ENV 6438: Physical & Chemical Processes for Drinking Water Treatment
Department of Civil & Environmental Engineering
University of South Florida

Cunningham **Spring 2020**

Homework #2 Due Wednesday, Feb. 5

Chemical Reactions, Reactor Theory, Reactor Analysis

1. (30 pts) Answer any three of the following problems in your text book: 5-6, 5-7, 6-2, 6-4, 6-9, 6-12, 6-14. Note: 6-14 is only for math nerds.

2. (50 pts) *adapted from a problem created by Paul Roberts, Stanford University*
A hydraulic study of the flow characteristics of a reactor was conducted by injecting a pulse of NaCl tracer at the reactor inlet and measuring the concentration of Cl^- in the effluent. The reactor volume is 400 m^3, the volumetric flow rate of water through the reactor is 10 m^3/min, and 40 kg of Cl^- are injected in the tracer pulse. The Cl^- concentration in the influent water is negligible other than the pulse injection. The concentration of Cl^- in the reactor effluent is measured, and the following results are obtained.

time (min)	Cl^- conc. (g/m^3)	time (min)	Cl^- conc. (g/m^3)
0	0	60	45
10	2	70	25
20	50	80	10
30	95	90	3
40	95	100	0
50	70	110	0

a. Estimate/calculate the theoretical average hydraulic residence time in the reactor.
b. Calculate the zeroth moment of the effluent concentration distribution. Use it to estimate the total mass of chloride that exits the reactor. What fraction of the injected chloride mass was recovered? Hint: trapezoidal rule is better than rectangle rule.
c. Calculate the first moment of the effluent concentration data. Use it to estimate the average hydraulic residence time. How does it compare to the theoretical value from part a? Hint: trapezoidal rule is better than rectangle rule.
d. Calculate the second (central) moment of the effluent concentration data. Use it to estimate the variance with respect to *t*. Then estimate the Peclet number of the reactor. Does this reactor exhibit a high degree of dispersion?
e. Draw a graph of the *residence time distribution* of fluid in the reactor. Your text calls it the *exit age distribution*. Also draw the *cumulative* residence time distribution (cumulative exit age distribution).

problem 2 continues →

2. continued
   f. On the graphs from part (e), sketch the residence time distributions you would expect for an ideal completely-mixed-flow reactor and for an ideal plug-flow reactor, each having the same average hydraulic residence time as the real reactor tested.
   g. What fraction of the fluid has a residence time of 20 minutes or less? By what time has 10% of the injected tracer left the reactor?
   h. Estimate the number of tanks for the tanks-in-series model of the reactor.
   i. Imagine that the reactor is operating at steady state, that a contaminant is entering the reactor with a concentration of 100 mg/L in the influent stream, that the contaminant undergoes first-order reaction in the reactor, and that the first-order reaction rate coefficient is 0.05 min^{-1}. Based on the tanks-in-series model, what effluent concentration would you expect from this reactor?
   j. What effluent concentration would you expect from an ideal plug-flow reactor with the same contaminant and the same hydraulic residence time? from an ideal completely-mixed-flow reactor?

3. (20 pts) One of my former students wrote his doctoral dissertation about a new technology to clean up soil contaminated by certain types of chemicals. One of the chemicals we tested in the lab was 1,2,4,5-tetrachlorobenzene (TeCB). When we started working on the project, we thought maybe TeCB would be destroyed according to first-order kinetics, but we weren't sure. Below are two tables of actual data that the student collected in a batch reactor in the laboratory. The two data sets were collected under different experimental conditions. For each of the two experiments, determine if the disappearance of TeCB is zero-order, first-order, second-order, or something else. Specify the value of the rate constant (k_0, k_1, or k_2, as appropriate). Be sure to give the right units of k!

   Table 1: Concentration of TeCB vs. time, experiment 1

time (min)	conc. (mg/L)
0	5.0
5	2.93
10	2.06
20	0.61
30	0.28
45	0.057

problem 3 continues →

3. continued

Table 2: Concentration of TeCB vs. time, experiment 2

time (min)	conc. (mg/L)
10	3.02
20	2.51
30	2.16
45	1.59
60	1.07

If you want to know more about this project, you can read the following papers:

Wee HY, Cunningham JA. **2008**. Palladium-catalyzed hydrodehalogenation of 1,2,4,5-tetrachlorobenzene in water-ethanol mixtures. *Journal of Hazardous Materials*, 155(1–2), 1–9. DOI: 10.1016/ j.jhazmat.2007.10.045

Wee HY, Cunningham JA. **2011**. Remediation of contaminated soil by solvent extraction and catalytic hydrodehalogenation: Semi-continuous process with solvent recycle. *Environmental Progress & Sustainable Energy*, 30(4), 589–598. DOI: 10.1002/ep.10513

Cone M, Osborn C, Ticknor JL, Cunningham JA. **2014**. Effects of solvent composition and hydrogen pressure on the catalytic conversion of 1,2,4,5-tetrachlorobenzene to cyclohexane. *Environmental Engineering Science*, 31(3), 156–166. DOI: 10.1089/ees.2013.0471