How much energy is required to remove the small amount of mass? For this, you may assume that  $\Delta C \ll C$ . Hint #1: you have a formula that tells you how much energy is required per mole of contaminant recovered. Hint #2: this is really simple, don't try to make it complicated.
- (c) (5 pts) Now suppose I have a volume  $V$  of water that initially contains a concentration  $C_0$  of the contaminant. I want to treat the water and reduce the contaminant concentration down to  $C_f$ . Argue that the energy required for this treatment is given by this formula:

$$V \frac{RT}{MW} \int_{C_f}^{C_0} \ln \left( \frac{C^{SL}}{C} \right) dC$$

where  $MW$  is the molecular weight of the contaminant, and  $C^{SL}$  is the solubility-limit concentration, in units of mass per volume.

- (d) (10 pts) Now let's perform a more realistic variant of part (a). Suppose I have water contaminated with PERC at a concentration of 5 mg/L. I want to treat this water to get the PERC concentration down to 5  $\mu\text{g/L}$ , which is the federal drinking-water standard. What is the minimum energy requirement to treat 1000 L of contaminated water? Hint #1: use the formula from part (c), and use an integral table if you are rusty on your integration. Hint #2, to help you with the integration: how is  $\ln(a/x)$  related to  $\ln(x/a)$ ? Which is easier to integrate?

(2) (20 pts)

- (a) (10 pts) Complete problem 7-2 in the Water Treatment text book. Hint: for each of the five bottles, you can calculate the adsorbed concentration  $q$  using methods given in the text book. Then, prepare a figure like Figure 7-2 in your text. Don't forget to specify the  $V/M$  ratios. The phase equilibrium line – that is, the graph of  $q$  versus  $C$  – is also called a *sorption isotherm*.
- (b) (10 pts) Graph  $q$  vs  $C$  on a log-log scale, i.e., graph  $\log(q)$  vs.  $\log(C)$ . If  $\log(q)$  is linear with respect to  $\log(C)$ , then the data are said to obey a *Freundlich isotherm*. Fit a straight line through the graph on the log-log plot. (You can do this in Excel, but it requires a little thought – if you do it wrong, you won't get a straight line on your log-log plot.) How good is the straight-line fit? Do you think a Freundlich isotherm applies to these data?

(3) (30 pts)

- (a) (9 pts) Use the Hayduk-Laudie method to estimate the aqueous diffusion coefficients for trichloroethene (TCE), 1,2-dichloroethane (DCA), and 1,1,1-trichloroethane (TCA) at 20 °C.
- (b) (4 pts) Compare the values that you get to the values listed in Table 7-4. Table 7-4 says the values are at 25 °C, but I think the table heading might be wrong...assume those values are for 20 °C. Do your estimates agree with the tabulated values within 1%? within 10%? within 20%?
- (c) (4 pts) When I was a graduate student in 1993, I was assigned a problem similar to this one, but using the Wilke-Chang method instead of the Hayduk-Laudie method. The answers I got were  $0.93 \times 10^{-5}$  cm<sup>2</sup>/s for TCE and  $0.89 \times 10^{-5}$  cm<sup>2</sup>/s for TCA. How do these values compare to the values you got with the Hayduk-Laudie method? Based on a comparison with values in Table 7-4, which of the two methods appears superior for these chemicals – the Hayduk-Laudie method or the Wilke-Chang method? Is there a significant difference, or do the two methods perform about the same?
- (d) (4 pts) Based on the comparison of the tabulated data, the Hayduk-Laudie approximations, and the Wilke-Chang approximations, how much uncertainty do you think there is in these estimation methods? Do you trust your estimated values to  $\pm 1\%$ ? to  $\pm 10\%$ ? to within a factor of two? Based on this, how many significant digits do you think are warranted when you report a diffusion coefficient estimated with the Hayduk-Laudie or Wilke-Change method?
- (e) (9 pts) Two of the chemicals in your design project this semester are cis-1,2-dichloroethene (DCE) and 1,1,2,2-tetrachloroethane (TeCA). Values for the aqueous diffusion coefficient are not listed in Table 7-4 for these chemicals. Use the Hayduk-Laudie method to estimate the aqueous diffusion coefficients for DCE and 1,1,2,2-TeCA. You can “calibrate” your answers based on your responses to parts (b)–(d). What values of  $D$  would you use for these two chemicals if, for instance, you needed to estimate a mass-transfer coefficient?

(4) (20 pts)

- (a) (8 pts) Using the method described in your text book, estimate the diffusion coefficient for tetrachloroethene (also called tetrachloroethylene, perchloroethene, perchloroethylene, PCE, or PERC) in air at 20 °C.
- (b) (8 pts) Repeat the calculation using the method of Arnold [Arnold, J.H., 1930; "Studies in Diffusion, I – Estimation of Diffusivities in Gaseous Systems." *Industrial and Engineering Chemistry*, vol. 22, no. 10, pp. 1091–1095]:

$$D_{12} = \frac{0.00837 T^{5/2} [(M_1 + M_2) / M_1 M_2]^{0.5}}{P (V_{b1}^{1/3} + V_{b2}^{1/3})^2 (T + S_{12})}$$

where  $D_{12}$  is the diffusion coefficient of gas 1 in gas 2, in units of  $\text{cm}^2/\text{s}$ ;  $T$  is the temperature in degrees Kelvin;  $M_1$  and  $M_2$  are the molecular weights (in g/mole) of compounds 1 and 2;  $P$  is the pressure in atmospheres;  $V_{b1}$  and  $V_{b2}$  are the molar volumes (in  $\text{cm}^3/\text{mole}$ ) of the gases at their normal boiling points; and  $S_{12}$  is given by the following.

$$S_{12} = 1.47 F \sqrt{T_{b1} T_{b2}}$$

$$F = \left[ \frac{2 \sqrt{V_{b1} V_{b2}}}{V_{b1} + V_{b2}} \right]^{(1/3)}$$

where  $T_{b1}$  and  $T_{b2}$  are the normal boiling points of the two gases, in degrees Kelvin.

For this problem, you can assume that the boiling point of air is 79 K, and the air is at 1 atmosphere. You can calculate the molecular weight of air based on knowing its composition, and you can look up its molar volume in Table 7-5 of your text. Also, you can estimate the molar volume of PCE using techniques given in the text, and you can look up the boiling point of PCE (it would be good to cite your source).

- (c) (4 pts) How well do the two methods agree? Which did you find easier? Based on the level of agreement, how many significant digits do you think are warranted in your estimates?
- (5) (5 pts) Based on your estimates in problems (3) and (4), what is the relative magnitude of the diffusion coefficient in air to the diffusion coefficient in water? i.e., what is (approximately) the ratio of  $D$  from problem (4) to those of problem (3)? (Although you considered different chemicals in problems 3 and 4, they are all of similar size and molecular weight, so comparing the values of  $D$  for the different chemicals is fine to give us a semi-quantitative estimate, which is all we want here.) Based on this, would you expect gas-phase mass transfer coefficients to be larger or smaller than liquid-phase mass transfer coefficients? By a little or by a lot?

(6) (15 pts)

- (a) (5 pts) Complete problem 7-13 in the text. Hint: if you read the text carefully, a lot of the work is done for you already.
- (b) (5 pts) Complete problem 7-17 in the text.
- (c) (5 pts) Are the mass transfer coefficients higher for oxygen, or for PCE? By how much? Why?