

Mixing Effects in Chemical Reactors—II

—Models for Nonideal Reactors

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OBJECTIVES

At the completion of this module, the student should be able to:

1. Understand the necessity for developing approximate models for nonideal reactors; itemize the flow models most often used to model continuous reactors; and recognize the forms of the impulse responses associated with each model.
2. Formulate and apply reactor models which account for stagnancy and channeling; quantifying the models on the basis of impulse response data.

PREREQUISITE MATHEMATICAL SKILLS

1. Understanding of semilogarithmic plots. First-order differential equations.

PREREQUISITE ENGINEERING AND SCIENCE SKILLS

1. Design and analysis of ideal plug flow reactors and ideal continuous stirred tank reactors. Impulse response measurements (Module E4.4).

The following problem statement is missing one important item of information--see if you can identify it.

"A reaction $A \rightarrow B$ whose rate law is $r = 0.05 C_A$ is carried out in a continuous isothermal reactor. The feed rate is 200 L/min and the concentration of A in the feed is 3.0 (mol/L). Calculate the reactor volume required to achieve a fractional conversion of 0.90."

The missing information, without which the problem cannot be solved, is the reactor type. If it were given that the reactor was either an ideal plug flow reactor (PFR) or an ideal continuous flow stirred tank reactor (CSTR), one would have no trouble solving the problem by writing the appropriate material balance equation and solving it for V .

Suppose, however, that the reactor is neither an ideal PFR nor an ideal CSTR. In principle, the calculation would be performed in the same manner—by writing and solving the reactor material balance equation. The problem is that for a nonideal reactor, this is more easily said than done. In a perfect mixer, the concentrations of all species are uniform, and the balance is a simple (or at least relatively simple) algebraic equation, and in an ideal plug flow reactor, the only variation is in the axial direction, and the balance equation contains nothing worse than a first derivative. In a nonideal reactor, however, reactant concentrations may vary in all directions; radially, as well as axially, in a tubular flow reactor, and arbitrarily with position in an imperfectly-mixed stirred tank; moreover, reactants move by diffusion, as well as by convection, in any direction in which spatial variations occur. The balance equation for a reactor in which all of these phenomena are taking place is a partial differential equation containing both first and second derivatives. The equation is not particularly hard to derive if enough assumptions are made (3), but it is frequently not clear what boundary conditions to apply; solutions are difficult or impossible to achieve (even using a computer), and generalizations of the results for design and scaleup calculations are usually out of the question.

What is done instead is to formulate a *model* for the nonideal reactor; a mathematical representation of the

unit which accounts to some extent for observed departures from ideal reactor conditions, but which can be analyzed without too much difficulty in order to derive relations between input and output variables. A powerful approach to nonideal reactor modeling is to perform an impulse response test on a flow unit, and to compare the measured response with responses characteristic of various relatively simple types of flow systems. When a correspondence is achieved, the simple system is used to model the real reactor.

The principal features of several of the most common flow reactor models, including their characteristic impulse responses, are given in the sections that follow. In the figures to be shown, the impulse injection is presumed to take place at a time $t=0$, and \bar{t} is the nominal mean residence time in the flow unit:

$$\bar{t}(s) = V(m^3)/q(m^3/s) \quad (1)$$

where V is reactor volume occupied by the reaction mixture and q is volumetric flow rate through the reactor.

IDEAL REACTOR MODELS: IDEAL PLUG FLOW AND PERFECT MIXING

These models, which by now should need no description, represent the extreme in simplicity. Their impulse responses (concentration curves of the tracer measured at the outflow in response to an instantaneous tracer injection in the inflow) are illustrated in Figures 1a and 1b, where $R(t)$ is the response proportional to the outlet concentration curve.

If an experimental impulse response appears as a sharp spike, the flow unit may be modeled as an ideal plug flow reactor with a mean residence time equal to the time at which the spike emerges, and if the response rises almost instantaneously and decays slowly, the unit may be considered a perfect mixer. It is not difficult to show that the impulse response of a perfect mixer is given by the formula

$$R(t) = R_0 \exp(-t/\bar{t}) \quad (2)$$

(see Homework Problem 4) so that a plot of $\ln R$ versus t (or a semilog plot of R versus t) should be a

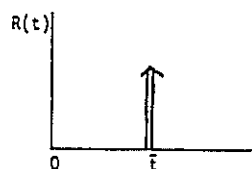


Figure 1a. Ideal plug flow.

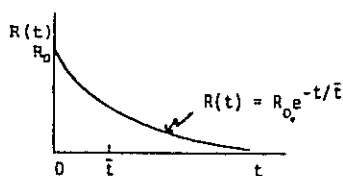


Figure 1b. Perfect mixing.

straight line with a slope of $-1/\bar{t}$. We will illustrate the application of this formula in the next section.

STAGNANCY

In any process unit with corners, baffles, or obstructions to flow, stagnant regions occur (Figure 2). When a tracer is injected into a unit where such a zone exists, some of the tracer diffuses into the zone and is slowly washed out (Figures 2a, 2b and 2c); the consequence is a long shallow tail in the response (See Figure 3). In the extreme case of the phenomenon, the stagnant region does not participate at all in the process taking place in the flow unit. The total volume V of the unit may then be divided into two regions as shown in Figure 4: an active region (volume V_a), through which all the flow passes, and a stagnant region, or *dead volume* (volume $V_s = V - V_a$), which simply occupies space in the unit. The impulse response for this model is that of the active region alone. The apparent mean residence time equals V_a/q and so is less than the nominal mean residence time $\bar{t} = V/q$; if the unit is a reactor, the conversion achieved is therefore lower than the conversion which the unit was designed to achieve. See



Figure 2a.

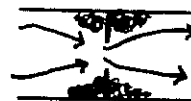


Figure 2b.

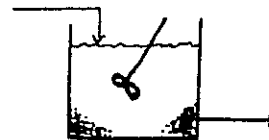


Figure 2c.

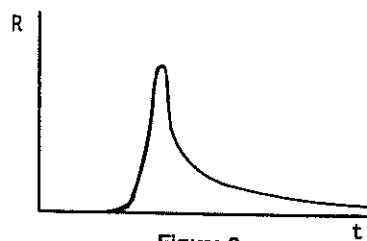


Figure 3.

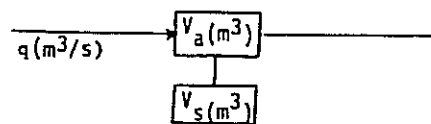


Figure 4.

Figure 5, which shows that the actual mean residence time is smaller than the design value.

Example: Determination of Stagnancy in a CSTR

The product yield from a continuous stirred-tank reactor is lower than the design specification calls for, and imperfect mixing is suspected to be the cause. A tracer impulse is injected at the tank inlet, and the response shown in Figure 6 is obtained at the outlet. The tank volume is 2.5 m^3 , and the volumetric flow rate of the fluid is $2.0 \text{ m}^3/\text{min}$. Determine whether a stagnant region exists, and if so, what fraction of the tank it occupies.

Solution:

It was previously observed that, for a perfect mixer, a plot of $\log R$ versus t should yield a straight line with slope $-1/\bar{t}$. Suppose that the measured response plotted in this manner is as follows (Figure 7). The shallow tail suggestive of a stagnant region appears clearly when the response is plotted in this manner, and the linearity of the earlier portion of the plot suggests that the active portion of the reactor behaves like a perfect mixer. The reactor can therefore be modeled as a perfect mixer and a dead volume (See Figure 4 again). The slope of the line corresponding to the active volume response is

$$-\frac{1}{\bar{t}_{\text{active}}} = -\frac{q}{V_a}$$

$$\frac{\ln(10/100)}{4.2 - 2.0} = -1.047 \text{ (min}^{-1}\text{)} = -\frac{2 \text{ (m}^3/\text{min)}}{V_a \text{ (m}^3\text{)}}$$

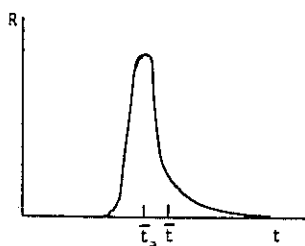


Figure 5.

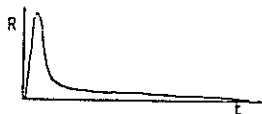


Figure 6.

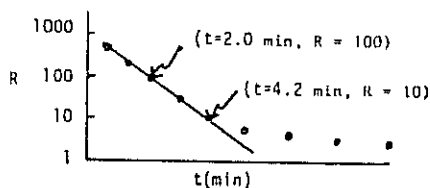


Figure 7.

The effective mean residence time of the unit is therefore only $(1/1.047) = 0.96 \text{ min}$ instead of the design value, $(2.5 \text{ m}^3)/(2.0 \text{ m}^3/\text{min}) = 1.25 \text{ min}$. This fact could very well account for the low reactant conversion.

The effective active volume may be determined as

$$V_a = 2 \text{ (m}^3/\text{min)} / 1.047 \text{ (min}^{-1}\text{)} = 1.91 \text{ m}^3$$

so that the fraction of the reactor which is active is

$$\frac{1.91 \text{ m}^3 \text{ (active)}}{2.5 \text{ m}^3 \text{ (total)}} = 0.764$$

Thus, almost 1/4 of the reaction volume does not participate in the process. This result suggests that increasing the stirrer speed, modifying the design of the baffles, or relocating the inlet and outlet ports to reduce the degree of stagnancy in the unit might remedy the problem.

CHANNELING

Just as stagnant pockets of fluid may have relatively long residence times in a reactor, it is possible for a portion of fluid entering a reactor to have an anomalously short residence time, a phenomenon known as *channeling*. Imperfect packing (Figure 8a) in a fixed bed reactor is one possible cause of this phenomenon; overly close placement of the inlet and outlet of a CSTR (Figure 8) is another. A tracer impulse injected at the inlet of one of these units would emerge in two peaks, the first corresponding to the channeling fluid and the second to the bulk fluid (Figure 9).

A model for a system of this sort would consist of two parallel branches, one corresponding to the bulk

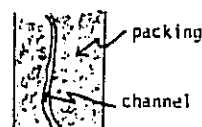


Figure 8a.

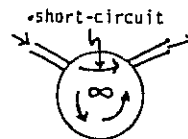


Figure 8b.

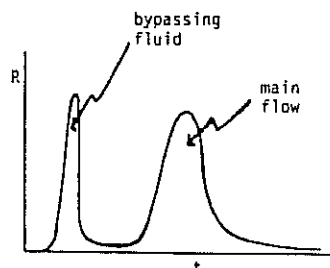


Figure 9.

fluid and the other corresponding to the channel (Figure 10). The shapes of the response peaks would suggest the type of unit to be inserted into each stream—ideal plug flow, perfect mixing, or one of the nonideal types still to be discussed. If the first response peak emerges almost instantaneously relative to the bulk fluid peak, the unit may be modeled as a single unit with a bypass stream (Figure 11). In any case, the fraction of the fluid which bypasses the main unit may be estimated as the ratio of the area under the bypass peak to the area under the total response curve. Remember $\int_0^\infty c(t)dt = m_i/q$ is the total area under the curve (why?). Thus the two individual areas above yield the fraction of the fluid that goes through the bypassing and through the main stream since the tracer behaves and distributes itself everywhere as the carrier fluid.

Example 2: Formulation of a Two-Region Model for a Packed Bed Reactor

An irreversible first-order reaction $A \rightarrow B$ is carried out in a packed-bed reactor. A conversion of 74% was predicted for a feed rate of 15 L/s, but the measured conversion is only 70%. An impulse response performed on the reactor yielded the following result. See Figure 12. From batch reactor measurements, the rate of reaction per unit void volume is

$$-r_A \text{ (mol/L} \cdot \text{s)} = 0.04 C_A$$

where C_A (mol/L) is the reactant concentration. The void volume in the reactor is 500 liters, and the concentration of A in the feed is $C_{A0} = 2$ (mol/L).

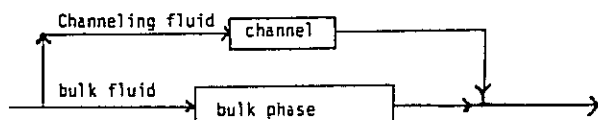


Figure 10.

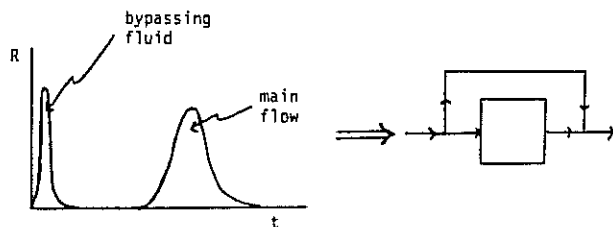


Figure 11.

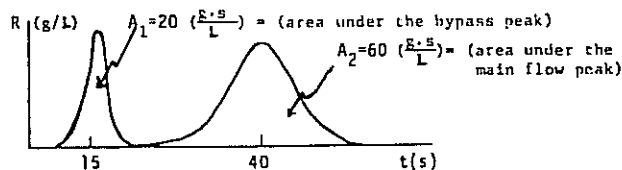


Figure 12.

Calculate:

- the expected conversion in the reactor based upon an assumption of ideal plug flow.
- the conversion which would be predicted by a model fitted to the experimental tracer response.

Solution:

- The mean residence time in the reactor is

$$\bar{t} = \frac{500 \text{ L}}{15 \text{ L/s}} = 33.3 \text{ (s)}$$

The ideal PFR design equation is

$$\bar{t} = \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-0.04 C_A}$$

$$\Downarrow$$

$$-0.04 \bar{t} = \ln \frac{C_{Af}}{C_{A0}}$$

$$\Downarrow \bar{t} = 33.3 \text{ (s)}$$

$$\Downarrow C_{A0} = 2 \text{ (mol/L)}$$

$$C_{Af} = C_{A0} \exp(-0.04 \cdot 33.3) = 0.527 \text{ (mol/L)}$$

A conversion

$$x_A = \left(1 - \frac{C_{Af}}{C_{A0}}\right) = 0.74$$

is thus predicted assuming ideal plug flow.

- The shape of the impulse response suggests modeling the reactor as two plug flow reactors in parallel. In Figure 13 the fraction of the total flow that passes through the first reactor—for which $\bar{t} = 15$ seconds—is $20/(20+60) = 0.25$. In the reactor with smaller residence time, $q_1 = (0.25)[15(\text{L/s})] = 3.75(\text{L/s})$. The concentration of A in the exit stream from this reactor is

$$C_{A1} = C_{A0} \exp(-0.04 \bar{t}_1)$$

$$= 2 \exp(-0.04 \times 15) = 1.10 \text{ (mol/L)}$$

Similarly, for the second reactor, $q_2 = (0.75)(15.00) = 11.25$ (L/s), and

$$C_{A2} = C_{A0} \exp(-0.04 \bar{t}_2)$$

$$= 2 \exp(-0.04 \times 40) = 0.404 \text{ (mol/L)}$$

A material balance on A at the mixing point yields

$$q C_{Af} = q_1 C_{A1} + q_2 C_{A2}$$

$$\Downarrow$$

$$C_{Af} = \frac{(3.75)(1.10) + (11.25)(0.404)}{15} = 0.577 \text{ (mol/L)}$$

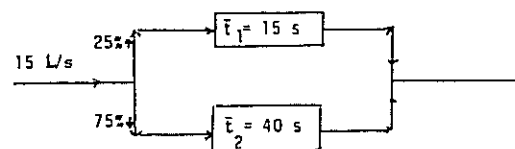


Figure 13.

The predicted conversion is

$$x_A = 1 - \frac{0.577}{2} = 0.71$$

or less than that predicted by the single ideal plug flow reactor model. The small remaining difference between the predicted conversion (0.71) and that actually measured (0.70) could be due to phenomena neglected in the two reactor model—intraphase diffusion and mass transfer between phases.

DISPERSION

When a slug of a tracer or a reactant enters a flow reactor, only in the case of ideal plug flow does the material in the slug pass through and emerge at nearly a single instant of time. Generally, velocity variations, molecular diffusion and (if the Reynolds number is high enough) turbulent mixing all tend to spread the tracer axially about its center of mass, so that the response signal downstream of the injection point appears as in Figure 14. The term *axial dispersion* is used to denote this axial spreading, regardless of its origin.

The symmetrical impulse response shown above is representative of units with slight degrees of dispersion—relatively close to ideal plug flow. In flow units with a high degree of axial dispersion, the flow pattern is closer to that of a perfect mixer—the impulse response rises rapidly and falls off slowly, as in Figure 15.

Two models are commonly used to simulate systems with varying degrees of axial dispersion. We will briefly describe them in the following sections, and discuss one of them in greater detail in Module E4.6.

Dispersion Model

The fluid flowing through the unit in Figure 16 is assumed to be in plug flow (that is, all radial variations

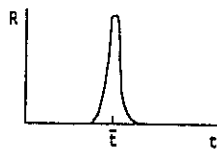


Figure 14.

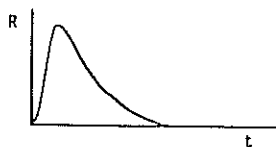


Figure 15.

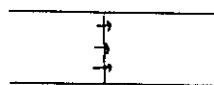


Figure 16.

in velocity and concentration are neglected) and the spread in the impulse response is accounted for by superimposing diffusion in the axial direction with an effective diffusivity D_e (called the *axial dispersion coefficient*). When $D_e = 0$ the model reduces to ideal plug flow, since no axial dispersion remains and a flat velocity profile was assumed. When $D_e \rightarrow \infty$ axial dispersion dominates over the convective movement of fluid. The mixing due to dispersion is much faster than the movement of the plug flow front, so that the contents of the tube are well mixed and the conditions in a perfect mixer (CSTR) are approached.

Tanks-in Series Model

One may recall that a series of N perfect mixers has a conversion versus total residence time relationship, between that of a single perfect mixer and that of an ideal plug flow reactor. Thus, by using a series of tanks (Figure 17) to represent a flow unit and letting the number of tanks vary from 1 to infinity (while keeping the total volume fixed), one can simulate any degree of axial dispersion, from perfect mixing ($N = 1$) to ideal plug flow ($N = \infty$).

In summary, impulse responses for flow systems with varying degrees of axial mixing appear as shown in Figure 18.

Equations and applications for the dispersion model will be developed in a later module (E4.6). For now, one should be able to recognize when they are applicable, and by inspection of an impulse response, one should be able to characterize a system as slightly dispersed, moderately dispersed or highly dispersed.

RECYCLE MODEL

Suppose a portion of the output of an ideal PFR (Figure 19) is recycled back to the inlet, with $\Psi = (\text{volume recycled})/(\text{volume withdrawn as product})$. As Ψ the recycle ratio approaches infinity, the recirculation rate is high enough so that the reactant and product concentrations approach uniformity in the reactor; the system then functions as a perfect mixer. Consequently, as the recycle ratio varies from $\Psi = 0$ (no recycle) to $\Psi \rightarrow \infty$ (nearly complete recycle), the reactor behavior varies from plug flow to perfect mixing.

The response of an ideal PFR with recycle to an impulse injection is quite different from the other responses we have seen so far. After the injection some tracer emerges after one mean residence time, and the rest is recycled; additional tracer emerges after another mean residence time elapses (but less tracer than appeared the first time); still more emerges after a third residence time elapses, and so forth. The impulse response appears as shown in Figure 20, where $\bar{t} = V/q$,

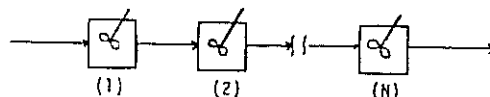


Figure 17.

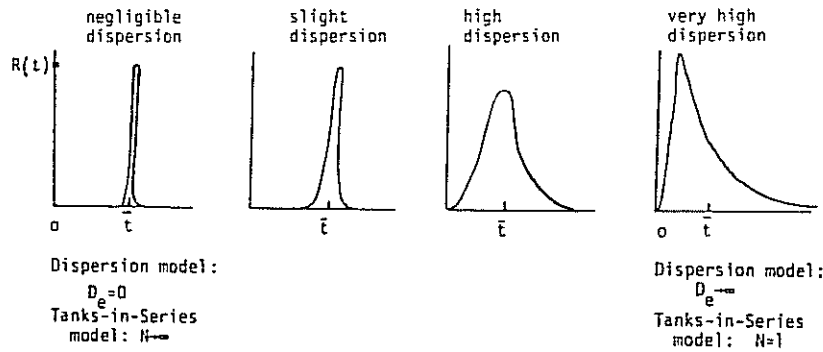


Figure 18.

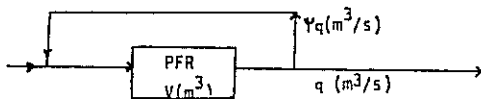


Figure 19.

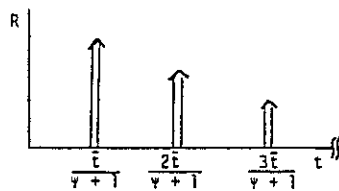


Figure 20.

as usual. (Why is the mean residence time for the first pass through the reactor $\bar{t}/(\Psi + 1)$, rather than \bar{t} ?)

A generalized recycle model can be formulated by replacing the ideal PFR with a nonideal reactor model (dispersed plug flow, or tanks-in-series). The impulse response for such a model would appear as in Figure 21.

Reactors with internal circulation (in particular, stirred tanks) often exhibit behavior of this sort. Consequently, the recycle model is a powerful tool for simulating such systems. The use of the model in reactor design is illustrated in one of the homework problems at the end of this module.

LAMINAR FLOW REACTOR

When the Reynolds number in a homogeneous tubular reactor is less than a certain critical value, the flow follows distinct streamlines, and a velocity profile is maintained across the flow channel cross section. For a Newtonian fluid flowing in a channel with a

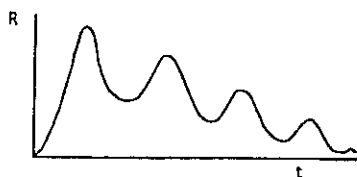


Figure 21.

circular cross section, the velocity profile is parabolic; $u(r)$ equals 0 at the tube wall and is at its maximum at the tube axis. A tracer injected into a fluid in laminar flow distributes itself in accordance with the flow streamlines; a slug of tracer injected proportionally to local flow rate across the flow channel cross section eventually appears as shown in Figure 22. Eventually, radial and axial diffusion of the tracer distort the shape of this figure, but as long as this does not occur, the impulse response appears as that shown in Figure 23. If L is the distance from the injection point to the detection point, and u_{max} is the maximum (centerline) velocity, then the *breakthrough time* t_0 (the time when tracer first appears at the detection point) equals L/u_{max} .

Analysis of laminar flow reactors is more complex than one might imagine. The precise shape of the impulse response depends not only on the velocity profile, but also on how the tracer is injected and detected, so that interpretation of the response is generally uncertain. Moreover, if the reactor is too short, entrance and exit effects dominate the reactor performance, while if it is too long, diffusion leads to deviations from the simple streamline flow behavior, which is the basis of the laminar flow reactor model.

See Reference (2) for further discussion of laminar flow reactors and reactor modeling in general.

NOMENCLATURE

C_A = reactant concentration
 C_{Af} = reactant concentration in the outflow

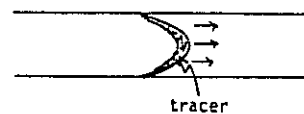


Figure 22.

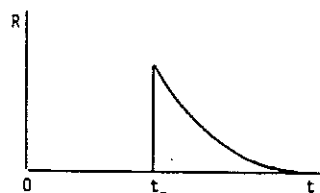


Figure 23.

C_{A_0}	= reactant concentration in the feed
c	= tracer concentration in the outflow
D_e	= axial dispersion coefficient
k	= reaction rate constant
L	= reactor length
m_i	= mass of tracer injected in an impulse injection
N	= number of tanks (CSTR's) in series
q	= volumetric flow rate
R	= system response proportional to exit tracer concentration
R_0	= initial system response
r	= intrinsic rate of reaction
$-r_A$	= rate of disappearance of reactant A
t	= time
\bar{t}	= mean residence time
$u(r)$	= velocity profile in laminar flow as function of radial position
u_{\max}	= maximum velocity
V	= volume of the reactor
V_a	= active volume
V_s	= stagnant volume
x_A	= fractional conversion of reactant A
ψ	= recycle ratio

LITERATURE CITED

- Levenspiel, O. "Chemical Reaction Engineering," 2nd Ed., Chap. 9, John Wiley & Sons, NY (1972).
- Wen, C. Y., and L. T. Fan, "Models for Flow Systems and Chemical Reactors," Marcel Dekker, Inc., NY (1975).
- Bird, R. B., W. E. Stewart and E. N. Lightfoot, "Transport Phenomena," John Wiley & Sons, New York (1960).

STUDY PROBLEMS

- What phenomena are responsible for deviations from ideal plug flow in a tubular reactor? Why must approximate models be used to analyze reactors in which these deviations occur?
- How would you determine from the results of an impulse response measurement whether a reactor can be treated as an ideal PFR, a perfect mixer, or neither?
- How would you determine the mean residence time in an ideal PFR from a measured impulse response? How would you determine \bar{t} for a perfect mixer?
- State several causes for the existence of stagnant regions in flow reactors. How are such reactors modeled?
- A CSTR containing a stagnant region is to be modeled as a perfect mixer with dead volume. How could the active volume fraction ($V_{\text{active}}/V_{\text{total}}$) be determined from a measured impulse response?
- Suppose the conversion achieved in the reactor of the previous question is not equal to the conver-

sion predicted by the model. What might be responsible for the discrepancy?

- What are some conditions that lead to channelling in a chemical reactor? How can such a reactor be modeled?
- Suppose an impulse response consists of two distinct peaks. How would you model the reactor? What is the significance of the ratio of the areas under each peak?
- What is meant by the term axial dispersion? What models may be used to represent a reactor in which dispersion is observed?
- Match each of the impulse responses in Figure 24 with the models you would use to represent the reactors in which they were obtained.
 - Ideal plug flow
 - Perfect mixer
 - Laminar flow
 - Dispersion model
 - Ideal plug flow with bypass
 - Ideal plug flow with dead volume
 - Ideal plug flow with recycle
 - Perfect mixer with dead volume

HOMEWORK PROBLEMS

- An impulse response test is carried out on a continuous stirred tank reactor using a radiotracer. The throughput rate is 5.0 L/s. The response plotted on semilog paper appears in Figure 25.
 - Is it appropriate to treat the tank as a perfect mixer? Explain.
 - Calculate the mean residence time in the tank.
 - If a mean residence time of one minute is desired, what volumetric throughput rate is required?
- A 45-liter CSTR is subjected to an impulse response

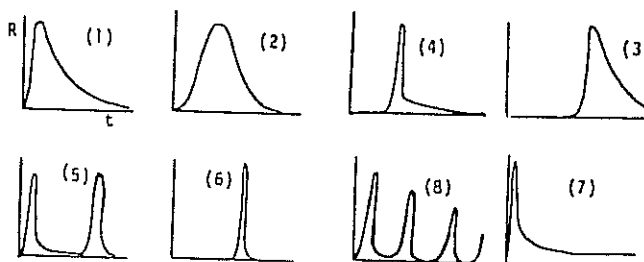


Figure 24.

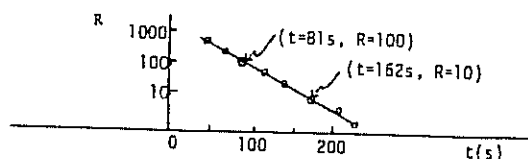


Figure 25.

test. The feed rate is 5 liters/second. The following response is obtained.

t (s)	R (arbitrary units)
5	49.0
10	24.0
15	11.7
20	5.7
25	3.2
30	2.0
35	1.6

- Use a semilog plot of the data to develop a two-region model for the tank. (See Example 1). Determine the volume associated with each region
- Suppose a chemical reaction $A \rightarrow B$ with a rate law

$$-r_A \text{ (mol/L} \cdot \text{s)} = 0.50 C_A$$

is to be carried out in the reactor, with a feed rate of 5 L/s. Calculate: i) the fractional conversion of A which would be predicted assuming that the reactor behaves like a perfect mixer; ii) the conversion which would actually be achieved, based on the results of the impulse response test.

- An experimental reactor (Figure 26) has a double pipe configuration: the feed enters and passes through the inner tube, then returns through the outer tube and passes out of the reactor. A liquid-phase, second-order reaction, $2A \rightarrow B$, is to be carried out in the reactor, which operates isothermally. The feed contains A at a concentration 10.0 mol/L, and no B . The mean residence time in the reactor is 2.00 minutes. In a batch run with an initial concentration of 12.5 mol/L, a 50% conversion was obtained in 20 seconds.
 - Calculate the reaction rate constant, and prove that the concentration of B in the product which should be achieved if the flow unit performs as an ideal plug flow reactor is 4.14 (mol/L).
 - In the first experimental test of the reactor the concentration of B in the product is found to be 3.43 (mol/L). An impulse response is performed, and a response approximately equal to that shown in Figure 27 is obtained. Use this response to formulate a model for the reactor. Use the model to predict the expected concentration of B in the product, and compare your result with the experimental value.
 - Suggest an explanation for the observed reactor behavior.

- Derive Equation 2 for the impulse response of a

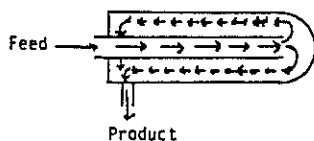


Figure 26.

perfect mixer. Consider a stirred tank of volume V (m^3) through which flows a fluid at a volumetric flow rate q (m^3/s), and suppose that at a time $t=0$ a quantity m (g) of a tracer is instantaneously present in the tank. Prove that a tracer mass balance yields the equation

$$\frac{dc}{dt} = -\frac{q}{V} c; c(0) = \frac{m}{V}$$

where c (g/m^3) is the concentration of tracer in the tank (and hence in the tank effluent). Finally, integrate the equation to derive Equation 2.

- Suppose a first-order liquid-phase reaction $A \rightarrow P$ is to be carried out in an isothermal reactor for which a recycle model is appropriate. See Figure 28.
 - Write the design equation for the reactor in terms of the variables shown on the diagram above, and integrate it to prove that

$$C_{Af} = C_{Ai} \exp \left[\frac{kV}{q(1+\Psi)} \right]$$

Then use a simple material balance about the feed mixing point to derive an expression for C_A in terms of C_{A0} , C_{Af} , q and Ψ , and substitute it in the above expression to derive a formula for C_{Af}/C_{A0} in terms of q , Ψ , k and V .

- Suppose an impulse response test is carried out on the reactor, with the result shown in Figure 29. If the reactor volume is $V=200\text{L}$ and the feed rate is $q=2$ (L/s) what is Ψ ?
- Next suppose $k=0.04 \text{ s}^{-1}$. Calculate the fractional conversion $(1 - C_{Af}/C_{A0})$ which would be achieved in the reactor, and compare it with the conversion which would be achieved if the same reactor were in ideal plug flow ($\Psi=0$).

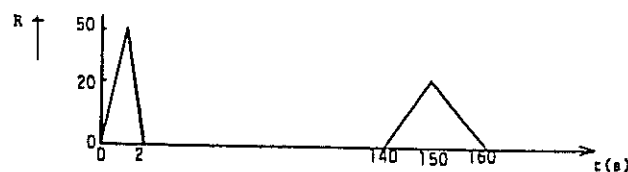


Figure 27.

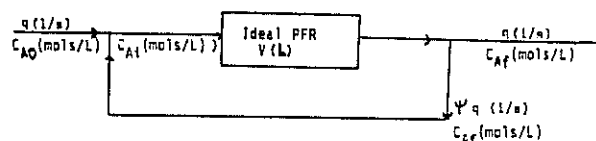


Figure 28.

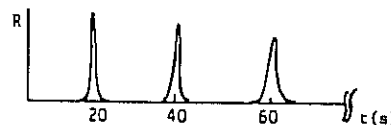
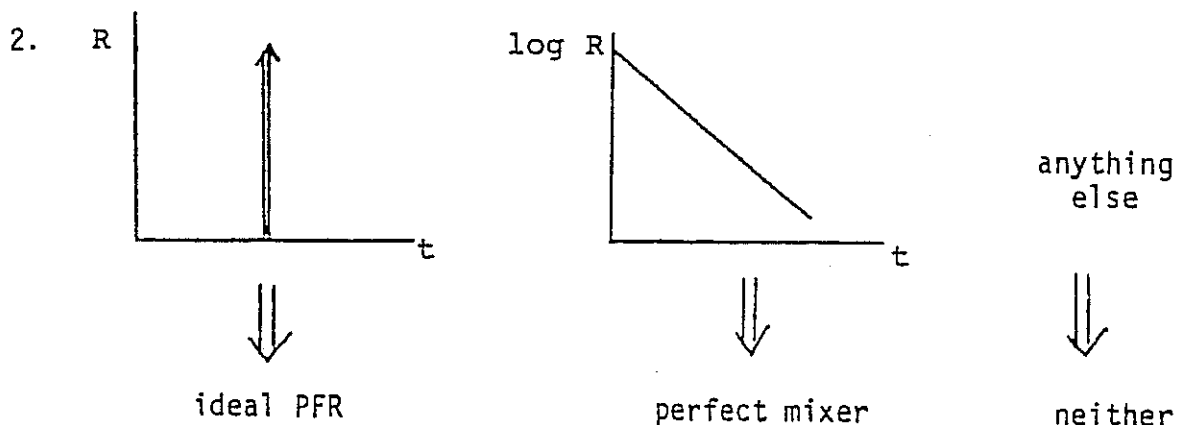


Figure 29.

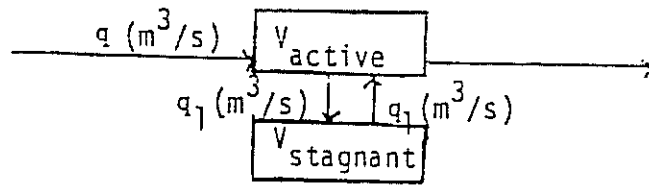
SOLUTIONS TO THE STUDY PROBLEMS

1. Departures from ideal plug flow are caused by nonuniform velocity profiles, turbulent mixing and molecular diffusion. An exact mathematical representation of a nonideal reactor is a second-order partial differential equation, which is difficult to derive in complete generality and impossible to solve analytically.



3. (a) (PFR) The time at which the peak emerges equals \bar{t} .
 (b) (PM) The slope of the plot of $\log R$ vs. t equals $-\frac{1}{\bar{t} \ln 10}$
4. Baffles or other obstructions to flow; expansions or contractions in a line; poor mixing in a stirred vessel. Model as an active region plus a dead volume.
5. Say q = the volumetric throughput rate. A plot of $\ln R$ vs t yields (at low t) a straight line with slope $\frac{-1}{\bar{t}_{\text{active}}} = \frac{-q}{V_{\text{active}}}$ so that V_{active} can be calculated as $q/|\text{slope}|$. Since V_{total} is presumably known independently, the active volume fraction (and by implication, the stagnant volume fraction) can then be determined.
6. The stagnant region is not truly a dead volume, but rather participates to a lesser extent in the reactive process. A more precise but more complex model would consist of an active zone and a stagnant zone with

mass transfer occurring between them.



7. Imperfect packing in a fixed bed; short circuiting between a tank inlet and outlet. Model as a parallel arrangement of ideal or other reactor types.
8. Two parallel branches. The total flow divides itself between the branches proportionally to the areas under the two peaks.
9. The collective phenomena which lead to axial mixing in a flow unit, viz. radial velocity variations and molecular and turbulent diffusion. Dispersion model and tanks-in series model.
10. 1b, 2d, 3c, 4f, 5e, 6a, 7h, 8g.