CE 597W FALL 2007 Example problems for Exam 3{PRIVATE }

Given:
Integration Formula:

For any ODE that takes the form:

$$\frac{dy}{dt} + p(t) \cdot y = q(t)$$

The following is the solution:

$$y = y_o \cdot e^{-P(t)} + e^{-P(t)} \int_{t_o}^{t} e^{P(t)} \cdot q(t) \cdot dt$$

where: $$P(t) = \int_{t_o}^{t} p(t) \cdot dt$$

1 (15 pts). Give specific example equilibrium equations and the units on the corresponding K.

1. acid dissociation:
2. complexation of a metal to a monodentate ligand:
3. chelation:
4. solubility of a divalent metal salt:
5. solubility of a neutral compound:
6. an oxidation-reduction half reaction (indicate each atoms oxidation state).
7. exchange across a liquid-gas interface:

2 (10 pts). Given the data below, calculate the first order decay constant in units of 1/min.

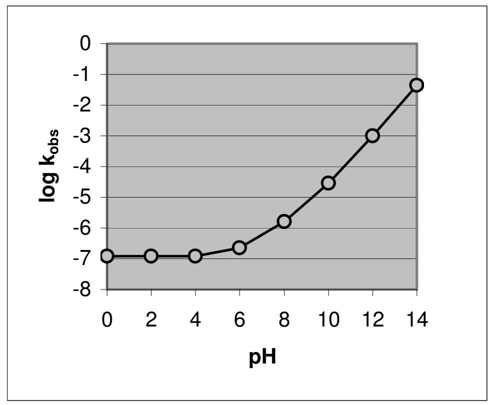
Time (days)	**Concentration of C (M)**
0	8.6×10^{-5}
1	4.7×10^{-5}
2	2.4×10^{-5}
3	1.4×10^{-5}

3 (20 pts) Chemical transfer from a liquid phase to a gas phase is often approximated with the following equation:

$$\frac{d[A]_{aq}}{dt} = -k([A]_{aq} - K_H P_A)$$

where k is a first-order transfer coefficient, K_H is Henry's constant (M/atm), and P_A is the partial pressure of the chemical in the gas phase. Assuming that the partial pressure remains constant and greater that zero over all conditions (i.e., a semi-infinite atmosphere), solve (the general solution) for C as a function of time, and constants (that is: k, K_H and P_A).

4 (10 pts). The figure below shows experimentally determined rate constants (k_{obs}) for the decay of the organic compound, AZ, as a function of pH. Quantitatively describe these data.



5. (20 pts). The organic compound trichlorophenol (pK_a = 6.0, log K_{ow} = 3.38 for the neutral species) is a contaminant in an aquifer whose solid phase contains 0.5 % organic carbon, and whose aqueous phase pH is 7.5. The compound exists as (i) HA in solution, (ii) A^- in solution, and (iii) HA sorbed to the solid phase (assume 0.5 K_{ow} = K_{oc}, and that sorption of the anion, A^-, may be neglected). If the aquifer is 50 % solids (density of solids = 2.0 g / cm^3), calculate the relative mass of TCP that exists in the liquid phase at equilibrium. What fraction of this is the neutral species. Start by listing all necessary and sufficient equations, knowns and unknowns.

6. (10 pts). Develop the two Euler's Method equations that can be used to solve for the concentrations of two species – A and B – that each react by first order kinetics to form the other.