CEN 786, Spring 2020
Project 5

Winter gray and falling rain
We'll see summer come again
Darkness falls and seasons change
Same old friends, the wind and rain
You'll see summer come again.

–Weir/Barlow

The following are all taken and/or adapted from problems in either Fogler (Elements) or Rawlings and Ekerdt.

1. Fogler, Problem 17-8: An experimental residence time distribution (E(t)) is given for an industrial reactor in the data file "P2DATA." The first column is the time in minutes, and the second column is the corresponding value of E, in units of min^{-1} at that time. You are carrying out the following, irreversible gas-phase reaction:

$$A + B \rightarrow C + D$$

The reaction is first order in A and second order in B. For this process, the feed concentrations of A and B are both equal to 0.0313 mol L^{-1}. The volume of the reactor is 1000L, the feed volumetric flowrate is 10 Liters s^{-1}, and the rate constant is 175 L^2 mol^{-2} s^{-1}. If the reactor operates isothermally at 320K, calculate conversion attained for:

   (a) An ideal (single) PFR operating at the mean residence time given by the RTD.

   (b) An ideal (single) CSTR operating at the mean residence time given by the RTD.

   (c) A laminar flow reactor using the complete segregation model.

   (d) The experimental RTD using the complete segregation model.

   (e) The experimental RTD using the maximum mixedness model

2. Fogler, 17-12

   The second-order, elementary liquid-phase reaction:

$$2A \rightarrow B$$

   is carried out in a nonideal CSTR. At 300K, the rate constant is k = 0.5 L mol^{-1} min^{-1}. In a pulse tracer test, the tracer concentration rose linearly up to 1 mg L^{-1} at 1 minute, and then decreased linearly to zero at exactly 2 minutes. Pure A enters the reactor at a temperature of 300K.

   (a) Calculate the conversion of A predicted by the segregation and maximum-mixedness models.

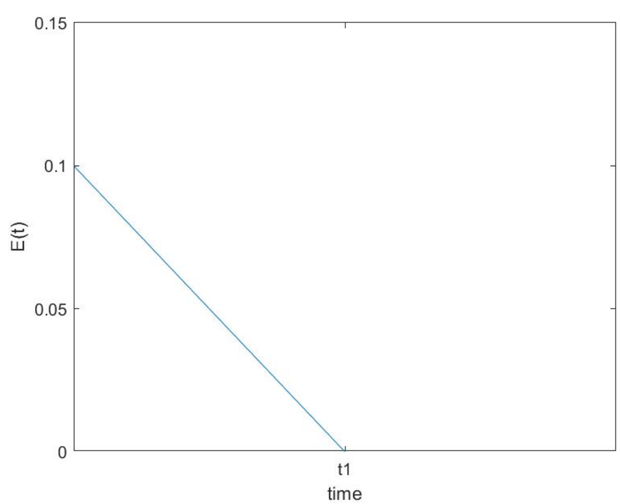
   (b) Now consider that a second elementary reaction also takes place

$$A + B \rightarrow C$$

   with a rate constant of k_2 = 0.12 L mol^{-1} min^{-1}. Compare the selectivities to B and C predicted by the segregation and maximum-mixedness models.

3. Folger 18-18:

   The following E-curve was obtained from a tracer test:



   (a) What is the mean residence time?

   (b) What is the Peclet number for a closed-closed system?

   (c) How many tanks in series are needed to model this reactor?

4. Fogler, Problem 16-11 and 18-12:

The volumetric flowrate through a reactor is 10 L min^{-1}. A pulse text gave the following tracer concentration (in units of mol L^{-1}) measurements at the outlet:

time (min)	$C \times 10^5$	time (min)	$C \times 10^5$
0	0	15	238
0.4	329	20	136
1	622	25	77
2	812	30	44
3	831	35	25
4	785	40	14
5	720	45	8
6	650	50	5
8	523	60	1
10	418		

(a) Plot the residence time distribution, E(t), as a function of time.

(b) Plot the cumulative distribution function, F(t), as a function of time.

(c) What are the mean residence time (t_m) and variance (σ^2) for this reactor?

(d) What fraction of the material spends between 2 and 4 minutes in the reactor?

(e) What fraction of the material spends longer than 6 minutes in the reactor?

(f) What fraction of the material spends less than 3 minutes in the reactor?

(g) What is the volume of this reactor?

(h) Use the segregation model to estimate the conversion for a second order reaction having k = 0.1 L mol^{-1} min^{-1} and C_{Af} = 1 mol L^{-1}

(i) Use the maximum mixedness model to estimate the conversion in this reactor for a second order reaction having k = 0.1 L mol^{-1} min^{-1} and C_{Af} = 1 mol L^{-1}

(j) If the reactor is modeled as a set of tanks-in-series, how many tanks are needed to represent this reactor? What is the conversion for a second order reaction having k = 0.1 L mol^{-1} min^{-1} and C_{Af} = 1 mol L^{-1}

(k) If the reactor is modeled as a PFR with axial dispersion, estimate the Peclet number that represents this reactor? What is the conversion for a second order reaction having k = 0.1 L mol^{-1} min^{-1} and C_{Af} = 1 mol L^{-1}

(l) Model this reactor as two identical CSTRs in series with backflow (Q_{bf}) from the second reactor back into the first reactor. What is the rate of backflow that describes this RTD, and what is the conversion predicted in this reactor configuration for a second order reaction having k = 0.1 L mol^{-1} min^{-1} and C_{Af} = 1 mol L^{-1}.

5. Fogler, 18-8:

The following E(t) curve was obtained from a tracer test on a reactor.

$$E(t) = 0.25t \quad \text{for} \quad 0 < t < 2$$
$$E(t) = 1 - 0.25t \quad \text{for} \quad 2 < t < 4$$
$$E(t) = 0 \quad \text{for} \quad t > 4$$

Here, time is in minutes and E(t) is in inverse minutes. The elementary reaction below is performed in this reactor:

$$A \rightarrow B$$

The reaction has an activation barrier of 25,000 cal mol^{-1}, and the conversion predicted by the tanks-in-series model for this system is 50% at 300K.

(a) If the temperature is to be raised by 10°C, and the reaction is carried out isothermally, what will be the conversion predicted by the tanks-in-series model? The maximum mixedness model?

(b) The elementary reactions:

$$A \rightarrow B$$
$$B \rightarrow C$$
$$A \rightarrow D$$

are carried out isothermally at 300K in the same reactor. At this temperature, $k_1 = k_2 = k_3 = 0.1$ min^{-1}. If $C_{Af} = 1$ mol L^{-1}, what is the concentration of B in the exit stream predicted by the maximum mixedness model?

(c) For the multiple reactions given in part (b), what is the conversion of A predicted by the dispersion model in an isothermal, closed-closed system?

6. Fogler, 18-13

   A second order reaction is to be carried out in a real reactor that gives the following outled concentration for a step input:

$$C = 10 \cdot \left(1 - e^{-0.1t}\right) \quad \text{for} \quad 0 \leq t < 10 \text{ minutes}$$
$$C = 5 + 10 \cdot \left(1 - e^{-0.1t}\right) \quad \text{for} \quad t \geq 10 \text{ minutes}$$

   Additional information: $Q_f = 1$ L min^{-1}, k $= 0.1$ L mol^{-1} min^{-1}, $C_{Af} = 1.25$ mol L^{-1}

   (a) What model do you propose and what are your model parameters, α and β

   (b) What conversion of A can you expect in the real reactor?

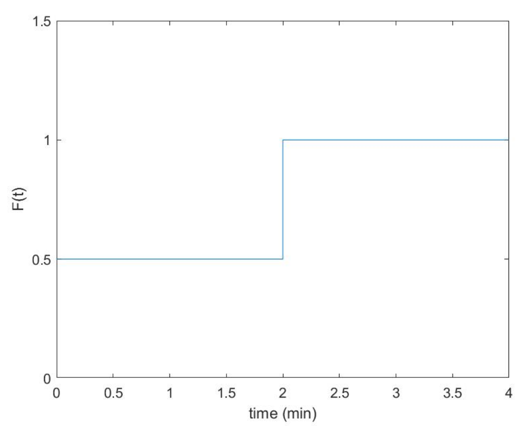
   (c) How would your model and conversion change if your outlet tracer concentration was as follows:

$$C = 0 \quad \text{for} \quad t \leq 10 \text{ minutes}$$
$$C = 5 + 10 \cdot \left(1 - e^{-0.2 \cdot (t-10)}\right) \quad \text{for} \quad t > 10 \text{ minutes}$$

7. Fogler, 18-17:

   There is a 2 m^3 reactor that is to be used to carry out the liquid phase, second order reaction. A and B are fed in equimolar amounts at $Q_f = 1$ m^3 min^{-1}. The entering concentration of A is 2 molar, and the rate constant is 1.5 m^3 kmol^{-1} min^{-1}. A tracer experiment was carried out and reported in terms of F as a function of time in minutes as shown below:

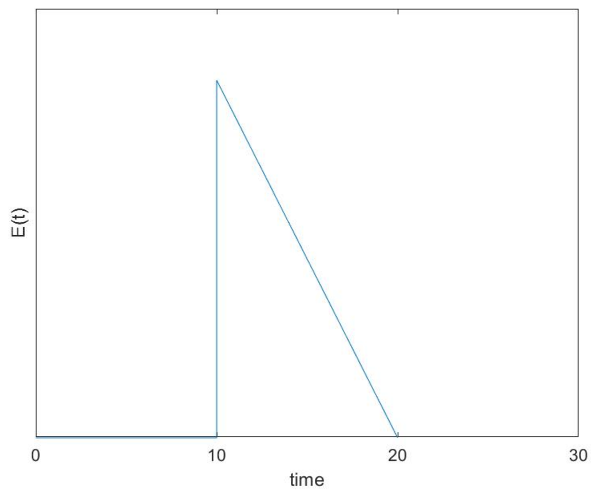
$$A + B \rightarrow C$$



   Suggest a two-parameter model that is consistent with the tracer test. Determine the model parameters, and use it to calculate the expected conversion in this reactor.

8. Folger 18-19:

The following E-curve was obtained for a reactor using a tracer test:



A first order reaction with a rate constant k = 0.1 min^{-1} is carried out in this reactor. Summarize the conversions predicted by the models below. For each case where you are able to do so (i.e., where you have to fit an RTD to the data), plot the residence time distribution associated with that model against the one observed experimentally in the figure above. Comment on the "goodness of fit" for each case. Which do you think best describes the data?

(a) Ideal PFR

(b) Ideal CSTR

(c) Ideal Laminar Flow Reactor

(d) Segregation Model

(e) Maximum Mixedness Model

(f) Dispersion Model

(g) Tanks in Series Model

9. Rawlings, Exercise 8.5:

The residence time distribution is tabulated below for a flow reactor that has a feed rate of 16.2 $\text{ft}^3\ \text{min}^{-1}$. Under the feed conditions ($C_{Af} = 0.02$ lbmol ft^{-3} and $C_{Bf} = 2.34$ lbmol ft^{-3}), the reaction

$$A + B \to C$$

is essentially first order in A with a rate constant of 0.23 min^{-1} at the temperature of the reactor. Determine the effluent concentration of reactant A in any two ways that you think are appropriate.

t (min)	E	t (min)	E	t(min)	E
0	0.0000	18.5	0.0604	37.0	0.0026
3.7	0.0005	22.2	0.0437	40.7	0.0010
7.4	0.0120	25.9	0.0259	44.4	0.0004
11.1	0.0415	29.6	0.0133	48.1	0.0001
14.8	0.0627	33.3	0.0061	51.8	0.0000