Reactor Engineering Week 10 Problem Set

Question 1

Tim's non-ideal, liquid-phase reactor has a residence time distribution, $E(t)$, of:

$$E(t) = \frac{\sin(t)}{2}; \quad 0 \leq t \leq \pi; \qquad E(t) = 0; \quad \text{elsewhere.} \tag{1}$$

The inlet concentration of A is C_{A0}, the reactor volume is V, and the volumetric flow rate through the reactor is v. Calculate the mean outlet concentration under the following conditions:

Question 1a

A undergoes a first order chemical reaction with reaction rate constant k_1. Do we care whether the reactor undergoes macro- or micromixing? Why not?

Question 1b

A is consumed in a second-order chemical reaction with reaction rate constant k_2, and the reactor is macro-mixed.

Question 1c

A is consumed in a second-order chemical reaction with reaction rate constant k_2, and the reactor is micro-mixed. Do we get the same answer as in part b? Explain physically why mixing is important for second-order reactions, but not for first-order reactions.

Question 1d

A undergoes an equilibrium reaction

$$\text{A} \underset{\text{k}_{-1}}{\overset{\text{k}_1}{\rightleftharpoons}} B \tag{2}$$

$C_{B0} = 0$ and the reaction is first-order in both directions.

Question 2

Tim has a few more experiments he wants to conduct on the reactor from Question 1d! All questions below refer to this case.

Question 2a

Tim's non-ideal reactor has been running smoothly in steady-state operation, undergoing the reversible equilibrium reaction. Tim is getting a little bored, and so at $t = 0$ he doubles the concentration of A in the inlet stream. Find an expression for the concentration of A in the outlet stream as a function of time, and the new equilibrium conversion.

Question 2b

Tim now sets $C_{A0} = C_{B0} = 0$ while keeping v constant, and waits long enough for all the A and B to be flushed out of the system. At $t = 0$ he then adds 1 mol of A in a short pulse, and then returns C_{A0} to zero. Find an expression for the outlet concentration of A.

Question 2c

Tim is interested in how the concentration at the outlet of his reactor changes as he oscillates C_{A0} over time. If he varies C_{A0} according to

$$C_{A0}(t) = C_{A0,0}(1 + \sin(t)) \tag{3}$$

and he has been doing so for some time (so the transient terms have died down) find an expression for the outlet concentration of A.
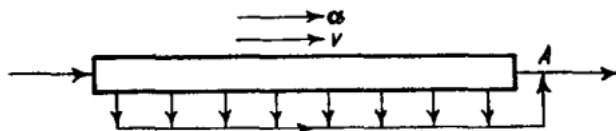
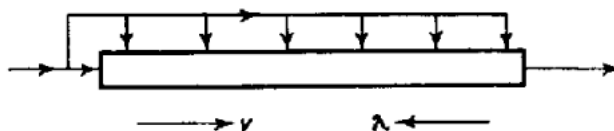Fɪɢ. 2. Plug flow reactor with side exits. A case of complete segregation.

Fɪɢ. 3. Plug flow reactor with side entrances. A case of maximum mixedness.

Question 3

If the liquid-phase, second order reaction A $\xrightarrow{k_2}$ B were conducted in a PFR and an MFR in series, is it more efficient to place the MFR first or the PFR first? Explain this by discussing the relative merit of macro- and micro- mixing.

Fredo-Frog-Challenge-Question

Note: This is a tricky question. Any student who can solve this question within a week may claim a Fredo Frog.

Mixing is a broad and complicated topic in reactor engineering - one which we can only brush past in this course. For first-order or pseudo-first order reactions, mixing inside the reactor is irrelevant, and only the residence time distribution is required to predict reaction conversion. However, for reactions of other order, or when two separate liquid streams are combined into one, we need information about mixing inside the reactor before we can predict the outlet conversion. The classic papers in this field were published by Danckwerts in 1958 and Zwietering in 1959, both in Chemical Engineering Science - I'm sure you can find them. The following questions explore some of the ideas discussed in these papers.

Question 1. Imagine a plug-flow reactor with one entrance and many small 'side-exits' along its length (see the figures from Zwietering above.) Show that, by choosing the location, number and flow-rates at these exits, the residence time distribution inside the reactor can be made arbitrarily close to any desired residence-time distribution function. Show the same for a plug flow reactor with many 'side-entrances' and one exit at its end.

Question 2. Explain why the PFR with side entrances may be considered the reactor with maximal mixedness for a given RTD. Explain why the PFR with side exits may be considered the reactor with complete segregation, or purely macroscopic mixing.

Question 3. The following residence time distribution describes the flow through 2 well-mixed MFR's in series:

$$E(t) = (4t/\tau^2)e^{-2t/\tau}. \tag{4}$$

Consider the second-order reaction A $\xrightarrow{k_2}$ B. If the initial concentration of A is C_{A0}, calculate the outlet conversion from (a) two MFRs in series (b) a PFR with side exits with residence time distribution given by (4), and (c) a PFR with side entrances and residence time distribution given by (4).

Question 4. Which reactor had the greatest outlet conversion? Explain intuitively why this is a reasonable result.