Exercises for Chapter 8

1. Find the residence time distribution, that is, the effluent concentration of tracer A after an impulse input at t = 0, for the following system of equivolume CSTRs with a volumetric flow rate of liquid into the system equal to v:



Chapter 8

Exercise 1:

Find the effluent concentration of a tracer after in impulse input for the following system:



A balance on CSTR #1 yields the following concentration of the tracer as a function of time (equation (h) in example 8.2.1):

$$C(t) = \frac{n}{v} \frac{\exp(-\frac{t}{\tau})}{\tau}$$
(1)

Next, write a balance on CSTR #2 (accumulation = in - out)

$$V\frac{dC_{out}}{dt} = 0.5 \text{v}C - 0.5 \text{v}C_{out}$$
(2)

Substitute equation (1) into equation (2):

$$\frac{dC_{out}}{dt} + \frac{0.5}{\tau}C_{out} = \frac{0.5n}{\tau^2 v} \exp(-\frac{t}{\tau})$$
(3)

Solve this first-order differential equation (with the initial condition $C_{out}(0) = 0$)

$$C_{out} = \frac{n}{v\tau} \exp(-\frac{0.5t}{\tau}) - \frac{n}{v\tau} \exp(-\frac{t}{\tau})$$
(4)

Write a mass balance at point X (in = out)

$$0.5vC + 0.5vC_{out} = vC_A \tag{5}$$

Therefore,

$$C_A = 0.5C + 0.5C_{out} \tag{6}$$

After substituting equations (1) and (4) into equation (6),

$$C_A = \frac{n}{2v\tau} \exp\left(-\frac{0.5t}{\tau}\right)$$

The RTD, E(t), can be found from the following equation:

$$E(t) = \frac{C_A}{\int\limits_0^\infty C_A dt}$$
(7)

Therefore,

$$E(t) = \frac{\exp\left(-\frac{0.5t}{\tau}\right)}{2\tau}$$
(8)

For a single CSTR with a volume equal to 2V, define

$$V' = 2V$$
$$\tau' = \frac{2V}{v} = 2\tau$$

Therefore,

$$C_A = \frac{n}{2v\tau} \exp(-\frac{t}{2\tau}) \tag{9}$$

The concentration of a tracer (C_A) for a single CSTR with V' = 2V is the same as the first system. Therefore, the RTD is the same also.

Exercise 2:

The RTD of a PFR is τ_p (not a function of time). Therefore, it does not matter if the PFR is first or the CSTR is first. The RTD of either of these systems is that of a CSTR shifted by τ_p units later.

4. Calculate the mean concentration of A at the outlet (z = L) of a laminar flow, tubular reactor (\overline{C}_{A}^{L}) accomplishing a second-order reaction (kC_{A}^{2}) , and compare the result to that obtained from a PFR when $[(C_{A}^{0}kL)/u] = 1$. Referring to Example 8.1.1, is the deviation from PFR behavior a strong function of the reaction rate expression (i.e., compare results from first- and second-order rates)?

$$\langle C_A \rangle = \int_0^\infty C_A(t) E(t) dt \tag{14}$$

After substituting equations (13) and (8) into equation (14), the mean concentration of A in the outlet is:

$$\langle C_A \rangle = \frac{C_A^o}{\left(1 + k\tau\right)^3} \tag{15}$$

This result confirms that the RTD analysis will yield the same result as a material balance on the system (Example 3.4.3).

Exercise 4:

For a PFR accomplishing a second-order reaction, the material balance is:

$$u\frac{dC_A}{dz} = -kC_A^2 \tag{1}$$

Non-dimensionalize the material balance:

Let $y = \frac{C_A}{C_A^o}$ and Z = z/L

Therefore, equation (1) becomes

$$\frac{dy}{dZ} = -\alpha y^2 \text{ where } \alpha = \frac{kLC_A^o}{u}$$
(2)

The boundary conditions are: y = 1 at Z = 0, and y = 0.5 at Z = 1 (average concentration at the outlet is half of that at the inlet).

$$y = \frac{1}{1 + \alpha Z}$$
 (where $\alpha = 1$) (3)

For a second-order reaction taking place in a laminar flow tubular reactor, the average concentration and the concentration at any radial position are the following:

$$\overline{C_A} = \frac{\int_{0}^{r_t} C_A(\bar{r})\bar{u}(\bar{r})2\pi\bar{r}d\bar{r}}{\int_{0}^{\bar{r}_t} \bar{u}(\bar{r})2\pi\bar{r}d\bar{r}}$$
(4)

$$\frac{-}{u(r)}\frac{dC_{A}}{dz} = -kC_{A}^{2}, \ z = 0 \text{ at } C_{A} = C_{A}^{o}$$
(5)

Notice that equation (5) is the material balance on a PFR with second-order reaction. The solution is given in equation (3).

The velocity profile for laminar flow in a tubular reactor is the following:

$$\overline{u}(\overline{r}) = 2u_{\max} \left[1 - \left(\frac{\overline{r}}{r_t} \right)^2 \right]$$
(6)

where $\overline{r_t}$ is the radius of the tubular reactor.

After substitution of equations (6) and (3) into equation (4) and letting $\rho_r = \frac{\bar{r}}{r_t}$, the denominator is the following:

$$\int_{0}^{1} 2u_{\max} \left(1 - \rho_r^2 \right) 2\pi \overline{r_t}^2 \rho_r d\rho_r = \pi \overline{r_t}^2 u_{\max}$$
⁽⁷⁾

In order to evaluate the numerator, $C_A(\vec{r})$ must be determined from equation (3):

$$C_A(\bar{r}) = \frac{C_A^o}{1 + \frac{kC_A^o z}{u(\bar{r})}}$$
(8)

The velocity profile is determined from equation (6), and the equation is again nondimensionalized and the concentration is evaluated at L. The result is the following:

numerator =
$$4\pi u_{\text{max}} C_A^o r_r^{-2} \int_{0}^{1} \frac{\rho_r (1 - \rho_r^2) d\rho_r}{1 + \left(\frac{1}{2(1 - \rho_r^2)}\right)}$$
 (9)

After solving the integral,

numerator = $8\pi u_{\text{max}} C_A^o r_t^{-2} (0.0687)$

Therefore, the average concentration of A at the outlet of the reactor is the following:

$$\overline{C_A} = \frac{8\pi C_A^o(0.0687)u_{\max}\overline{r_t^2}}{\pi u_{\max}\overline{r_t^2}} = 8(C_A^o)(0.0687) = 0.55C_A^o$$

Therefore, the conversion (for a second-order reaction) is 45% in a laminar flow tubular reactor whereas it is 50% in a PFR.

As shown in example 8.1.1, the conversion in a laminar flow tubular reactor for a firstorder reaction is 55.7% and in a PFR it is 63.2%. Therefore, the deviation from PFR is not a large function of the reaction-rate expression.

Exercise 5:

The following recycle reactor can represent the Berty reactor.



A material balance at the mixing point marked with an X, is the following:

$$\mathbf{v}_o C_o + \mathbf{v}_r C = \mathbf{v}_1 C_1 \tag{1}$$

Additionally,

$$\mathbf{v}_{o} + \mathbf{v}_{r} = \mathbf{v}_{1} \tag{2}$$

If $\alpha = \frac{V_r}{V_o}$, then equations (1) and (2) can be combined and the result is the following: