# 14. Models for Nonideal Reactors

## Professional Reference Shelf

### R14.2 Real Reactor Modeled as an Ideal CSTR with an Exchange Volume

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 R14.2-1). 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 highly agitated region as one CSTR, the quieter region as another CSTR, with material transfer between the two. The material balances describing the steady-state behavior of the two reactors are

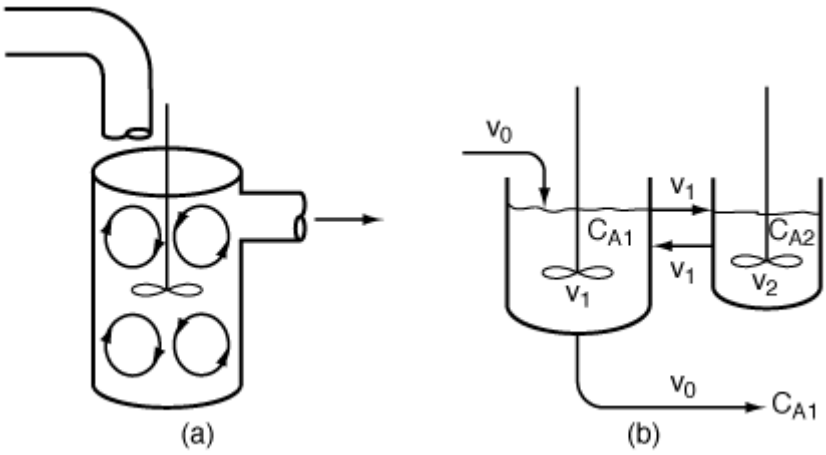


Figure R14.2-1
(a) Real reaction systems; (b) model reaction system

Mole balances

| | in | − | out | + | generation | = | accumulation | |
|---|---|---|---|---|---|---|---|---|
| Reactor 1: | $(v_0 C_{A0} + v_1 C_{A2})$ | − | $(v_0 C_{A1} + v_1 C_{A1})$ | + | $r_{A1} V_1$ | = | 0 | (R14.2-1) |
| Reactor 2: | $v_1 C_{A1}$ | − | $v_1 C_{A2}$ | + | $r_{A2} V_2$ | = | 0 | (R14.2-2) |

The two parameters in this model are the exchange flow rate $v_1$ and the volume of the highly agitated region, $V_1$. Note that the measured volume $V$ is just the sum of $V_1$ and $V_2$.

These two simultaneous algebraic equations can readily be solved for most rate laws. We shall first consider the case of a first-order reaction:

$$-r_A = kC_A \tag{R14.2-3}$$

Let $\beta$ represent that fraction of the total flow that is exchanged between reactors 1 and 2:

$$v_1 = \beta v_0 \quad \text{(R14.2-4)}$$

and let $\alpha$ represent that fraction of the total volume *V* occupied by the highly
agitated region:

Two parameters: $\alpha$ and $\beta$

$$V_1 = \alpha V \quad \text{(R14.2-5)}$$

Then

$$V_2 = (1 - \alpha)V \quad \text{(R14.2-6)}$$

The space-time is

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

With these specifications the balance on reactor 2 becomes

$$\beta v_0 C_{A1} - \beta v_0 C_{A2} - (1 - \alpha)VkC_{A2} = 0 \quad \text{(R14.2-7)}$$

Solving for $C_{A2}$ gives us

$$C_{A2} = \frac{\beta C_{A1}}{\beta + (1 - \alpha)\tau k} \quad \text{(R14.2-8)}$$

Substituting this value for $C_{A2}$ into the mole balance on reactor 1, Equation (R14.1-1) yields

$$v_0 C_{A0} + \beta v_0 \frac{\beta C_{A1}}{\beta + (1 - \alpha)\tau k} - v_0 C_{A1} - \beta v_0 C_{A1} - kC_{A1}\alpha V = 0 \quad \text{(R14.2-9)}$$

Solving for $C_{A1}$ we have

$$C_{A1} = \frac{C_{A0}}{1 + \beta + \alpha\tau k - \{\beta^2/[\beta + (1 - \alpha)\tau k\}} \quad \text{(R14.2-10)}$$

In terms of conversion,

Conversion for the two-CSTR model

$$X = 1 - \frac{C_{A1}}{C_{A0}} = \frac{(\beta + \alpha\tau k)[\beta + (1 - \alpha)\tau k] - \beta^2}{(1 + \beta \quad \alpha\tau k)[\beta + (1 - \alpha)\tau k] - \beta^2} \quad \text{(R14.2-11)}$$

For large values of the product $\tau k$,

$$C_{A1} \cong \frac{C_{A0}}{1 + \beta \quad \alpha\tau k \quad 0} \cong \frac{C_{A0}}{\alpha\tau k} \qquad \text{(R14.2-12)}$$

we observe that the exit concentration is a function of the relative sizes of the reactor volumes but not of the fluid exchanged between the two volumes. This statement will also be true for the case where. $\beta \gg (1-\alpha)\tau k$. For small values of the product $\tau k$,

$$C_{A1} \cong \frac{C_{A0}}{1 + \beta + 0 - \beta^2/\beta} = C_{A0} \qquad \text{(R14.2-13)}$$

Limiting situations

which shows the consistency of our equation. If $\tau k$ is very small, we should expect no significant amount of reaction. Let's examine the case where the Damköhler number, $\tau k$, has an intermediate value, say $\tau k = 1$; then

$$\text{If } \alpha = 0.5, \beta = 0.5: \qquad \frac{C_{A1}}{C_{A0}} = 0.57 \,(43\% \text{ conversion})$$

$$\text{If } \alpha = 1.0, \beta = 0: \qquad \frac{C_{A1}}{C_{A0}} = 0.50 \,(50\% \text{ conversion})$$

We shall soon show how the two parameters $\alpha$ and $\beta$ may be determined from tracer tests.

Determination of the Parameters $\alpha$ and $\beta$.

In more complex models, unfortunately, the determination of the parameters in the model is not straightforward, and they usually must be calculated by nonlinear regression using the predicted tracer response curve directly. Exceptions do exist to this general rule, though: Consider, for example, the two-CSTRs-with-interchange model described earlier (shown in Figure R14.2-2 in simplified form). A mole balance on a tracer pulse injected at $t = 0$ for each of the tanks is

Unsteady-state balance of inert tracer

$$\text{accumulation} = \text{rate in} - \text{rate out}$$

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

$$\text{Reactor 2:} \qquad V_2 \frac{dC_{T2}}{dt} = v_1 C_{T1} - v_1 C_{T2}$$

Model system

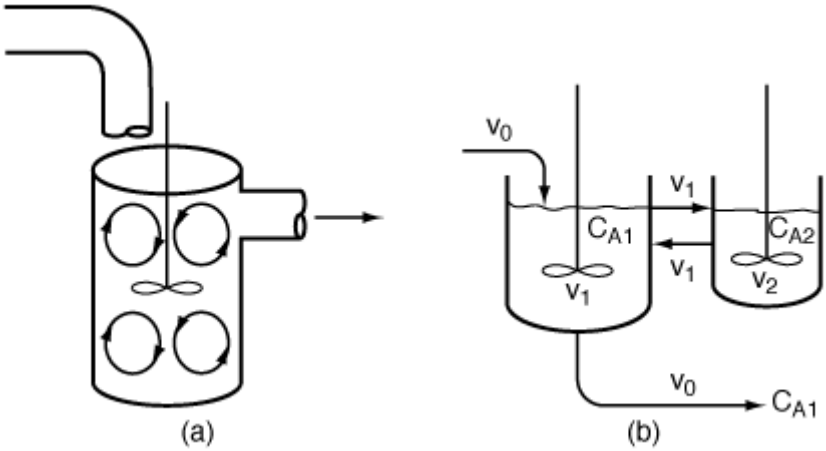


Figure R14.2-2
Model system: two CSTRs with interchange

$C_{T1}$ and $C_{T2}$ are the tracer concentrations in reactors 1 and 2, respectively, with $C_{T10} = N_{T0}/V_1$ and $C_{T20} = 0$. As before,

$$v_1 = \beta v_0 \qquad \text{(R14.2-4)}$$

$$V_1 = \alpha V$$

$$\theta = \frac{tv_0}{V} \qquad \text{(R14.2-5)}$$

Substituting, we arrive at two coupled differential equations describing the unsteady behavior of the tracer that must be solved simultaneously.

$$\alpha \frac{dC_{T1}}{d\theta} = \beta C_{T2} - (1+\beta) C_{T1} \qquad \text{(R14.2-14)}$$

$$(1-\alpha)\frac{dC_{T2}}{d\theta} = \beta C_{T1} - \beta C_{T2} \qquad \text{(R14.2-15)}$$

To obtain a solution, we first differentiate Equation (R14.2-14) with respect to u and then multiply through by (1 - $\alpha$) to get

$$\alpha(1-\alpha)\frac{d^2C_{T1}}{d\theta^2} = \beta\left[(1-\alpha)\frac{dC_{T2}}{d\theta}\right] - (1-\alpha)(1+\beta)\frac{dC_{T1}}{d\theta} \qquad \text{(R14.2-16)}$$

Substituting Equation (R14.2-15) for the bracketed term on the right-hand side gives us

$$\alpha(1-\alpha)\frac{d^2C_{T1}}{d\theta^2} = \beta(\beta C_{T1} - \beta C_{T2}) - (1-\alpha)(1+\beta)\frac{dC_{T1}}{d\theta} \qquad \text{(R14.2-17)}$$

The term $C_{T2}$ in Equation (R14.2-17) is eliminated by solving Equation (R14.2-14) for $\beta C_{T2}$:

(R14.2-

Solution technique commonly encountered in reactor modeling

$$\beta C_{T2} = \alpha \frac{dC_{T1}}{d\theta} + (1+\beta) C_{T1} \qquad (18)$$

Combining Equations (R14.2-17) and (R14.2-18) and rearranging, we get

$$\frac{\alpha(1-\alpha)}{1+\beta-\alpha}\left(\frac{d^2C_{T1}}{d\theta^2}\right) + \frac{dC_{T1}}{d\theta} + \frac{\beta}{1+\beta-\alpha} C_{T1} = 0 \qquad (R14.2\text{-}19)$$

which is of the form

$$a\frac{d^2C_{T1}}{d\theta^2} + b\frac{dC_{T1}}{d\theta} + cC_{T1} = 0$$

the solution to which is

$$C_{T1} = Ae^{m_1\theta} + Be^{m_2\theta}$$

$$m_1, m_2 = \frac{-b \quad \sqrt{b^2-4ac}}{2a}$$

For the problem at hand, the initial conditions at $\theta = 0$ are:

1. $C_{T1} = C_{T10}$
2. $C_{T20} = 0$; then, from Equation (CD14-26), we obtain
3. $\left(\frac{dC_{T1}}{d\theta}\right)_0 = -\frac{1+\beta}{\alpha} C_{T10}$

The corresponding solution for the tracer outlet concentration is

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

where

$$m_1, m_2 = \frac{1-\alpha+\beta}{2\alpha(1-\alpha)}\left[-1 \pm \sqrt{1 - \frac{4\alpha\beta(1-\alpha)}{(1-\alpha+\beta)^2}}\right] \qquad (R14.2\text{-}20)$$

Plot in $C_{T1}$ as a function of time find $\alpha$ and $\beta$

When tank 1 is rather small in comparison with tank 2 (small $\alpha$), and the rates of transfer between the two reactors are small (small $\beta$), then during the first portion of the response to a pulse input the second exponential term approximates to 1. During the second portion of the response, the first exponential term approximates to zero. If the logarithm of the tracer concentration is plotted as a function of time, the response curve will approach a straight line at the two ends of the curve, and the parameters may be obtained from the slopes and intercepts of these lines. This concept has been used in physiological systems.[2]

See Example R14-1.

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Fogler & Gurmen

# UNIT D

## Process Modelling and Simulation

# Real CSTR modeled using by passing and dead space

# 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

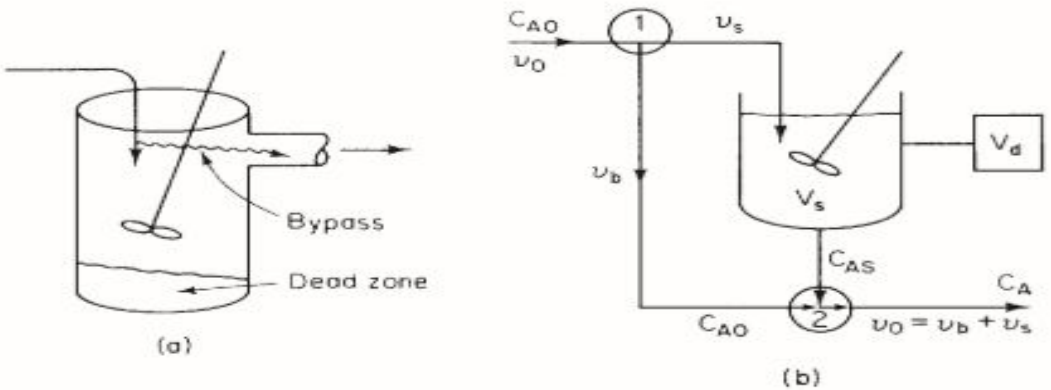


**Figure 18-1** (a) Real system; (b) model system.

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

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

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

Mole balance on CSTR

$$v_s C_{A0} - v_s C_{As} - kC_{As}V_s = 0 \tag{18-61}$$

or, in terms of $\alpha$ and $\beta$

$$C_{As} = \frac{C_{A0}(1-\beta)v_0}{(1-\beta)v_0 + \alpha V k} \tag{18-62}$$

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

Conversion as a function of model parameters

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

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## Real CSTR modelled using Bypassing and dead space.

A real CSTR is believed to be modelled 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 flowrate $v_b$.

Total volume $V_s$ and volumetric flowrates $v_s$ are known.

We can readily find $v_b$ and $V_d$

Solving for the concentration of A leaving the reactor.

$$v_0 C_A = v_b C_{A0} + C_{AS} v_s \quad \text{--- (a)}$$

$$C_A = \frac{v_b C_{A0} + C_{AS} v_s}{v_b + v_s} \quad (\text{as } v_0 = v_b + v_s)$$

Let $\alpha = \frac{V_s}{V}$ & $\beta = v_b / v_0$

$$C_A = \frac{v_b}{v_0} C_{A0} + \left(\frac{v_0}{v_0} - \frac{v_b}{v_0}\right) C_{AS}$$

$$C_A = \beta C_{A0} + (1-\beta) C_{AS} \quad \text{--- (1)}$$

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Applying mole balance on CSTR.

$$v_s C_{A0} - v_s C_{AS} - k C_{AS} V_s = 0.$$

$$(v_0 - v_b) C_{A0} - (v_s - v_b) C_{AS} - k C_{AS} V_s$$

$$(v_0 - v_b) C_{A0} = \left[(v_0 - v_b) + k V_s\right] C_{AS}.$$

$$C_{AS} = \frac{(v_0 - v_b) C_{A0}}{\left[(v_0 - v_b) + k \alpha V\right]}$$

multiplying and dividing the numerator and denominator by $v_0$

$$C_{AS} = \frac{(1-\beta) v_0 C_{A0}}{(1-\beta) v_0 + \alpha V k}. \quad \text{--- (2)}$$

from eq (2) writing $C_{A0}$ in terms of $C_{AS}$

$$C_{A0} = \frac{\left[(1-\beta) v_0 + \alpha V k\right] C_{AS}}{(1-\beta) v_0}$$

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also we know $\frac{V}{v_0} = \tau$.

∴ solving for conversion X.

$$\frac{C_A}{C_{A0}} = 1 - X = \frac{\beta C_{A0}}{C_{A0}} + (1-\beta)\frac{C_{AS}}{C_{A0}}.$$

$$\frac{C_A}{C_{A0}} = 1 - X = \beta + (1-\beta)\frac{C_{AS}}{\left[(1-\beta)v_0 + \alpha V K\right]C_{AS}}$$

$$\frac{C_{A0}}{C_{A0}} = \beta + \frac{(1-\beta)^2}{\left[(1-\beta) + \left(\alpha \frac{V}{v_0} K.\right)\right]}$$

$$1 - X = \beta + \frac{(1-\beta)^2}{(1-\beta) + \alpha\tau K.}$$

Notes

# Real CSTR modeled as two CSTRs with Interchange

### 18.7.2 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 18-16). 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 highly agitated region as one CSTR, the quieter region as another CSTR, with material transfer between the two.

The model system

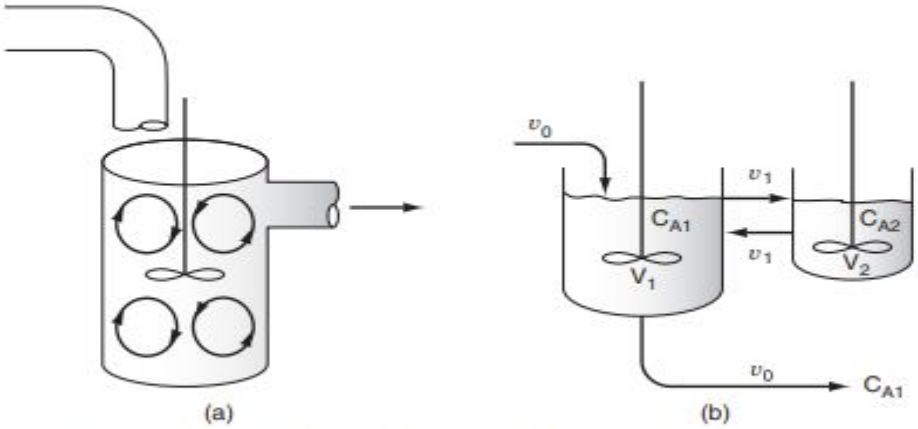


**Figure 18-16** (a) Real reaction system; (b) model reaction system.

#### *18.7.2A 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 $\alpha$ represent that fraction of the total volume, $V$, occupied by the highly agitated region:

Two parameters: $\alpha$ and $\beta$

$$V_1 = \alpha V$$

Then

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

The space time is

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

for a first-order reaction, the exit concentration and conversion are


$$C_{A1} = \frac{C_{A0}}{1 + \beta + \alpha\tau k - \{\beta^2/[\beta + (1 - \alpha)\tau k]\}} \tag{18-67}$$

and

Conversion for two-CSTR model

$$\boxed{X = 1 - \frac{C_{A1}}{C_{A0}} = \frac{(\beta + \alpha\tau k)[\beta + (1 - \alpha)\tau k] - \beta^2}{(1 + \beta + \alpha\tau k)[\beta + (1 - \alpha)\tau k] - \beta^2}} \tag{18-68}$$

where $C_{A1}$ is the reactor concentration exiting the first reactor in Figure 18-17(b).