Mixing Effects in Chemical Reactors—I
—Nonideal Reactors and Tracer Response Analysis

M. P. Dudukovic
Washington University
St. Louis, Missouri

and

R. M. Felder
North Carolina State University
Raleigh, North Carolina

OBJECTIVES
At the completion of this module the student should be able to:
1. State several causes for deviations from ideal flow conditions in real reactors.
2. Describe an impulse response measurement, and recognize characteristic impulse responses for ideal plug flow, perfect mixing, and dispersed plug flow.
3. Derive the tracer balance equation, state the conditions under which it is valid, and apply it to the measurement of a volumetric flow rate.
4. Define the concept of mean residence time, calculate a mean residence time from a measured impulse response, and use the result to determine a volumetric flow rate or the fluid volume between injection and detection points.
5. Use an impulse response to derive an ideal flow model for a continuous process vessel, and combine the model with a kinetic rate law to determine an expected extent of reaction.

PREREQUISITE MATHEMATICAL SKILLS
1. Differential and integral calculus.

PREREQUISITE ENGINEERING AND SCIENCE SKILLS
1. Understand the concept of a kinetic rate law. Have studied the design and analysis of ideal plug flow reactors and ideal continuous stirred-tank reactors.

A continuous reactor may behave very much like a plug flow reactor or a perfect mixer, but it can never completely achieve either of these ideal states. In an ideal plug flow reactor, all reactant and product molecules at a given axial position move at the same rate in the direction of the bulk fluid flow, while in real flow reactors, fluid velocity profiles, turbulent mixing and molecular diffusion cause molecules to move with a variety of speeds and directions. In an ideal continuous stirred-tank reactor, the reactant concentration is uniform throughout the reaction vessel, while in a real stirred tank, the reactant concentration is relatively high at the point where the feed enters, and low in the stagnant regions that develop in corners and behind baffles.

These inevitable deviations from ideal reactor conditions lead to several fundamental problems in reactor design and analysis:

1. Can an existing or planned reactor be treated as one of the ideal types (PFR or CSTR), or must nonidealities be considered when predicting the conversion which will result from a given feed rate and composition?
2. If nonidealties are important, what are they, and how can they be taken into account?

This module, and several that follow it, describe a technique called tracer response analysis, which is used to characterize the type of flow and mixing that takes place in a continuous process vessel. The technique is also applicable to biological systems, like organs and blood vessels, to hydrological systems, like rivers and estuaries; in general, to any system through which a fluid flows continuously.

THE TRACER-RESPONSE TECHNIQUE: QUALITATIVE DISCUSSION

Suppose the continuous process unit in Figure 1 operates at steady state, and that it is possible to measure the rate at which individual fluid molecules leave the unit in the outlet stream. There is no way to tell what kind of flow and mixing takes place in the unit simply by observing the outlet; fluid molecules leave at a rate equal to the rate at which they enter, whether the unit is an ideal plug flow reactor, an ideal CSTR, or any real unit. Why must this be so?

Suppose, however, that 100 molecules of a different species are abruptly injected at the inlet, and that it is possible to distinguish between these molecules and those of the bulk species at the outlet. For ease of discussion, let us call the molecules of the original species "white," and those of the injected species, "red." What would an observer instructed to watch for red molecules at the reactor outlet see?

The rate at which red molecules emerge depends upon the type of flow and mixing in the reactor. In ideal plug flow (Figure 2), all of the molecules would move through at the same velocity, and therefore all would emerge at once, after a time from injection equal to the mean residence time \( t \) in the unit (\( t = \text{tube length/velocity or volume/volumetric flow rate} \)).

On the other hand, in anything but an ideal plug flow reactor, a distribution of residence times would be observed—some red molecules would reach the outlet relatively quickly, emerging at times less than the mean residence time \( t \), while others would remain in the reactor for times considerably longer than \( t \). If the observer at the reactor outlet counts the number of red molecules that emerge in 1 second intervals, he might obtain a curve resembling one of the types shown in Figures 3a, b, and c. The shape of the curve depends strongly on how much mixing takes place in the reactor. In a slightly mixed tubular reactor, some molecules move faster than the mean fluid velocity, and others move slower, but the bulk moves close to the mean velocity and a relatively narrow distribution of residence times results (Figure 3). In a well-mixed system, the red molecules become distributed throughout the reactor relatively quickly, and emerge at a rate proportional to the number contained in the reactor—a high rate initially, when all are contained, and a steadily decreasing rate as the number remaining decreases (Figure 3a). For a reactor which is neither unmixed (PFR), nor perfectly mixed (CSTR), a response resembling that in Figure 3b might be obtained.

What has just been described in a qualitative way, is known as an impulse response test. An impulse is an injection that takes place instantaneously. The injected species functions as a tracer. In real experiments, the tracer is a radioactive substance or a dye or any other material whose outlet concentration can easily be measured. The injection at the inlet takes a finite time, but if the time it takes (typically 0.1 second) is much less than the mean residence time in the process unit, it is reasonable to consider it instantaneous. Techniques for analyzing responses to tracer inputs, other than impulses, will be discussed later.

The next section of this module formally introduces some terminology of impulse response testing, and outlines calculations that can be performed using the results of impulse response tests.

THE TRACER BALANCE EQUATION

Let us consider a continuous process unit operating at steady-state with a single input and output. In Figure 4, at a time \( t = 0 \), \( m_i \) grams of a tracer are injected into the inflow stream just before the entrance to the unit, and the concentration of tracer in the exit

![Figure 1. Schematic of process unit.](image)

![Figure 2. Tracer response for ideal plug flow reactor.](image)

![Figure 3. Characteristic impulse responses.](image)

![Figure 4. Schematic of impulse response measurement experiment.](image)
stream \( c(t) \) [g tracer/liter] is measured as a function of time. The following assumptions are made.

1. The tracer is perfect—i.e., the tracer molecules behave identically to the process fluid molecules within the process unit—and no tracer is lost within the system by reaction or adsorption on the walls.
2. The fluid velocity profiles at the inlet and outlet are flat.
3. The tracer enters and leaves the unit at the bulk inlet and outlet fluid velocities, which is to say the rate of diffusion of the tracer at the inlet and outlet is negligible compared to the rate of bulk convective flow. (However, any extent of mixing or diffusion may take place within the unit.) The term closed vessel is used to signify a process unit for which this condition is satisfied. The mass flow rate of tracer at the outlet is

\[
q \text{ [L/min]} \int_0^\infty c(t) dt \text{ [g/L]} = q c(t) \text{ [g/min]}
\]

In the infinitesimal time interval from \( t \) to \( t + dt \), the amount of tracer that leaves the unit is

\[
q c(t) dt \text{ [g tracer]}
\]

If the amounts that leave in each such time interval from \( t = 0 \) to \( t = \infty \) are summed (integrated), the total must be the total amount of tracer injected, or

\[
q \int_0^\infty c(t) dt = \int_0^\infty q \int_0^\infty c(t) dt = m_i \quad (1)
\]

Equation 1 is a fundamental relationship in tracer response analysis. The integral of \( c(t) \) can be determined by numerically integrating the experimental response curve (see Appendix). If both \( q \) and \( m_i \) are known independently, Equation 1 functions as a material balance (tracer out = tracer in); if it is not satisfied, then the assumption that tracer is not lost due to adsorption or reaction is invalid. If only \( m_i \) is known and the tracer is indeed conserved, Equation 1 may be used to determine the volumetric flow rate \( q \).

This technique has been used to measure flow rates in conduits ranging in size from blood vessels to rivers.

Example 1: Flow Rate Measurement Using a Tracer Balance

10 mg of a dye are injected at the inlet of a continuous reactor. Small samples are then periodically withdrawn from the reactor outlet stream, and the dye concentrations in the samples are measured using a photometer. The response curve shown in Figure 5 is obtained. The area under the curve determined by numerical integration is 7.5 (mg/L) · min. What is the

\[
\text{volumetric flow rate? If the reactor volume is 10 liters, what is the mean residence time in the reactor?}
\]

Solution:

From Equation 1,

\[
q = \frac{m_i}{\int_0^\infty c(t) dt} = \frac{10 \text{ mg}}{7.5 \text{ mg/L} \cdot \text{min/L}} = 1.33 \text{ L/min}
\]

\[
\bar{t} = V/q = \frac{10 \text{ L}}{1.333 \text{ L/min}} = 7.5 \text{ min}
\]

It can be seen from the shape of the output curve that this process vessel cannot be considered an ideal PFR or CSTR (see Figure 3).

MEAN RESIDENCE TIME

If a total of four tracer molecules were injected at the inlet of a process unit, and one emerged after one minute, two after two minutes, and the last one after three minutes, the average residence time for all four molecules would be

\[
\bar{t} = \frac{(1 \times 1 \text{ min}) + (2 \times 2 \text{ min}) + (1 \times 3 \text{ min})}{1 + 2 + 1} = 2 \text{ min}
\]

The mean residence time of the tracer molecules in the impulse response test described in the preceding section can be obtained in a similar manner. The number of tracer molecules that emerge in the time interval from \( t \) to \( t + dt \) is

\[
\frac{dm_i}{dt} = q \left[ \frac{\text{L/min}}{\text{L}} \right] \left[ \frac{\text{g/L}}{\text{L}} \right] dt \text{ [min]}
\]

The mean residence time is

\[
\bar{t} = \frac{\int_0^\infty \frac{dm_i}{dt} dt}{\int_0^\infty \frac{dm_i}{dt} dt}
\]

Substitute for \( dm_i \),

\[
\bar{t} = \frac{\int_0^\infty \frac{t c(t) dt}{\int_0^\infty c(t) dt}}{\int_0^\infty \frac{t c(t) dt}{\int_0^\infty c(t) dt}}
\]

Equation 2 gives the mean residence time for tracer molecules in the process unit, but since we have assumed that the tracer molecules behave identically to the process fluid molecules, \( \bar{t} \) must also be the mean residence time for all molecules in the unit.

We have not shown that \( \bar{t} \) determined from Eq. (2) is equal to the previously defined value of the mean residence time, \( V[\text{liters}] / q[\text{liters/second}] \). We will temporarily assume that this is the case, and prove it in a later module when the concept of age distributions

Figure 5. Impulse response for the system in Example 1.
is introduced. Therefore
\[ \bar{t} = \frac{\int_0^\infty t c(t) dt}{\int_0^\infty c(t) dt} \]

The right-hand side of Equation 3 can be calculated by numerical integration of a measured impulse response to yield \( \bar{t} \) directly. If the reactor volume \( V \) is known, \( q \) may then be determined, and conversely the volume may be calculated from a known value of \( q \). Notice that this method of determining \( q \) (unlike the method of Equation 1) does not require a knowledge of the amount of tracer injected; also, any measured signal proportional to \( c(t) \) may be used directly in place of \( c(t) \) itself. (Why?)

**Example 2: Determination of Mean Residence Time**

A tracer is injected at the inlet of a process unit, and the response in Figure 6 is obtained.

\[ c(t) = \begin{cases} 0.1 (t-1) & 1 \leq t \leq 2 \\ 0.1 (3-t) & 2 \leq t \leq 3 \\ 0 & \text{everywhere else} \end{cases} \]

(The form of the response was chosen for illustrative purposes; real tracer responses never look like this.) Calculate the mean residence time in the reactor. If the reactor volume is 2 liters, what is the volumetric flow rate of the fluid passing through it?

**Solution:**

\[ \int_0^\infty c(t) dt = \frac{1}{2} (2)(0.1) = 0.1 \text{ (g/cm}^3) \cdot \text{min} \]

\[ \int_0^\infty t c(t) dt = 0.1 \int_1^2 (t-1) dt \\
= 0.1 \int_2^3 (3-t) dt = 0.2 \text{ (g/cm}^3) \cdot \text{min}^2 \]

so that,

\[ \bar{t} = \frac{\int_0^\infty t c(t) dt}{\int_0^\infty c(t) dt} = 2 \text{ min} \]

**Figure 6. Impulse response (Example 2).**

\[ q = \frac{V}{\bar{t}} = \frac{20 \text{ L}}{2 \text{ min}} = 10 \text{ L/min} \]

**NOMENCLATURE**

\[ c = \int c(t) dt \text{ tracer concentration measured in the outflow of the system} \]

\[ m_i = \text{ mass of tracer injected in an impulse injection} \]

\[ q = \text{ volumetric flow rate through the system} \]

\[ t = \text{ time} \]

\[ \bar{t} = \text{ mean residence time} \]

\[ V = \text{ volume of the system} \]

**LITERATURE CITED**


**STUDY PROBLEMS**

1. Why are the conditions of ideal plug flow and perfect mixing never achieved in real reactors, however closely they may be approached?

2. What is a perfect tracer? A closed vessel? An impulse injection?

3. If a tracer impulse is injected at the inlet of an ideal plug flow reactor and the tracer concentration at the outlet is measured and plotted as a function of time from injection, what would the plot look like?

4. Repeat Question 3 for an ideal CSTR. Explain the shape of the response.

5. The following tracer impulse responses were obtained for continuous reactors. In each case, indicate whether you would model the reactor as an ideal PFR, an ideal CSTR, or neither.

**Response 1.**

<table>
<thead>
<tr>
<th>( t )</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c )</td>
<td>10</td>
<td>3.7</td>
<td>1.4</td>
<td>0.5</td>
<td>0.2</td>
<td>0.07</td>
</tr>
</tbody>
</table>

**Response 2.**

<table>
<thead>
<tr>
<th>( t )</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c )</td>
<td>0</td>
<td>0.01</td>
<td>10.0</td>
<td>0.02</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

**Response 3.**

<table>
<thead>
<tr>
<th>( t )</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c )</td>
<td>0</td>
<td>1.0</td>
<td>3.0</td>
<td>6.3</td>
<td>4.7</td>
<td>2.6</td>
<td>1.8</td>
</tr>
</tbody>
</table>

6. According to Equation 1,

\[ \int_0^\infty q c(t) dt = m_i \]

where \( m_i \) is the total mass of tracer injected in an impulse test. Suppose a response obtained using a
radioactive tracer in a very long channel is integrated numerically, and it is found that

\[ \int_0^\infty q(t) \, dt < m_i \]

Suggest an explanation for this result which might be true for any tracer, and a second explanation applicable specifically to a radioisotope.

7. Ten grams of a tracer are injected at the inlet of a reactor. Samples are withdrawn at the outlet and the concentration of the tracer in each sample is measured. The results are shown in Figure 7. The area under the curve is determined by numerical integration to be 50 mg · s/mL. What is the volumetric flow rate of fluid in the reactor? If the reactor volume is 10 liters, what is the mean residence time in the reactor?

8. How could you calculate \( t \) from the experiment of Question 7 without knowing the quantity of tracer injected?

**HOMEWORK PROBLEMS**

1. In Figure 8, a process fluid passes through a continuous tubular reactor with a 3 cm inner diameter. One gram of a tracer is injected instantaneously at the reactor inlet, and the following symmetrical outlet response is measured at a point 175 cm from the injection point.
   a) Is this reactor closer to being an ideal plug flow reactor or a perfect mixer?
   b) Calculate the volumetric flow rate using the tracer balance equation.
   c) Calculate the volumetric flow rate by first calculating the mean residence time.

2. Consider the following simplified biomedical experiment performed on a dog's kidney which is being artificially perfused by a pump at a constant flow rate of 100 mL/min. Two tracers are injected in the inflow and their concentrations are monitored in the major vein leaving the kidney. Tracer 1 cannot penetrate across the walls of the blood vessels and remains confined to the blood. Tracer 2 readily penetrates through all the fluids and tissues of the kidney but is not removed by urine. Ten grams of each tracer are injected at time \( t = 0 \) and an idealized response is presented Figure 9. Find the volume of distribution of tracer 1 (blood volume, \( V_b \)), and of tracer 2 (total kidney volume, \( V_k \)). Assume that the partition coefficient for tracer 2 is one, i.e. that the tracer is equally soluble in all kidney fluids.

3. An impulse response test is performed on a continuous reactor. The following is measured.

<table>
<thead>
<tr>
<th>( \Delta t = 5 ) seconds</th>
<th>( \Delta t = 30 ) seconds</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{time from injection} )</td>
<td>( \text{tracer concentration in outlet stream} )</td>
</tr>
<tr>
<td>( t ) (seconds)</td>
<td>( \text{mg/mL} )</td>
</tr>
<tr>
<td>5</td>
<td>0.400</td>
</tr>
<tr>
<td>10</td>
<td>0.383</td>
</tr>
<tr>
<td>15</td>
<td>0.367</td>
</tr>
<tr>
<td>20</td>
<td>0.353</td>
</tr>
<tr>
<td>25</td>
<td>0.338</td>
</tr>
<tr>
<td>30</td>
<td>0.325</td>
</tr>
<tr>
<td>60</td>
<td>0.253</td>
</tr>
<tr>
<td>90</td>
<td>0.197</td>
</tr>
<tr>
<td>120</td>
<td>0.153</td>
</tr>
<tr>
<td>150</td>
<td>0.119</td>
</tr>
<tr>
<td>180</td>
<td>0.093</td>
</tr>
<tr>
<td>210</td>
<td>0.072</td>
</tr>
<tr>
<td>240</td>
<td>0.056</td>
</tr>
<tr>
<td>270</td>
<td>0.044</td>
</tr>
<tr>
<td>300</td>
<td>0.034</td>
</tr>
<tr>
<td>330</td>
<td>0.027</td>
</tr>
<tr>
<td>360</td>
<td>0.021</td>
</tr>
<tr>
<td>390</td>
<td>0.016</td>
</tr>
<tr>
<td>420</td>
<td>0.013</td>
</tr>
<tr>
<td>450</td>
<td>0.010</td>
</tr>
<tr>
<td>480</td>
<td>0.008</td>
</tr>
<tr>
<td>510</td>
<td>0.006</td>
</tr>
</tbody>
</table>

a) Extrapolate the data back to the \( c \) axis to estimate the value of \( c \) at \( t = 0 \), and calculate the mean residence time in the reactor, either by graphical integration or using the computer program in the Appendix.

b) If the volumetric flow rate in this experiment was 4 L/min, what is the reactor volume, and how much tracer was injected?

c) Suppose a first-order reaction \( A \rightarrow B \), \( k = 0.5 \) min\(^{-1}\) is carried out in the reactor with the same volumetric flow rate used in the impulse response test. Use the results of Part (a) to choose and
evaluate the parameters of an ideal reactor model, and calculate the fractional conversion of \( A \) which would be achieved in the reactor.

Notes: 1. If \( \bar{r} \) is calculated using the computer program, you will have to apply the program twice for each integral from \( t = 0 \) to \( t = 510 \) seconds—once for \( 0 \leq t \leq 30 \), and again for \( 30 \leq t \leq 510 \).
2. The true response continues to \( t \rightarrow \infty \).

\( A \) truncation error is introduced when the response is cut off at \( t = 510 \) seconds; this is an unavoidable error in any tracer response experiment.

**APPENDIX: SIMPSON'S RULE FOR NUMERICAL INTEGRATION**

Suppose one wished to calculate

\[
I = \int_a^b y(x)dx
\]

where \( y(x) \) is a plotted or tabulated function, as in Figure 10.

\[
\begin{align*}
  x_1 & \quad y_1 \\
  x_2 & \quad y_2 \\
  x_3 & \quad y_3 \\
  x_4 & \quad y_4 \\
  x_5 & \quad y_5
\end{align*}
\]

Numerical integration is a procedure whereby simple analytical functions are fit to adjacent data points, and these approximate functions are integrated analytically to estimate the area under the true curve. If lines are fit to adjacent pairs of data points, the procedure is called the trapezoidal rule. If instead, parabolas are fit to adjacent triplets of equally spaced points, the procedure is Simpson's rule.

The area under a parabola through three points, whose \( x \) values are separated by a distance \( h \) (see Figure 11), is \( h/3 \left[ y_1 + 4y_2 + y_3 \right] \). Using this result, it is easy to show (see Figure 12) that the area under \( n \) equally spaced points (note: \( n \) must be odd) is

\[
I = \frac{h}{3} \left[ (y_1 + 4y_2 + y_3) + (y_3 + 4y_4 + y_5) + \ldots + (y_{n-2} + 4y_{n-1} + y_1) \right]
\]

or Simpson's rule formula, which is:

\[
\int_{x_1}^{x_n} y(x)dx \\
\approx \frac{h}{3} \left[ y_1 + y_n + 4(y_2 + y_4 + \ldots + y_{n-1}) + 2(y_3 + y_5 + \ldots + y_{n-2}) \right]
\]

For example, suppose it is desired to estimate the integral

\[
I = \int_1^5 c(t)dt
\]

from the following tabulated data:

<table>
<thead>
<tr>
<th>( t )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c )</td>
<td>5</td>
<td>12</td>
<td>31</td>
<td>68</td>
<td>129</td>
</tr>
</tbody>
</table>

Then \( n = 5 \), \( h = 1 \), and

\[
\int_1^5 c(t) \approx \frac{1}{3} \left[ 5 + 129 + 4(12 + 68) + 2(31) \right] = 172
\]

The integral of any function of \( c \) and \( t \), such as

\[
\int_1^5 tc(t)dt
\]

could easily be calculated by determining this function for each entry in the data table, and substituting the calculated values in the Simpson's rule formula.

**COMPUTER PROGRAM**

Program Name: SIMPR
Language: FORTRAN IV

Object: Evaluate

\[
F_0 = \int_{x_1}^{x} y_1 x dx
\]
\[ F_1 = \int_{x_1}^{x_n} x f(x) \, dx \]

using Simpson's rule for an array of equally-spaced points \( x_1, x_2, \ldots, x_n \). If \( n \) is even, the program uses Simpson's rule for the interval from \( x_1 \) to \( x_{n-1} \), and the trapezoidal rule for the interval from \( x_{n-1} \) to \( x_n \). The program calculates and prints out \( F_0, F_1, \) and \( F_1/F_0 \).

The following data must be supplied:

- \( NDS = \) Number of sets of \( y(x) \) data for which the program is to be run, and for each data set.
- \( N = \) Number of points.
- \( X(1) = \) First \( x \) value \( (x_1) \).
- \( H = \) Difference between successive \( x \) values.
- \( Y(1), Y(2), \ldots, Y(N) = \) dependent variable values \( (y_1, y_2, \ldots, y_n) \).

### Data Format

Card 1: \( NDS \) (Format 110)
Card 2: \( N, X(1), H \) (Format 110, 2F10.3)
Card(s) 3, 4, \ldots: \( Y(1), Y(2), \ldots, Y(N) \) (Format 8E10.3)

### Example

Impulse response data for a continuous reactor are as follows.

| \( t \) | 1 3 5 7 9 11 13 15 17 19 |
|---|---|---|---|---|---|---|---|---|---|---|
| \( c \) | 0 2 5 9 8 6.5 4.5 2 0.5 0.0 |

Calculate

\[
F_0 = \int_0^t \, c(t) \, dt \\
F_1 = \int_0^1 \, c(t) \, dt \\
\bar{t} = F_1/F_0
\]

Input data: (All numbers in fields of 10, integers right-adjusted)

Card 1: 1
Card 2: 10 1.0 2.0
Card 3: 0.0E0 2.0E0 5.0E0 9.0E0 8.0E0 6.5E0 4.5E0 2.0E0
Card 4: 0.5E0 0.0E0

C *** PROGRAM SIMFR
C *** EVALUATE INTEGRALS OF Y*DX(=F0) AND X*Y*DX
C *** (=F1) FROM X(1) TO X(N)
DIMENSION X(201),Y(201),YC(201)
C *** IF N EXCEEDS 201, INCREASE THE DIMENSIONS OF X,
C *** Y AND YC
READ(1,1) NDS

1 FORMAT(110)
WRITE(3,2) NDS
2 FORMAT(1H13X,'PROGRAM SIMFR'//1X'I3,'DATA
* SET(S) TO BE ANALYZED'//2X'INPUT DATA'//8X,
* 'X', 'X', 'X', 'Y', 'A(I2,'X', 'X', 'X', 'Y', 'Y')")
DO 500 J=1,N
READ (1,3) N,N,X(1),H
3 FORMAT(1H13X,'READ(I4,Y(J),J=1,N)
4 FORMAT(1H13X,'I4')
35 DO 40 I=2,N
40 X(1)=X(1)-1+H
WRITE(3,5)X(1),Y(J),J=1,N
5 FORMAT(1H13X,'WRITE(I4,F0.3)')
6 FORMAT(1H13X,'F0=F0.05*H*(Y(NF)+Y(N))")
200 F1=F1+0.5*X*Y(NF)+YC(N)
100 FR=F1/F0
WRITE(3,6)F0,F1,FR
6 FORMAT(1H13X,'F0=','E12.5','/4X'F1=','E12.5")
100 CONTINUE
WRITE(3,7)
7 FORMAT(1')
STOP
END

SUBROUTINE SIMP(Y,N,H,F)
DIMENSION Y(N)
NM1=N-1
NM2=N-2
S1=0.0
DO 200 J=2,NM1
100 S1=S1+Y(J)
S2=0.0
DO 200 J=2,NM2
200 S2=S2+Y(J)
F=F0*(Y(J)+Y(N)+4.0*S1+S2)/3.0
RETURN
END

American Institute of Chemical Engineers
SOLUTIONS TO THE STUDY PROBLEMS

1. Departures from ideal plug flow are caused by nonuniform velocity profiles, turbulent mixing and molecular diffusion. Departures from perfect mixing are caused by spatial inhomogeneities at the reactor inlet and stagnant regions in corners and behind baffles.

2. **Perfect tracer:** tracer molecules behave identically with the process fluid molecules within the process unit.

   **Closed vessel:** rate of diffusion across the vessel entrance and exit boundaries is negligible compared to the rate of convective motion across the boundaries.

   **Impulse injection:** takes place instantaneously (or nearly instantaneously on the time scale of the process).

3. 

4. 

---

American Institute of Chemical Engineers
The tracer is instantly dispersed throughout the reaction vessel, before any has a chance to emerge. The concentration of tracer in the outlet stream is proportional to the amount of tracer in the vessel; since this quantity has its maximum value at \( t=0 \) and thereafter declines, the shape of the response curve follows the same pattern.

5. (a) ideal CSTR; (b) ideal PFR; (c) neither

6. (a) irreversible adsorption on or reaction with the vessel walls
   (b) activity decay

7. \[ q \int c(t) \, dt = m_i \]
   \[ q = \frac{10000 \text{ (mg)}}{50 \text{ (mg·s/mL)}} = 200 \text{ (mL/s)} = 0.2 \text{ (L/s)} \]
   \[ \tau = \frac{10 \text{ (L)}}{0.2 \text{ (L/s)}} = 50 \text{ (s)} \]

8. Calculate the first moment of the response, and then determine \( \bar{t} \) as
   \[ \bar{t} = \frac{\int_0^\infty tc(t) \, dt}{\int_0^\infty c(t) \, dt} \]