## ENV 6002: Physical & Chemical Principles of Environmental Engineering

Fall 2021 Homework #9 Due Tues., Nov. 16 University of South Florida Civil & Environmental Engineering J.A. Cunningham

## Assignment for 2021: Complete problem 1. Then choose any 2 of the remaining problems.

1. (70 pts) modified from a problem that I acquired from Paul Roberts, Stanford University

ADVICE: Set up an Excel spreadsheet or a Matlab program for this problem, rather than doing it all by hand. This is not required, but I think it will make your life easier in the long run.

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<sup>3</sup>, the volumetric flow rate of water through the reactor is 10 m<sup>3</sup>/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	Cl <sup>-</sup> conc.	time	Cl <sup>−</sup> conc.
(min)	$(g/m^3)$	(min)	(g/m <sup>3</sup> )
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,  $\bar{t}$ , in the reactor. Hint: it's really easy. If you are making it difficult, you are doing it incorrectly.
- b. Calculate the zeroth moment,  $\mu_0$ , of the effluent concentration distribution. Use it to estimate the total mass of chloride that exits the reactor. Compare the recovered mass to the injected mass are they close? Hint: use the trapezoidal rule or Simpson's rule to perform the integration. (Rectangle rule doesn't work that well use trapezoidal or Simpson's.)

Once you know  $\mu_0$ , you can transform the concentration data  $C_{\text{out}}$  into E data, using  $E = C/\mu_0$ . This is useful because when we use E, we can calculate some important properties about the reactor.

c. Estimate/calculate  $t_m$ , the average residence time of the tracer. How does it compare to the theoretical value of  $\bar{t}$  from part a? Hint: you can use either the  $C_{out}$  data or the E data to estimate  $t_m$  -- I gave you two different formulae in class for  $t_m$ , one using  $C_{out}$  and the other using E -- you should get the same answer either way. Use trapezoidal rule or Simpson's rule -- I think Simpson's rule is a little better for this part.

## 1. continued

- d. Using equation 9-71 or 9-72 from your text, estimate/calculate  $\sigma^2$ , the variance of the residence time distribution. This is also called the "normalized central second moment". Simpson's rule is probably better than trapezoidal rule for this part.
- e. Draw a graph of the *residence time distribution* (exit age distribution) of fluid in the reactor. You can either graph E vs t, or you can graph  $E_{\theta}$  vs  $\theta$  – you choose. Recall that the definition of E and the definition of  $E_{\theta}$  are slightly different – they need to be different to ensure that the area under the curve equals 1 in either case. I did my graph in the fully normalized form,  $E_{\theta}$  vs  $\theta$ , but you can choose which way you want to do it.
- f. Make another graph of the *cumulative* residence time distribution (cumulative exit age distribution). If your graph from part (e) is E vs t, then make this graph F vs t. If your graph from part (e) is  $E_{\theta}$  vs  $\theta$ , then make this graph F vs  $\theta$ . To calculate F, you'll need to integrate  $C_{\text{out}}$  or E. For this part, trapezoidal rule actually works better than Simpson's rule.
- g. On the graphs from parts (e) and (f), add in 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.
- h. What fraction of the fluid has a residence time of 20 minutes or less? By what time has 20% of the injected tracer left the reactor?
- i. Suppose we want to model our reactor as *n* CMFRs in series (tanks-in-series model), with a total residence time equal to  $t_{\rm m}$ . (Each tank in the series has a residence time  $t_{\rm m}/n$ .) Using equation 9-117, along with your answer from part (d), estimate *n*, the number of tanks that correspond to our reactor.
- j. Make a graph of  $E_{\theta}$  vs  $\theta$  for our reactor. Maybe you already did this in part (e) if so, no problem, but make another one, because now we are going to add something to it. Using equation 9-111, along with your estimate of *n* from part (i), add a curve that corresponds to  $E_{\theta}$  for the tanks-in-series model. Does the residence-time distribution for the tanks-in-series model look pretty close to the residence-time distribution for the real reactor? If so, then we can use the tanks-in-series model to estimate the behavior of our real reactor! (See part k, below.)
- k. 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<sup>-1</sup>. Based on the tanks-in-series model, what effluent concentration would you expect from this reactor?
- 1. 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? Does it appear that our real reactor behaves more like a CMFR or more like a PFR in terms of contaminant removal?

- 2. (15 points) This one is only for serious math nerds. Derive equation 9-109 or 9-111 in the text. If you don't really like taking integrals, then skip this one. I really like taking integrals, so I thought it was pretty fun.
- 3. (15 points) Answer problem 9-10 in the text.
- 4. (15 points) Answer problem 9-12 in the text. Where the problem says "segregated flow model," they mean that you should use equation 9-114. You can do that easily enough because you know *E*(*t*) for an ideal CMFR. So using equation 9-114, along with the known formula for *E*(*t*), you will derive a formula for C<sub>out</sub>. Then, as the problem says, answer "how does this equation compare to that derived from a masterial balance written for a CMFR in the usual way?" you will notice something very interesting! This problem is actually a really classic problem in reactor engineering. (Amazingly, it doesn't work for zero-order reactions, only for first-order reactions I have been trying for years to figure out why it doesn't work for zero-order, and I haven't figured it out yet. But you don't have to do the zero-order case, only the first-order case, so don't worry about that.)
- 5. (15 points) Answer problem 9-17 in the text.
- 6. (15 points) We know the residence-time distributions for an ideal CMFR is  $E(t) = (1/\bar{t}) \exp(-t/\bar{t})$ , where  $\bar{t}$  is the theoretical residence time *V/Q*. We also know the residence-time distribution for an ideal PFR is  $E(t) = \delta(t-\bar{t})$ , where  $\delta$  is the Dirac delta function.
  - a. For the ideal CMFR, show that the zeroth temporal moment of E(t) is 1. That is, if you take the area under the whole E(t) curve, it is 1. You don't have to show it for the ideal PFR, because we already know that is a property of the Dirac delta function, so it's a given.
  - b. For the ideal CMFR, show that the first temporal moment of E(t) is  $\bar{t}$ . In other words, the residence-time distribution agrees with the fact that the average hydraulic residence time is  $\bar{t}$ . I think you'll probably have to integrate by parts. For the PFR, it is once again a property of the Dirac function, so it's a given and we don't have to derive it.
  - c. Find the second temporal moment (central) of E(t) for the ideal CMFR and for the ideal PFR. In other words, find  $\sigma^2$  for the CMFR and the PFR. This is a measure of the spread of the residence-time distribution.