# Reactor Engineering Week 9 Problem Set

## Question 1

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

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

## Question 1a

Calculate the mean residence time for Tim's reactor, and derive expressions for the  $F(\cdot)$  and  $E_{\theta}(\cdot)$ .

## Question 1b

If the volumetric flow rate of the liquid flowing through the reactor were  $v = 10 \,\mathrm{L\,min^{-1}}$ , calculate the volume of the reactor.

# Question 1c

If 5 mol of A were added in a pulse at time t = 0, derive a function for the concentration of A in the outlet stream as a function of time. You may assume the conditions in part b hold true.

## Question 1d

If Tim were to buy an ideal plug-flow reactor with the same volume as his original reactor, and if he were to place it in front of his non-ideal reactor and run them in series, what would be the E(t) function of the combined system? (hint: how will an ideal PFR affect the mean time a molecule stays inside the system?)

## Question 1e

What if Tim were to place the plug-flow reactor after his non-ideal reactor? Do we get the same overall residence time distribution as in part (d)?

## Question 1f

What if Tim were to place an MFR of equal volume as his original reactor in series before or after his original reactor? What would be the residence time distribution, E(t), of the combined reactors? Does it matter which order you place the reactors? (hint: the output of a pulse test from the first reactor will have a certain distribution, which will be the input to the second reactor. The two may be combined by a convolution integral.)

#### Question 1g

In general, when two reactors with residence time distributions  $E_a(t)$  and  $E_b(t)$ , respectively, are placed in series, does the combined residence time of the two reactors placed in series,  $E_{\{a,b\}}(t)$ , depend on the order the reactors are placed (i.e. a before b or b before a)? Provide an example where the order is important, or prove that the order is irrelevant.

# Question 2

A non-ideal reactor was investigated via a tracer-step experiment. From time t=0, A was continually added to the input stream so it had constant concentration of  $5 \,\mathrm{mol}\,\mathrm{m}^{-3}$ . This stream was flowing at a volumetric flow rate of  $v=1\,\mathrm{m}^3\,\mathrm{s}^{-1}$  and at a velocity of  $u=10\,\mathrm{m}\,\mathrm{s}^{-1}$ . The output concentration of A was measured, and fitted to the following curve:

$$\frac{C_{\text{out}}(t)}{\text{mol/m}^3} = \begin{cases}
0 & \text{if } t \ge 50 \\
\frac{5}{2}(1 - \cos(\pi t/5)) & \text{if } 50 \le t \le 55 \\
5 & \text{if } t \ge 55
\end{cases}$$
(2)

where t is measured in seconds.

## Question 2a

Find an expression for F(t), E(t) and  $E_{\theta}(t)$ , and calculate the mean residence time, volume, and length of the reactor.

#### Question 2b

What is the variance of the reactor,  $\sigma^2$ ?

## Question 2c

If 5 of these reactors were placed in series, what would be the mean residence time and variance of the overall system?

#### Question 2d

Calculate the dispersion coefficient,  $\mathcal{D}$ , for this reactor. You may be able to use the approximation of Aris (1959), mentioned in your notes, which is valid when  $\mathcal{D}/uL < 0.01$ .

## Question 3

In probability theory, a *Poisson process* is a random process in which an event is equally likely to happen at any instant of time. For example, in queueing theory (yes, that is a thing that people are paid to study) a new customer is just as likely to arrive in one second as in any other second. In a similar way, a Geiger counter measuring radiactive decay from a block uranium is just as likely to beep during one millisecond as in any other millisecond.

For any Poisson process, it is possible to prove that, if events occur on average every  $\bar{t}$  seconds, then the time between events (which is a random variable) is governed by the following probability distribution function:

$$f(t) = \frac{e^{-t/\bar{t}}}{\bar{t}}. (3)$$

This is identical to the residence time distribution for an MFR reactor with mean residence time  $\bar{t}$ . Explain intuitively why this should be the case.

# 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.

At time t = 0, a pulse of  $50 \,\mathrm{mol}$  of the radioactive dye A is added to the feed stream of a non-ideal, liquid-phase reactor. This dye is not a standard dye: as it passes through the reactor, it reacts according to the following reaction:

$$A \xrightarrow{k_1} B \tag{4}$$

Because A breaks down via radioactive decay, we know this reaction is first order with respect to A, and we will say it has reaction rate constant  $k_1$ . However, we don't yet know the value of  $k_1$ .

The concentration of A in the outlet stream was measured over time, and it was found to fit the following curve:

$$C^{\text{out}}(t) = \begin{cases} 1 & \text{if } 0 \le t \le 1\\ 0 & \text{if } t > 1 \end{cases}$$
 (5)

where t is measured in seconds, and  $C^{out}(t)$  is measured in mol m<sup>-3</sup>. The volumetric flow rate through the reactor, v, was  $10 \,\mathrm{m}^3 \,\mathrm{s}^{-1}$ .

Calculate the value of the first-order reaction rate constant,  $k_1$ , and the residence time distribution inside the reactor, E(t).

## Solutions

# Fredo Frog Challenge Question

We know that, if the were no reaction, the outlet concentration of A from a pulse test is of the form:

$$C^{\text{out}}(t) = \frac{N}{v} E(t) \tag{6}$$

where N is the number of moles added, and v is the volumetric flow rate. Now, if there is a reaction, some fraction of the A that would have come out will instead come out as B. Thus the concentration of A in the outlet stream,  $C^{\text{out}}(t)$ , will be smaller. But by how much? Well, because this is a first-order reaction, the conversion is independent of the degree of mixing in the reactor, and instead depends only on the time the atoms have stayed in the reactor. For atoms that have been in for time t, the fraction that haven't yet reacted away will be  $e^{-kt}$ , where k is the first-order reaction constant. Thus, with a first-order reaction occurring,  $C^{\text{out}}(t)$  will be of the form:

$$C^{\text{out}}(t) = \frac{N}{v} e^{-kt} E(t) \tag{7}$$

Now, we have measured that

$$C^{\text{out}}(t) = \begin{cases} 1 & \text{if } 0 \le t \le 1\\ 0 & \text{if } t > 1 \end{cases}$$
 (8)

We must find a k and an E(t) that will make this work. At first it seems impossible, as we are free to choose both k and E, however we must also remember that E(t) must have total area 1. Equating (7) and (8) gives

$$E(t) = \begin{cases} \frac{v}{N}e^{kt} & \text{if } 0 \le t \le 1\\ 0 & \text{if } t > 1 \end{cases}$$
 (9)

The area under this curve is:

$$1 = \int_0^\infty E(t) = \int_0^1 \frac{v}{N} e^{kt} = \frac{v}{N} \frac{e^k - 1}{k}$$
 (10)

We know that N = 50 mol and v = 10m<sup>3</sup>/s, so

$$5 \text{ seconds} = \frac{e^k - 1}{k} \tag{11}$$

solving this gives  $k = 2.66 \text{ s}^{-1}$ , and substituting this back into (9) gives

$$E(t) = \begin{cases} \frac{1}{5}e^{2.66t} & \text{if } 0 \le t \le 1\\ 0 & \text{if } t > 1 \end{cases}$$
 (12)