University of Anbar

College of Engineering

Chemical and Petrochemical Engineering Department

Chemical Reacior Design

Third Year

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Lecture No. 8

C STEADY-STATE PLUG FLOW REACTOR:

$$\text{input} = \text{output} + \text{disappearance by reaction} + \overset{=0}{\cancel{\text{accumulation}}} \qquad \textbf{(10)}$$

Referring to Fig. 5.5, we see for volume dV that

input of A, moles/time = F_A

output of A, moles/time = $F_A + dF_A$

disappearance of A by reaction, moles/time = $(-r_A)dV$

$$= \left(\frac{\text{moles A reacting)}}{\text{(time)(volume of fluid)}}\right)\left(\begin{array}{c}\text{volume of}\\ \text{element}\end{array}\right)$$

Introducing these three terms in Eq. 10, we obtain

$$F_A = (F_A + dF_A) + (-r_A)dV$$

Noting that

$$dF_A = d[F_{A0}(1 - X_A)] = -F_{A0}dX_A$$

We obtain on replacement

$$F_{A0}dX_A = (-r_A)dV \qquad \textbf{(16)}$$

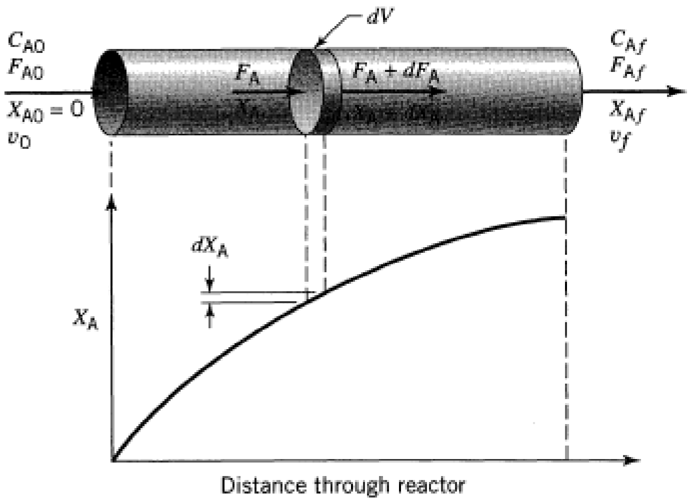

Figure 5.5 Notation for a plug flow reactor.

This, then, is the equation which accounts for A in the differential section of reactor of volume dV. For the reactor as a whole the expression must be integrated. Now F_{A0}, the feed rate, is constant, but r_A is certainly dependent on the concentration or conversion of materials. Grouping the terms accordingly, we obtain

$$\int_0^V \frac{dV}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

, Thus;

or

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{-r_A} \qquad \text{any } \varepsilon_A \qquad \textbf{(17)}$$

$$\frac{V}{F_{A0}} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

(18)

$$\tau = C_{A0}\int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

in which case the performance equation can be expressed in terms of concentrations, or

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}}\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A} \qquad \varepsilon_A = 0 \qquad \textbf{(19)}$$

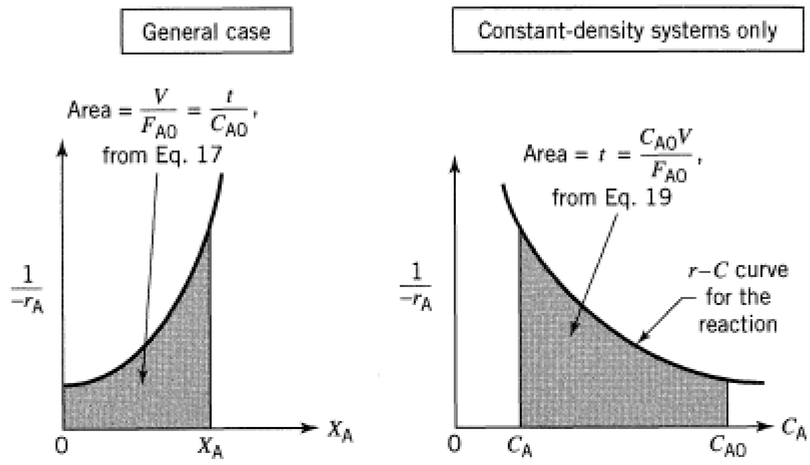

Figure 5.6 Graphical representation of the performance equations for plug flow reactors.

To do this, insert the kinetic expression for r_A in Eq. 17 and integrate. Some of the simpler integrated forms for ***plug flow*** are as follows:

Zero-order homogeneous reaction, any constant ε_A

$$k\tau = \frac{kC_{A0}V}{F_{A0}} = C_{A0}X_A \qquad \textbf{(20)}$$

First-order irreversible reaction, A → products, any constant ε_A,

$$\boxed{k\tau = -(1+\varepsilon_A)\ln(1-X_A) - \varepsilon_A X_A} \qquad \textbf{(21)}$$

First-order reversible reaction, $A \rightleftarrows rR$, $C_{R0}/C_{A0} = M$, kinetics approximated or fitted by $-r_A = k_1C_A - k_2C_R$ with an observed equilibrium conversion X_{Ae}, any constant ε_A,

$$k_1\tau = \frac{M + rX_{Ae}}{M + r}\left[-(1+\varepsilon_A X_{Ae})\ln\left(1 - \frac{X_A}{X_{Ae}}\right) - \varepsilon_A X_A\right] \qquad \textbf{(22)}$$

Second-order irreversible reaction, A + B → products with equimolar feed or 2A → products, any constant ε_A,

$$C_{A0}k\tau = 2\varepsilon_A(1+\varepsilon_A)\ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2\frac{X_A}{1-X_A} \qquad \textbf{(23)}$$

EXAMPLE 5.4 PLUG FLOW REACTOR PERFORMANCE

A homogeneous gas reaction A → 3R has a reported rate at 215°C

$$-r_A = 10^{-2}C_A^{1/2}, \qquad [\text{mol/liter}\cdot\text{sec}]$$

Find the space-time needed for 80% conversion of a 50% A–50% inert feed to a plug flow reactor operating at 215°C and 5 atm (C_{A0} = 0.0625 mol/liter).

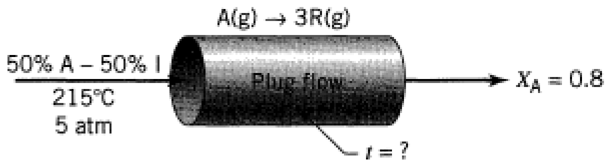

Figure E5.4*a*

SOLUTION

For this stoichiometry and with 50% inerts, two volumes of feed gas would give four volumes of completely converted product gas; thus

$$\varepsilon_A = \frac{4-2}{2} = 1$$

in which case the plug flow performance equation, Eq. 17, becomes

$$\tau = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{-r_A} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{kC_{A0}^{1/2}\left(\frac{1-X_A}{1+\varepsilon_A X_A}\right)^{1/2}} = \frac{C_{A0}^{1/2}}{k}\int_0^{0.8}\left(\frac{1+X_A}{1-X_A}\right)^{1/2} dX_A \qquad \textbf{(i)}$$

The integral can be evaluated in any one of three ways: graphically, numerically, or analytically. Let us illustrate these methods.

Table E5.4

X_A	$\dfrac{1+X_A}{1-X_A}$	$\left(\dfrac{1+X_A}{1-X_A}\right)^{1/2}$
0	1	1
0.2	$\frac{1.2}{0.8} = 1.5$	1.227
0.4	2.3	1.528
0.6	4	2
0.8	9	3

Graphical Integration. First evaluate the function to be integrated at selected values (see Table E5.4) and plot this function (see Fig. E5.4*b*).

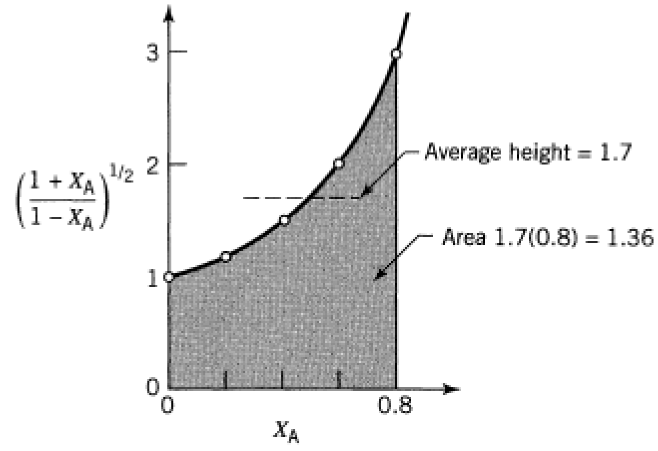

Figure E5.4*b*

Counting squares or estimating by eye we find

$$\text{Area} = \int_0^{0.8} \left(\frac{1+X_A}{1-X_A}\right)^{1/2} dX_A = (1.70)(0.8) = \underline{\underline{1.36}}$$

Numerical Integration. Using Simpson's rule, applicable to an even number of uniformly spaced intervals on the X_A axis, we find for the data of Table E5.4,

$$\int_0^{0.8} \left(\frac{1+X_A}{1-X_A}\right)^{1/2} dX_A = \text{(average height)(total width)}$$

$$= \left[\frac{1(1) + 4(1.227) + 2(1.528) + 4(2) + 1(3)}{12}\right](0.8)$$

$$= \underline{\underline{1.331}}$$

Analytical Integration. From a table of integrals

$$\int_0^{0.8} \left(\frac{1+X_A}{1-X_A}\right)^{1/2} dX_A = \int_0^{0.8} \frac{1+X_A}{\sqrt{1-X_A^2}} dX_A$$

$$= \left(\arcsin X_A - \sqrt{1-X_A^2}\right)\Big|_0^{0.8} = \underline{\underline{1.328}}$$

The method of integration recommended depends on the situation. In this problem probably the numerical method is the quickest and simplest and gives a good enough answer for most purposes.

So with the integral evaluated, Eq. (i) becomes

$$\underline{\underline{\tau}} = \frac{(0.0625 \text{ mol/liter})^{1/2}}{(10^{-2} \text{ mol}^{1/2}/\text{liter}^{1/2} \cdot \text{sec})}(1.33) = \underline{\underline{33.2 \text{ sec}}}$$