Fate & Transport of Chemicals in the Environment

Homework #2 | University of South Florida
Due Monday, Jan. 31, 2022 | Prof J A Cunningham

This assignment is designed to get you accustomed to different types of units that we use in environmental engineering, particularly for reporting concentrations of chemicals in air, water, and soil. (…and a little bit in non-aqueous-phase liquids, too.)

(1) (20 pts) On a molar basis, the composition of dry air is approximately 78.03% N_2, 20.99% O_2, 0.94% Ar, and 0.04% CO_2.

(a) Estimate/calculate the molar mass of dry air, in units of g/mol. Report your answer to four significant digits. Hint: use the periodic table.

(b) Estimate/calculate the density of dry air at sea level on a cold day (5 °C) and on a warm day (35 °C). Hint: use the ideal gas law and your answer from part (a). Report your answers in units of kg/m^3, and report three significant digits.

(c) For 35 °C, estimate/calculate the concentration of CO_2 in units of mg/m^3 (assuming dry air at sea level). Hint: use the partial pressure of CO_2 along with the ideal gas law.

(d) For 35 °C, estimate/calculate the mass fraction of CO_2 in dry air. Hint: use your answers from the parts above. There is more than one way to solve this part.

(2) (10 pts) A dilute aqueous solution of benzene (C_6H_6) has a benzene concentration of 15 mg/L. Estimate/calculate the *mole fraction* of benzene in the solution. Hint: you can make use of the fact that the solution is dilute – this implies that the solution is mostly water, so you can estimate the density and the molar mass of the solution.

(3) (15 pts) A volume of benzene, V_{ben}, is mixed with a volume of toluene, V_{tol}. The resultant solution has a benzene concentration of 150 g/L. Estimate/calculate the mole fraction of benzene in the solution.

Hint #1: Benzene and toluene are both liquids. Benzene has a molar mass of 78.11 g/mol and a liquid density of 875 g/L. Toluene has a molar mass of 92.14 g/mol and a liquid density of 866 g/L.

Hint #2: This solution is not dilute, so you can't use the same approach as problem (2). However, you can *neglect the volume change of mixing*. This means that when you mix V_{ben} with V_{tol}, the resultant solution has a final volume of $V_{\mathrm{ben}} + V_{\mathrm{tol}}$. (That might sound obvious, but it actually isn't always true. It is OK here.)

Hint #3: There is more than one way to approach this problem. I found that one simple way is to assume that you have a total solution volume of 1.00 L. Then it is not difficult to figure out how much benzene and how much toluene must be in there – and hence the mole fractions of each.

(4) (25 pts) In problem (3), we had a solution in which it was OK to ignore the volume change of mixing. That is fine for mixtures of benzene and toluene. Now let's look at the dissolution of a strong electrolyte (salt) in water, and we'll see what happens.

An aqueous saline solution is 12.0% NaCl by mass and has a density of 1084 g/L.

(a) *Estimate/calculate the molar concentration of NaCl in the solution*. Report your answer to three significant digits. Hint: you can start by assuming that you have 1.0 L of solution. Then what is the mass of the solution? What mass of NaCl is present?

(b) Suppose you made the solution in the following way. You took the necessary mass of dry NaCl and you dissolved it into 100.0 mL of pure water. When you were done, you had a solution that is 12.0% NaCl by mass, with a density of 1084 g/L. *What is the final volume of the solution*? Hint: assume that the density of pure water is 998.0 g/L at the temperature of this problem. So what mass of water did you start with? – and therefore what mass of NaCl did you start with? – and therefore what is the total mass of the solution? – and therefore what is the total volume of the solution?

(c) The density of NaCl salt is 2165 g/L. In part (b), what volume of dry NaCl did you start with? Therefore, what total volume (volume of water plus volume of dry NaCl) did you start with? What total volume did you end up with after the NaCl dissolved (i.e., what was your answer to part (b))? What can you conclude about the volume change of mixing when NaCl dissolves into water?

(5) (10 pts) The molecular formula for lactose is $C_{12}H_{22}O_{11}$. Suppose we have an aqueous solution of lactose with a concentration of 100 mg/L. Estimate/calculate the concentration of dissolved oxygen (in mg/L) that would be required to completely oxidize the lactose. Hint: you will have to write the stoichiometry for the oxidation of lactose. What are the products when a carbohydrate is oxidized?

(6) (20 pts) Imagine that the soil and groundwater in a nearby area are contaminated with cadmium, a toxic heavy metal. We excavated 1.0 m^3 of soil from beneath the water table (which means that the pore spaces of the soil are filled with groundwater). There are two *phases* present in the collected sample – solid grains and liquid water. Cadmium is present in both of those phases – it is dissolved in the liquid water, and it is adsorbed onto the surfaces of the solid grains. Here is some information about the collected soil sample.

- The mass of the 1.0 m^3 sample is 2,120 kg.
- The soil has a porosity of 0.30. That means that, by volume, 30% of the sample is pores, and the other 70% is solid grains. The pores are filled with water.
- The total mass of cadmium found in the 1.0 m^3 sample was 109 g.
- The concentration of cadmium in the aqueous phase (i.e., in the groundwater) is 3.4 mg/L.

problem 6 continues →

6. continued

Each of the following parts of the problem is pretty short – if you are making any of them very long or complicated, then you are over-thinking it.

(a) Estimate/calculate the volume of water and the mass of water that are present in the soil sample. Remember that water is one of the two phases present.

(b) Estimate/calculate the volume of solid grains and the mass of solid grains that are present in the soil sample. Remember that solid grains are one of the two phases present.

(c) Estimate/calculate the mass of cadmium in the water phase, in units of g. All the rest of the cadmium must be adsorbed onto the solid grains. Remember that cadmium is present in both of the two phases – dissolved in the water, and adsorbed onto the solid surfaces.

(d) Estimate/calculate the concentration of cadmium adsorbed to the solid phase of the soil. Report your answer in units of mg/kg, which is the same thing as ppm. Hint: use your answers from parts (b) and (c).

(e) Assume that the system is at equilibrium. Estimate/calculate the distribution coefficient, K_d, for adsorption of cadmium from water onto the soil. K_d is the ratio of the adsorbed concentration (in mg/kg) to the aqueous concentration (in mg/L). K_d has units of L/kg.

(*Note*: I don't actually know if an aqueous concentration of 3.4 mg/L is realistic for cadmium at a contaminated site. I just made it up for this problem. I usually like to use realistic numbers for my made-up problems, but I couldn't find a reliable number for cadmium, so I just made it up. The other numbers in the problem should all be pretty realistic. I think *probably* the given value is realistic, but I am not certain. Naturally occurring concentrations of cadmium are far below 3.4 mg/L, but at a contaminated site, I think 3.4 mg/L is probably pretty realistic?)