18.8 Two-Parameter Models—Modeling Real Reactors with Combinations of Ideal Reactors

Creativity and engineering judgment are necessary for model formulation.

We now will see how a real reactor might be modeled by different combinations of ideal reactors. Here, an almost unlimited number of combinations that could be made. However, if we limit the number of adjustable parameters to two (e.g., bypass flow rate, v_b, and dead volume, V_D), the situation becomes much more tractable. After reviewing the steps in Table 18-1, choose a model and determine if it is reasonable by qualitatively comparing it with the RTD and, if it is, determine the model parameters. Usually, the simplest means of obtaining the necessary data is some form of a tracer test. These tests have been described in Chapters 16 and 17, together with their uses in determining the RTD of a reactor system. Tracer tests can be used to determine the RTD, which can then be used in a similar manner to determine the suitability of the model and the value of its parameters.

A tracer experiment is used to evaluate the model parameters.

In determining the suitability of a particular reactor model and the parameter values from tracer tests, it may not be necessary to calculate the RTD function $E(t)$. The model parameters (e.g., V_D) may be acquired directly from measurements of effluent concentration in a tracer test. The theoretical prediction of the particular tracer test in the chosen model system is compared with the tracer measurements from the real reactor. The parameters in the model are chosen so as to obtain the closest possible agreement between the model and experiment. If the agreement is then sufficiently close, the model is deemed reasonable. If not, another model must be chosen.

What is sufficiently close?

The quality of the agreement necessary to fulfill the criterion "*sufficiently close*" again depends on creativity in developing the model and on engineering judgment. The most extreme demands are that the maximum error in the prediction not exceed the estimated error in the tracer test, and that there be no observable trends with time in the difference between prediction (the model) and observation (the real reactor). In the *Expanded Material* on the CRE Web site we illustrate how the modeling is carried out, we will now consider two different models for a CSTR.

### 18.8.1 Real CSTR Modeled Using Bypassing and Dead Space

A real CSTR is believed to be modeled as a combination of an ideal CSTR with a well-mixed volume V_s, a dead zone of volume V_d, and a bypass with a volumetric flow rate v_b (Figure 18-1). We have used a tracer experiment to evaluate the parameters of the model V_s and v_s. Because the total volume and volumetric flow rate are known, once V_s and v_s are found, v_b and V_d can readily be calculated.

18.8.1.1 Solving the Model System for C_A and X

$$[C_A(v_b + v_s)] = [C_{As}v_s] \tag{18-64}$$

We can solve for the concentration of A leaving the reactor

$$C_A = \frac{v_b C_{A0} + C_{As}\,v_s}{v_b + v_s} = \frac{v_b C_{A0} + C_{As}\,v_s}{v_0}$$
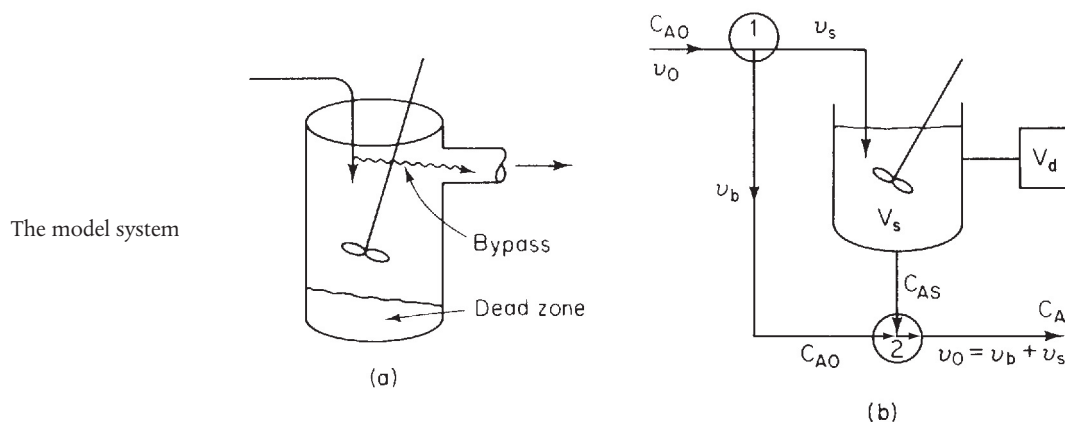
The model system

Figure 18-1   (a) Real system; (b) model system.

Let $\alpha = V_s/V$ and $\beta = v_b/v_0$. Then

$$C_A = \beta C_{A0} + (1 - \beta)C_{As} \qquad (18\text{-}60)$$

For a first-order reaction, a mole balance on V_s gives

Mole balance on
CSTR

$$v_s C_{A0} - v_s C_{As} - kC_{As}V_s = 0 \qquad (18\text{-}61)$$

or, in terms of α and β

$$C_{As} = \frac{C_{A0}(1 - \beta)v_0}{(1 - \beta)v_0 + \alpha Vk} \qquad (18\text{-}62)$$

Substituting Equation (18-62) into (18-60) gives the effluent concentration of species A:

Conversion as a
function of model
parameters

$$\frac{C_A}{C_{A0}} = 1 - X = \beta + \frac{(1 - \beta)^2}{(1 - \beta) + \alpha\tau k} \qquad (18\text{-}63)$$

We have used the ideal reactor system shown in Figure 18-1 to predict the conversion in the real reactor. The model has two parameters, α and β. The parameter α is the dead zone volume fraction and parameter β is the fraction of the volumetric flow rate that bypasses the reaction zone. If these parameters are known, we can readily predict the conversion. In the following section, we shall see how we can use tracer experiments and RTD data to evaluate the model parameters.

18.8.1.2   Using a Tracer to Determine the Model Parameters in a CSTR-with-Dead-Space-and-Bypass Model

Model system

In Section 18.8.1.1, we used the system shown in Figure 18-2, with bypass flow rate, v_b, and dead volume, V_d, to model our real reactor system. We shall inject our tracer, T, as a positive-step input. The unsteady-state balance on the nonreacting tracer, T, in the well-mixed reactor volume, V_s, is
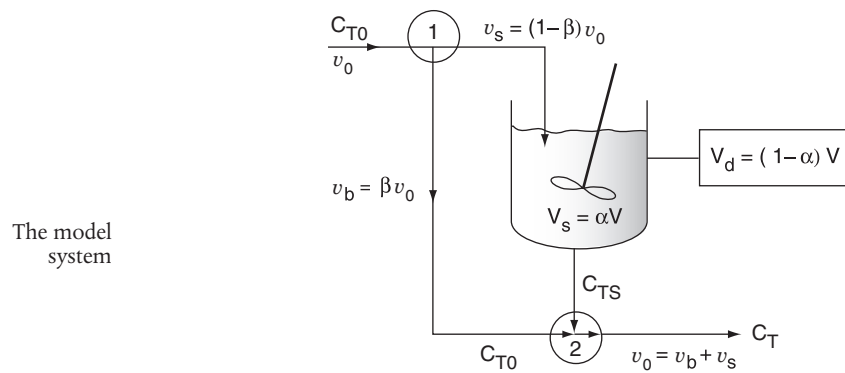
Figure 18-2 Model system: CSTR with dead volume and bypassing.

$$\text{In} - \text{out} = \text{accumulation}$$

Tracer balance for
step input

$$v_s C_{T0} - v_s C_{Ts} = \frac{dN_{Ts}}{dt} = V_s \frac{dC_{Ts}}{dt} \tag{18-64}$$

The conditions for the positive-step input are

$$\text{At } t < 0 \quad C_T = 0$$

$$\text{At } t \geq 0 \quad C_T = C_{T0}$$

A balance around junction point 2 gives

The junction
balance

$$C_T = \frac{v_b C_{T0} + C_{Ts} v_s}{v_0} \tag{18-65}$$

As before

$$V_s = \alpha V$$

$$v_b = \beta v$$

$$\tau = \frac{V}{v_0}$$

Integrating Equation (18-64) and substituting in terms of α and β gives

$$\frac{C_{Ts}}{C_{T0}} = 1 - \exp\left[-\frac{1-\beta}{\alpha}\left(\frac{t}{\tau}\right)\right] \tag{18-66}$$

Combining Equations (18-65) and (18-66), the effluent tracer concentration is

$$\frac{C_T}{C_{T0}} = 1 - (1 - \beta) \exp\left[-\frac{1-\beta}{\alpha}\left(\frac{t}{\tau}\right)\right] \tag{18-67}$$

We now need to rearrange this equation to extract the model parameters, α and β, either by regression (Polymath/MATLAB/Excel) or from the proper plot of the effluent tracer concentration as a function of time. Rearranging yields

Evaluating the
model parameters

$$\ln \frac{C_{T0}}{C_{T0} - C_T} = \ln \frac{1}{1 - \beta} + \left(\frac{1 - \beta}{\alpha} \right) \frac{t}{\tau} \qquad (18\text{-}68)$$

Consequently, we plot $\ln[C_{T0}/(C_{T0} - C_T)]$ as a function of t. If our model is correct, a straight line should result with a slope of $(1 - \beta)/\tau\alpha$ and an intercept of $\ln[1/(1 - \beta)]$.

Example 18–4   Parameter Evaluation for a CSTR with Dead Space and Bypass

The elementary reaction

$$A + B \longrightarrow C + D$$

is to be carried out in the CSTR shown schematically in Figure 18-2. There is both bypassing and a stagnant region in this reactor. The tracer output for this reactor is shown in Table E18-4.1. The measured reactor volume is 1.0 m³ and the flow rate to the reactor is 0.1 m³/min. The reaction-rate constant is 0.28 m³/kmol·min. The feed is equimolar in A and B with an entering concentration of A equal to 2.0 kmol/m³. Calculate the conversion that can be expected in this reactor (Figure E18-4.1).

TABLE E18-4.1   TRACER DATA FOR STEP INPUT

C_T (mg/dm³)	1000	1333	1500	1666	1750	1800
t (min)	4	8	10	14	16	18

The entering tracer concentration is C_{T0} = 2000 mg/dm³.

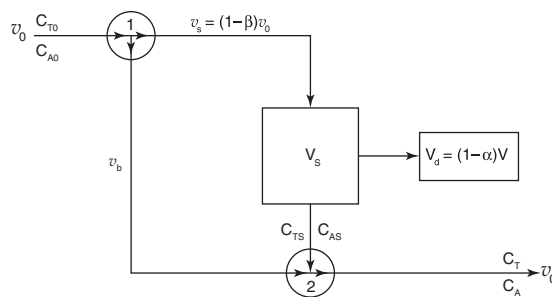Two-parameter
model

Figure E18-4.1   Schematic of real reactor modeled with dead space (V_d) and bypass (v_b).

Solution

One of the keys is to determine **what** to plot as function of **what** in order to determine the system parameters, e.g., v_b, α, β.
Recalling Equation (18-68)

$$ln \frac{C_{T0}}{C_{T0} - C_T} = ln \frac{1}{1 - \beta} + \frac{(1 - \beta)}{\alpha} \frac{t}{\tau} \qquad (18\text{-}68)$$

Equation (18-68) suggests that we construct Table E18-4.2 from Table E18-4.1 and plot $C_{T0}/(C_{T0} - C_T)$ as a function of time on semilog paper. Using this table we get Figure E18-4.2.

TABLE E18-4.2   PROCESSED DATA

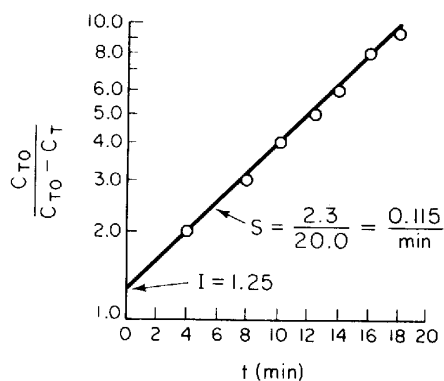| t (min)	4	8	10	14	16	18
$\dfrac{C_{T0}}{C_{T0} - C_T}$	2	3	4	6	8	10

Figure E18-4.2   Response to a step input.

We can find α and β from either a semilog plot, as shown in Figure E18-4.2, or by regression using Polymath, MATLAB, or Excel.

The volumetric flow rate to the well-mixed portion of the reactor, v_s, can be determined from the intercept, I

$$\frac{1}{1 - \beta} = I = 1.25$$

$$\boxed{\beta = \frac{v_b}{v_0} = 0.2}$$

The volume of the well-mixed region, V_s, can be calculated from the slope, S,

$$\frac{1 - \beta}{\alpha \tau} = S = 0.115 \text{ min}^{-1}$$

$$\alpha \tau = \frac{1 - 0.2}{0.115} = 7 \text{ min}$$

$$\tau = \frac{V}{v_0} = \frac{1 \text{ m}^3}{(0.1 \text{ m}^3/\text{min})} = 10 \text{ min}$$

$$\boxed{\alpha = \frac{7 \text{ min}}{\tau} = 0.7}$$

We now proceed to determine the conversion corresponding to these model parameters.

1. **Balance on reactor volume V_s:**

$$[\text{In}] - [\text{Out}] + [\text{Generation}] = [\text{Accumulation}]$$

$$v_s C_{A0} - v_s C_{As} + r_{As} V_s \qquad = 0 \qquad \text{(E18-4.1)}$$

2. **Rate law:**

$$-r_{AS} = k C_{As} C_{Bs}$$

Equalmolar feed $\therefore C_{As} = C_{Bs}$

$$-r_{As} = k C_{As}^2 \qquad \text{(E18-4.2)}$$

3. **Combining** Equations (E18-4.1) and (E18-4.2) gives

$$v_s C_{A0} - v_s C_{As} - k C_{As}^2 V_s = 0 \qquad \text{(E18-4.3)}$$

Rearranging, we have

$$\tau_s k C_{As}^2 + C_{As} - C_{A0} = 0 \qquad \text{(E18-4.4)}$$

Solving for C_{As} yields

$$\boxed{C_{As} = \frac{-1 + \sqrt{1 + 4\tau_s k C_{A0}}}{2\tau_s k}} \qquad \text{(E18-4.5)}$$

4. **Balance around junction** point 2:

$$[\text{In}] = [\text{Out}]$$

$$[v_b C_{A0} + v_s C_{As}] = [v_0 C_A] \qquad \text{(E18-4.6)}$$

Rearranging Equation (E18-4.6) gives us

$$\boxed{C_A = \frac{v_0 - v_s}{v_0} C_{A0} + \frac{v_s}{v_0} C_{As}} \qquad \text{(E18-4.7)}$$

5. **Parameter evaluation:**

$$v_s = 0.8\, v_0 = (0.8)(0.1\ \text{m}^3/\text{min}) = 0.08\ \text{m}^3/\text{min}$$

$$V_s = (\alpha\tau)\, v_0 = (7.0\ \text{min})(0.1\ \text{m}^3/\text{min}) = 0.7\ \text{m}^3$$

$$\tau_s = \frac{V_s}{v_s} = 8.7\ \text{min}$$

$$C_{As} = \frac{\sqrt{1 + 4\tau_s k C_{A0}} - 1}{2\tau_s k} \qquad \text{(E18-4.8)}$$

$$= \frac{\sqrt{1 + (4)(8.7\ \text{min})(0.28\ \text{m}^3/\text{kmol}\cdot\text{min})(2\ \text{kmol}/\text{m}^3)} - 1}{(2)(8.7\ \text{min})(0.28\ \text{m}^3/\text{kmol}\cdot\text{min})}$$

$$= 0.724\ \text{kmol}/\text{m}^3$$

Substituting into Equation (E18-4.7) yields

Finding the conversion

$$C_A = \frac{0.1 - 0.08}{0.1}\, (2) + (0.8)(0.724) = 0.979$$

The predicted conversion for the real reactor using the CSTR dead volume and bypassing is

$$X = 1 - \frac{0.979}{2.0} = 0.51$$

If the real reactor were acting as an ideal CSTR, the conversion would be

$$C_A = \frac{\sqrt{1 + 4\tau k C_{A0}} - 1}{2\tau k} \qquad \text{(E18-4.9)}$$

$$C_A = \frac{\sqrt{1 + 4(10)(0.28)(2)} - 1}{2(10)(0.28)} = 0.685$$

$$\boxed{X_{model} = 0.51}$$
$$\boxed{X_{Ideal} = 0.66}$$

$$X = 1 - \frac{C_A}{C_{A0}} = 1 - \frac{0.685}{2.0} = 0.66 \qquad \text{(E18-4.10)}$$

Analysis: In this example we used a combination of an ideal CSTR with a dead volume and bypassing to model a nonideal reactor. If the nonideal reactor behaved as an ideal CSTR, a conversion of 66% was expected. Because of the dead volume, not all the space would be available for reaction; also, some of the fluid did not enter the space where the reaction was taking place and, as a result, the conversion in this nonideal reactor was only 51%.

Example web 18–2   Two CSTRs with interchange

The elementary first-order liquid-phase reaction

$$A \xrightarrow{\ k\ } B$$
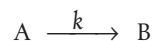
is carried out in a nonideal CSTR with k = 0.03 min^{-1}. The flow patterns seem to approximate two CSTRs with interchange (Figure web E18-2.1). Species A enters the reactor at a rate of 25 dm^3/min and a concentration of 0.02 mo1/dm^3. The total reactor volume is 1000 dm^3. The results of a pulse tracer test are shown in Table web 18-2.1 Using the results of these tests, determine the conversion.

$$\tau = \frac{V}{v_0} = \frac{1000 \text{ dm}^3}{25 \text{ dm}^3/\text{min}} = 40 \text{ min}$$
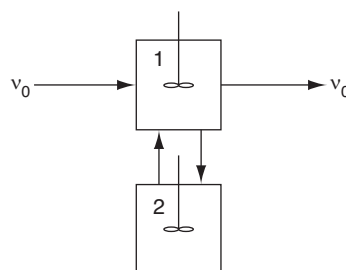
$$C_{10} = 2000 \text{ mg/dm}^3$$

Figure web E18-2.1

TABLE WEB 18-2.1

t (min)	C (mg/dm³)
0	2000
20	1050
40	520
60	280
80	160
120	61
160	29
200	16.4
240	10.0
280	6.4
320	4.0

Solution

t (min)	0.0	20	40	60	80	120	160	200	240	280	320
$\theta = t/\tau$	0.0	0.5	1.0	1.5	2.0	3.0	4.0	5.0	6.0	7.0	8.0
C	2000	1050	520	280	160	61	29	16.4	10.0	6.4	4.0
C/C_{10}	1.0	0.525	0.26	0.14	0.08	0.03	0.0145	0.0082	0.005	0.0032	0.002

A tracer balance yields
(mass added at $t = 0$) = (mass out over all time)

$$C_{10}\alpha V = v_0 \int_0^\infty C(t) \; dt \qquad \text{(Web 18-1.1)}$$

$$\alpha = \frac{1}{C_{10}} \int_0^\infty C(\theta)d\theta = \int_0^\infty \frac{C(\theta)}{C_{10}}d\theta \qquad \text{(Web 18-1.2)}$$

$$\alpha = \frac{b_1}{3}(f_1' + 4f_2' + 2f_3' + 4f_4' + f_5')$$

$$+ \frac{b_2}{3}(f_1' + 4f_2' + 2f_3' + 4f_4' + f_5' + 4f_6' + f_7')$$

$$= \frac{0.5}{3}[1 + 4(0.525) + 2(0.26) + 4(0.14) + 0.08]$$

$$+ \frac{1}{3}[0.08 + 4(0.03) + 2(0.0145) + 4(0.0082)$$

$$+ 2(0.005) + 4(0.0032) + 0.002]$$
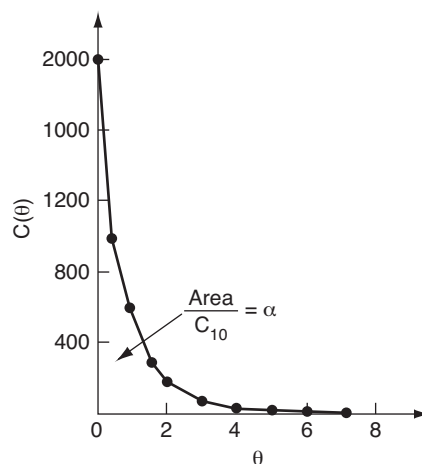
$$= 0.71 + 0.09 = 0.80$$

We could also have evaluated Equation (web E18-1.2) by taking the area under the curve of a plot of $C(\theta)$ versus θ (Figure web E18-2.2)
We will now determine the decay constants, m_1 and m_2, from which the fraction exchanged, β, can be determined. The dimensionless concentration is obtained from Equation (web 18-75)

$$\frac{C}{C_{10}} = \frac{(\alpha m_1 + \beta + 1)e^{m_2\theta} - (\alpha m_2 + \beta + 1)e^{m_1\theta}}{\alpha(m_1 - m_2)} \qquad \text{(Web E18-1.3)}$$

$$|m_2| > |m_1|$$

Figure web E18-2.2   Dimensionless tracer concentration as a
function of dimensionless time

Plotting the ratio $C(t)/C_{10}$ as a function of θ on semilog coordinates, we get the graph shown in Figure web E18-1.3. At long times, the first term containing m_2 in the exponent is negligible with respect to the second term. Consequently, if we extrapolate the portion of the curve for long times back to $\theta = 0$, we have

$$\text{Intercept} = I = -\frac{\alpha m_2 + \beta + 1}{\alpha(m_1 - m_2)} = 0.066 \qquad \text{(Web E18-2.4)}$$

$$0.066 = \frac{-(0.8)(-1.44) + \beta + 1}{(0.8)[-0.434 - (-1.44)]}$$

Solving for β, we obtain $\beta = 0.1$. The two parameters for this model are then

$$\alpha = 0.8 \text{ and } \beta = 0.1$$

$$\tau k = (40 \text{ min})(0.03 \text{ min}^{-1}) = 1.2$$

Substituting for τk, α, and β in Equation (18-69) yields

$$\frac{C_A}{C_{A0}} = 1 - X = \frac{1}{1 + \beta + \alpha\tau k - \dfrac{\beta^2}{\beta + (1 - \alpha)\tau k}} \qquad \text{(Web E18-2.5)}$$

$$1 - X = \frac{1}{1 + 0.1 + (0.8)(1.2) - \dfrac{(0.1)^2}{0.1 + (1 - 0.8)(1.2)}} \qquad \text{(Web E18-2.6)}$$
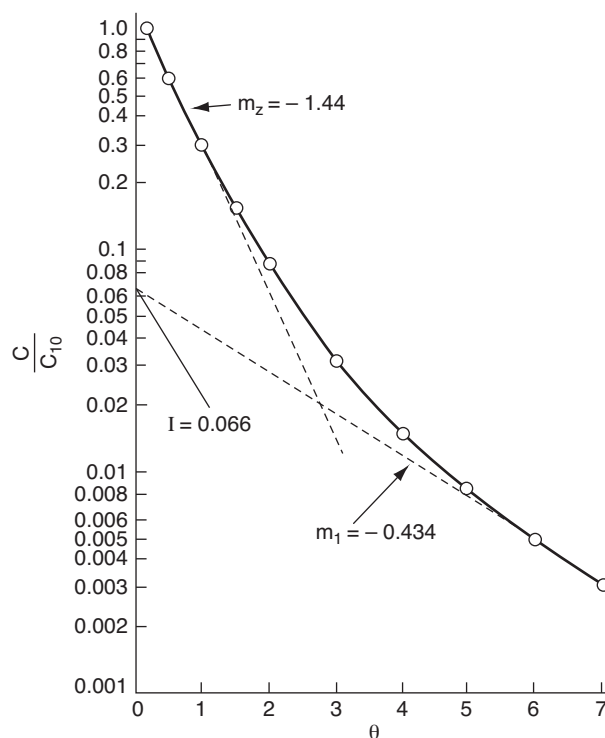
So $X = 0.51$. For a single ideal CSTR,

$$X = \frac{\tau k}{1 + \tau k} = \frac{1.2}{2.2} = 0.55 \qquad \text{(Web E18-2.7)}$$

For a single ideal plug-flow reactor,

$$X = 1 - e^{-\tau k} = 1 - e^{-12} = 0.70 \qquad \text{(Web E18-2.8)}$$

$$\boxed{(X_{\text{model}} = 0.51) < (X_{\text{CSTR}} = 0.55) < (X_{\text{PFR}}) = 0.70}$$

Figure web E18-1.3   Dimensionless tracer concentration as a
function of dimensionless time

Other Models.   In Section 18.8.1 it was shown how we formulated a model consisting of ideal reactors to represent a real reactor. First, we solved for the exit concentration and conversion for our model system in terms of two parameters, α and β. We next evaluated these parameters from data on tracer concentration as a function of time. Finally, we substituted these parameter values into the mole balance, rate law, and stoichiometric equations to predict the conversion in our real reactor.

To reinforce this concept, we will use one more example.

18.8.2   Real CSTR Modeled as Two CSTRs with Interchange

In this particular model there is a highly agitated region in the vicinity of the impeller; outside this region, there is a region with less agitation (Figure 18-3). There is considerable material transfer between the two regions. Both inlet and outlet flow channels connect to the highly agitated region. We shall model the

The model system
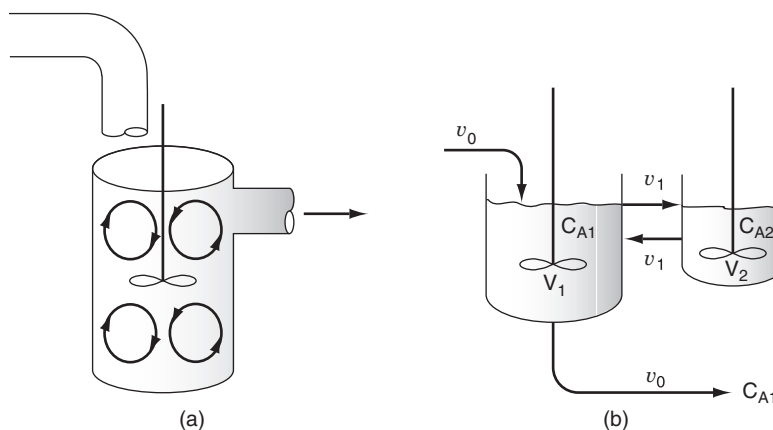
Figure 18-3   (a) Real reaction system; (b) model reaction system.

highly agitated region as one CSTR, the quieter region as another CSTR, with material transfer between the two.

18.8.2.1 Solving the Model System for C_A and X

Let β represent that fraction of the total flow that is exchanged between reactors 1 and 2; that is,

$$v_1 = \beta v_0$$

and let α represent that fraction of the total volume, V, occupied by the highly agitated region:
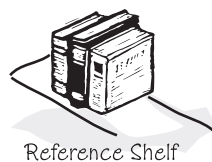
Two parameters:
α and β

$$V_1 = \alpha V$$

Then

$$V_2 = (1 - \alpha)V$$

The space time is

$$\tau = \frac{V}{v_0}$$

As shown on the CRE Web site *Professional Reference Shelf R18.2,* for a first-order reaction, the exit concentration and conversion are

Reference Shelf

$$C_{A1} = \frac{C_{A0}}{1 + \beta + \alpha\tau k - \{\beta^2/[\beta + (1-\alpha)\tau k]\}} \qquad (18\text{-}69)$$

and

Conversion for
two-CSTR model

$$\boxed{X = 1 - \frac{C_{A1}}{C_{A0}} = \frac{(\beta + \alpha\tau k)[\beta + (1-\alpha)\tau k] - \beta^2}{(1 + \beta + \alpha\tau k)[\beta + (1-\alpha)\tau k] - \beta^2}} \qquad (18\text{-}70)$$

where C_{A1} is the reactor concentration exiting the first reactor in Figure 18-3(b).

18.8.2.2 *Using a Tracer Experiment to Determine the Model Parameters in a CSTR with an Exchange Volume*

The problem now is to evaluate the parameters α and β using the RTD data for the reaction system shown in Figure 18-3. A mole balance on a tracer pulse injected at $t = 0$ for each of the tanks is

$$\text{Accumulation} = \text{Rate in} - \text{Rate out}$$

Unsteady-state balance of inert tracer

Reactor 1:
$$V_1 \frac{dC_{T1}}{dt} = v_1 C_{T2} - (v_0 C_{T1} + v_1 C_{T1}) \tag{18-71}$$

Reactor 2:
$$V_2 \frac{dC_{T2}}{dt} = v_1 C_{T1} - v_1 C_{T2} \tag{18-72}$$

and C_{T1} is the measured tracer concentration existing the real reactor. The tracer is initially dumped only into reactor 1, so that the initial conditions $C_{T10} = N_{T0}/V_1$ and $C_{T20} = 0$.

Substituting in terms of α, β, and τ, we arrive at two coupled differential equations describing the unsteady behavior of the tracer that must be solved simultaneously.

See Appendix A.3 for method of solution

$$\tau\alpha \frac{dC_{T1}}{dt} = \beta C_{T2} - (1 + \beta) C_{T1} \tag{18-73}$$

$$\tau(1 - \alpha) \frac{dC_{T2}}{dt} = \beta C_{T1} - \beta C_{T2} \tag{18-74}$$
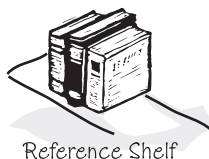
Analytical solutions to Equations (18-73) and (18-74) are given on the CRE Web site, in Appendix A.3 and in Equation (18-75), below. However, for more complicated systems, analytical solutions to evaluate the system parameters may not be possible.

Reference Shelf

$$\left(\frac{C_{T1}}{C_{T10}} \right)_{\text{pulse}} = \frac{(\alpha m_1 + \beta + 1)\, e^{m_2 t/\tau} - (\alpha m_2 + \beta + 1)\, e^{m_1 t/\tau}}{\alpha\,(m_1 - m_2)} \tag{18-75}$$

where

$$m_1,\, m_2 = \left[\frac{1 - \alpha + \beta}{2\alpha\,(1 - \alpha)} \right] \left[-1 \pm \sqrt{1 - \frac{4\alpha\beta\,(1 - \alpha)}{(1 - \alpha + \beta^2)}} \right]$$

By regression on Equation (18-75) and the data in Table E18-4.2 or by an appropriate semilog plot of C_{T1}/C_{T10} versus time, one can evaluate the model parameters α and β.

18.9 *Expanded Material on the Web Site:* Use of Software Packages to Determine the Model Parameters

If analytical solutions to the model equations are not available to obtain the parameters from RTD data, one could use ODE solvers. Here, the RTD data would first be fit to a polynomial to the effluent concentration–time data and then compared with the model predictions for different parameter values.

An example showing how to evaluate the model parameters for a CSTR with Bypassing and dead volume (*http://www.umich.edu/~elements/5e/18chap/learn-cd18-3.html*).

Example 18–4   CSTR with Bypass and Dead Volume

(a) Determine parameters α and β that can be used to model two CSTRs with interchange using the tracer concentration data listed in Table E18-4.1. The tracer was "thrown/injected" into the reactor at $t = 0$.

TABLE E18-4.1   RTD DATA

t (min)	0.0	20	40	60	80	120	160	200	240
C_{Te} (g/m³)	2000	1050	520	280	160	61	29	16.4	10.0

(b) Determine the conversion of a first-order reaction with $k = 0.03$ min^{-1} and $\tau = 40$ min.

Solution

First, we will use Polymath to fit the RTD to a polynomial. Because of the steepness of the curve, we shall use two polynomials.

For $t \leq 80$ min

$$C_{Te} = 2000 - 59.6t + 0.642t^2 - 0.00146t^3 - 1.04 \times 10^{-5}t^4 \qquad \text{(E18-4.1)}$$

For $t > 80$ min

$$C_{Te} = 921 - 17.3t + 0.129t^2 - 0.000438t^3 - 5.6 \times 10^{-7}t^4 \qquad \text{(E18-4.2)}$$

where C_{Te} is the exit concentration of tracer determined experimentally. Next we would enter the tracer mole (mass) balances Equations (18-68) and (18-69) into an ODE solver. The Polymath program is shown in Table E18-4.2. Finally, we vary the parameters α and β and then compare the calculated effluent concentration C_{T1} with the experimental effluent tracer concentration C_{Te}. After a few trials, we converge on the values α = 0.8 and β = 0.1. We see from Figure E18-4.1 and Table E18-4.3 that the agreement between the RTD data and the calculated data is quite good, indicating the validity of our values of α and β. We now substitute these values in Equation (18-70), and as shown on the CRE Web site, the corresponding conversion is 51% for the model system of two CSTRs with interchange

Trial and error using software packages

$$X = 1 - \frac{C_{A1}}{C_{A0}} = \frac{(\beta + \alpha\tau k)[\beta + (1-\alpha)\,\tau k] - \beta^2}{(1 + \beta + \alpha\tau k)[\beta + (1-\alpha)\,\tau k] - \beta^2} \qquad (18\text{-}70)$$

$$\tau k = (40 \text{ min})(0.03 \text{ min}^{-1}) = 1.2$$

$$X = \frac{[0.1 + (0.8)(1.2)][0.1 + (1-0.8)(1.2)] - (0.1)^2}{[1 + 0.1 + (0.8)(1.2)][0.1 + (1-0.8)(1.2) - (0.1)^2]}$$

$$X = 0.51$$

Comparing models, we find

$$(X_{\text{model}} = 0.51) < (X_{\text{CSTR}} = 0.55) < (X_{\text{PFR}} = 0.7)$$

TABLE E18-4.2   POLYMATH PROGRAM: TWO CSTRs WITH INTERCHANGE

ODE Report (RKF45)

Differential equations as entered by the user
[1] d(CT1)/d(t) = (beta*CT2-(1+beta)*CT1)/alpha/tau
[2] d(CT2)/d(t) = (beta*CT1-beta*CT2)/(1-alpha)/tau

Explicit equations as entered by the user
[1] beta = 0.1
[2] alpha = 0.8
[3] tau = 40
[4] CTe1 = 2000-59.6*t+0.64*t^2-0.00146*t^3-1.047*10^(-5)*t^4
[5] CTe2 = 921-17.3*t+0.129*t^2-0.000438*t^3+5.6*10^(-7)*t^4
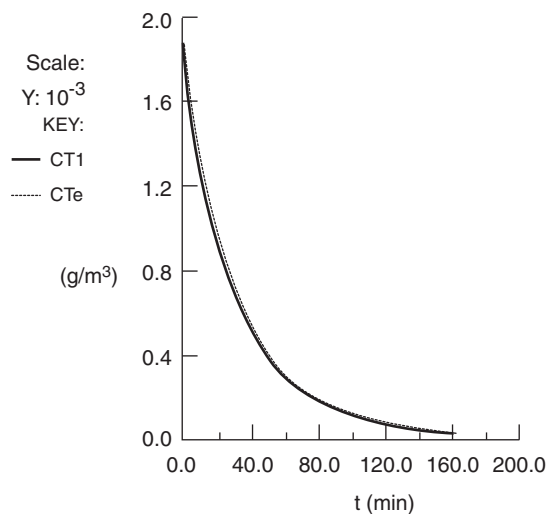[6] t1 = t-80
[7] CTe = if(t<80)then(CTe1)else(CTe2)

Figure E18-4.1   Comparison of model and experimental exit tracer concentrations.

TABLE E18-4.3   COMPARING MODEL (CT1) WITH EXPERIMENT (CTe)

t	CT1	CTe
0	2000	2000
10	1421.1968	1466.4353
20	1014.8151	1050.6448
30	728.9637	740.0993
40	527.4236	519.7568
50	384.9088	372.0625
60	283.7609	276.9488
70	211.6439	211.8353
80	159.9355	161.2816
100	95.43456	99
120	60.6222	61.8576
140	40.9209.3	40.6576
160	29.10943	28.3536

Two CSTRs with interchange

**Analysis:** For the two-parameter model chosen, we used the RTD to determine the two parameters' dead volume and fraction of fluid bypassed. We then calculated the exit trace concentration using the ideal CSTR balance equations but with a lesser reactor volume and a smaller flow rate through the reactor and compared it with the experimental data.