Ideal Reactors in Series

Plug flow reactors in series

$$\xrightarrow{C_{i-1}} \boxed{i} \xrightarrow{C_i} \boxed{i+1} \xrightarrow{C_{i+1}} \boxed{i+2} \xrightarrow{C_{i+2}} \cdots$$

$$\tau_i = \int_{C_{i-1}}^{C_i} \frac{dC_A}{r_A}, \quad \tau_{i+1} = \int_{C_i}^{C_{i+1}} \frac{dC_A}{r_A} \quad \cdots$$

$$\tau_{total} = \tau_i + \tau_{i+1} + \tau_{i+2} + \cdots \tau_n$$

$$= \int_{C_{i-1}}^{C_i} \frac{dC_A}{r_A} + \int_{C_i}^{C_{i+1}} \frac{dC_A}{r_A} + \cdots \int_{C_{n-1}}^{C_n} \frac{dC_A}{r_A}$$

$$= \int_{C_{i-1}}^{C_n} \frac{dC_A}{r_A}$$

$$\Rightarrow \tau_{total} = \sum \tau_i, \quad V_{total} = \sum V_i$$

$$K\tau_{total} = \sum K\tau_i$$

Multiple reactor systems

Plug flow

$$\tau = V/q = \int \frac{dc}{r}$$

$$\xrightarrow{C_0} \boxed{\;1\;} \xrightarrow{C_1} \boxed{\;2\;} \xrightarrow{C_2} \boxed{\;3\;} \xrightarrow{C_3}$$

$$\tau_1 = V_1/q = \int_{c_0}^{c_1} \frac{dc}{r}$$

$$\tau_2 = V_2/q = \int_{c_1}^{c_2} \frac{dc}{r}$$

$$\tau_3 = V_3/q = \int_{c_2}^{c_3} \frac{dc}{r}$$

$$\tau_{total} = \Sigma \tau_i = \frac{1}{q} \Sigma V_i = \int_{c_0}^{c_1} \frac{dc}{r} + \int_{c_1}^{c_2} \frac{dc}{r} + \int_{c_2}^{c_3} \frac{dc}{r}$$

$$= \int_{C_0}^{C_3} \frac{dc}{r}$$

For n reactors in series

$$\tau_{total} = \frac{1}{q} \sum_1^n V_i = \int_{C_0}^{C_n} \frac{dc}{r} = -C_0 \int_0^{x_n} \frac{dx}{r}$$

$\therefore$ Series of pfrs is simply additive.

1^{st} order

$$\tau = \frac{1}{k} \ln\left(\frac{1}{1-X}\right)$$

$$e^{\tau k} = \frac{1}{1-X} \Rightarrow X = 1 - e^{-\tau k}$$

for series pfr $\tau_{overall} = n\tau_i$

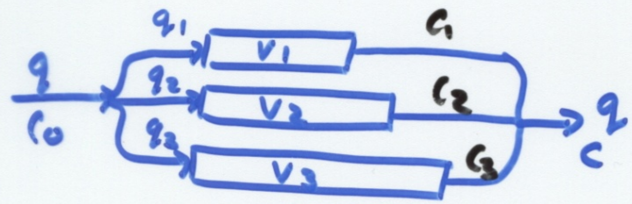
$$X_{overall} = 1 - e^{-n\tau_i k}$$

What about 2^{nd} order reactions?

pfr in parallel

1) X for each path must be the same
(any other system is less efficient)

2) Therefore, issue is how to split flows.



$\tau_1 = V_1/q_1 \qquad \tau_2 = V_2/q_2 \qquad \tau_3 = V_3/q_3$

for equal conversion, $\tau_1 = \tau_2 = \tau_3$

$$\frac{V_1}{q_1} = \frac{V_2}{q_2} = \frac{V_3}{q_3} \Rightarrow \quad q_2 = \frac{V_2}{V_1} q_1$$

$$q_3 = \frac{V_3}{V_1} q_1$$

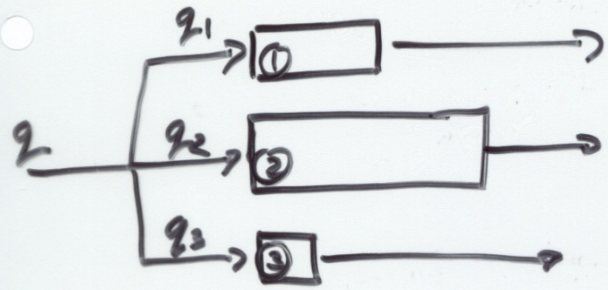
$$q = q_1 + \frac{V_2}{V_1} q_1 + \frac{V_3}{V_1} q_1 = \left(1 + \frac{V_2}{V_1} + \frac{V_3}{V_1}\right) q_1$$

∴ parallel pfrs must split flowrates in ratio to their volumes

general, n reactors in parallel

$$q = \left(1 + \Sigma \frac{V_i}{V_1}\right) q_1$$

3 reactors in parallel



$q = 1000\ \text{L/hr}$

$k = 0.5/\text{hr}$

$C_0 = 5\ \text{mol/L}$

$V_1 = 100\ \text{L}$

$V_2 = 500\ \text{L}$

$V_3 = 50\ \text{L}$

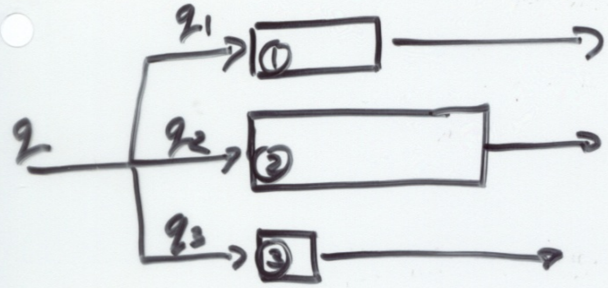
Split flow as

$$\left.\begin{aligned} q_1 &= 300\ \text{L/hr} \\ q_2 &= 500\ \text{L/hr} \\ q_3 &= 200\ \text{L/hr} \end{aligned}\right\} \Sigma = 1000\ \text{L/hr}$$

$X = 1 - e^{-k\tau}$

$X q C_0$ = total mols product

3 reactors in parallel



$q = 1000\ L/hr$

$k = 0.5/hr$

$C_0 = 5\ mol/L$

$V_1 = 100\ L$

$V_2 = 500\ L$

$V_3 = 50\ L$

Split flow as
$$\left.\begin{aligned} q_1 &= 300\ L/hr \\ q_2 &= 500\ L/hr \\ q_3 &= 200\ L/hr \end{aligned}\right\} \Sigma = 1000\ L/hr$$

$X = 1 - e^{-k\tau}$ $\qquad$ $X q C_0$ = total mols product

$\tau_1 = \frac{100}{300} = 0.3333$ $\qquad$ $\tau_2 = \frac{500}{500} = 1$ $\qquad$ $\tau_3 = \frac{50}{200} = 0.25$

$X_1 = 0.1535$ $\qquad$ $X_2 = 0.3935$ $\qquad$ $X_3 = 0.1175$

230.25 $\qquad$ 983.75 $\qquad$ 117.5

$$\frac{1331.5}{(5)(1000)} = 0.2663 = X_{net}$$

$$q = \left(1 + \frac{500}{100} + \frac{50}{100}\right) q_1 = 6.5\, q_1$$

$$q_1 = \frac{q}{6.5} = \frac{1000}{6.5} = 153.85\ L/hr$$

$$q_2 = \frac{500}{100} q_1 = 769.23\ L/hr$$

$$q_3 = 76.92\ L/hr$$

$$q_1 + q_2 + q_3 = 1000\ L/hr \checkmark$$

$$\tau_1 = \frac{100}{153.85} = \tau_2 = \frac{500}{769.23} = \tau_3 = \frac{50}{76.92}$$

$$= 0.65$$

$$X = 1 - e^{-k\tau} = \underline{\underline{0.2775}}$$

overall conversion

Better conversion by having equal τ

The reactor setup shown in Fig. E6.1 consists of three plug flow reactors in two parallel branches. Branch D has a reactor of volume 50 liters followed by a reactor of volume 30 liters. Branch E has a reactor of volume 40 liters. What fraction of the feed should go to branch D?

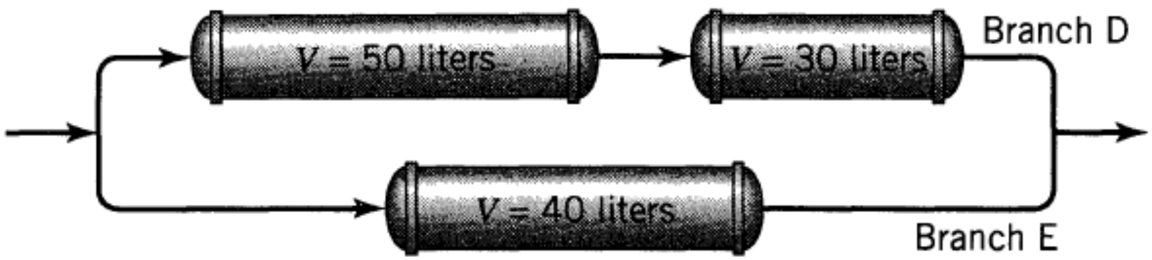


Figure E6.1

Branch D consists of two reactors in series; hence, it may be considered to be a single reactor of volume

$$V_D = 50 + 30 = 80 \text{ liters}$$

Now for reactors in parallel V/F must be identical if the conversion is to be the same in each branch. Therefore,

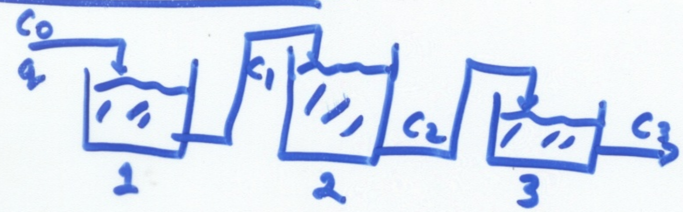
$$\left(\frac{V}{F}\right)_D = \left(\frac{V}{F}\right)_E$$

or

$$\frac{F_D}{\underline{\underline{F_E}}} = \frac{V_D}{V_E} = \frac{80}{40} = \underline{\underline{2}}$$

Therefore, two-thirds of the feed must be fed to branch D. $\blacksquare$

Mixedflow reactors



$q \Rightarrow$ cons't

$$\tau_i = \frac{C_{i-1} - C_i}{-r}$$

1^{st} order rxn, $-r = kC$

$$\tau_1 = \frac{C_0 - C_1}{kC_1} \Rightarrow \frac{C_0}{C_1} = 1 + k\tau_1$$

$$\tau_2 = \frac{C_1 - C_2}{kC_2} \Rightarrow \frac{C_1}{C_2} = 1 + k\tau_2$$

$$\tau_3 = \frac{C_2 - C_3}{kC_3} \Rightarrow \frac{C_2}{C_3} = 1 + k\tau_3$$

$$\left(\frac{C_0}{C_1}\right)\left(\frac{C_1}{C_2}\right)\left(\frac{C_2}{C_3}\right) = (1 + k\tau_1)(1 + k\tau_2)(1 + k\tau_3)$$

$$C_0/C_3 = \prod_{1}^{3} (1 + k\tau_i)$$

For equal volume mfr, $\tau_1 = \tau_2 = \tau_3 = \dots \tau_n$

$$C_0/C_n = (1 + k\tau_i)^n$$

$$\Rightarrow \tau_i = \frac{1}{k}\left[\left(\frac{C_0}{C_n}\right)^{1/n} - 1\right]$$

$$\tau_{overall} = n\tau_i = \frac{n}{k}\left[\left(\frac{C_0}{C_n}\right)^{1/n} - 1\right]$$

$$= \frac{n}{k}\left[\left(\frac{1}{1-x}\right)^{1/n} - 1\right]$$

Note: As $n \to \infty$, $n\left[\left(\frac{C_0}{C_n}\right)^{1/n} - 1\right] \to \ln C_0/C_n$

$\Rightarrow \tau_{overall} \to \frac{1}{k}\ln(C_0/C) \Rightarrow$ pfr

8 MFR in series

All same volume, $V = 10L$

$v = 1\ L/hr$, $C_0 = 10\ mol/L$, $k = 0.04\ \frac{1}{hr}$

What is overall conversion?

What are intermediate concentrations?

1st order rxn

$$C_1 = \frac{C_0}{1 + k\tau} \qquad k\tau = (.04)\left(\frac{10}{10}\right) = 0.4$$

$$\text{So, } C_1 = \frac{C_0}{1 + .4} = \frac{10}{1.4} = \underline{\underline{7.1429}}\ mol/L$$

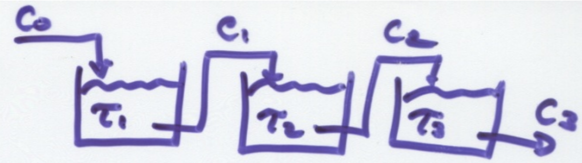
$$C_2 = \frac{C_1}{1 + 0.4} = \frac{7.1249}{1.4} = \underline{\underline{5.102}}\ mol/L$$

etc.

$$C_8 = \frac{C_0}{(1 + k\tau)^n} = \frac{C_0}{(1 + 0.4)^8} = 0.6776\ \frac{mol}{L}$$

$$X = \frac{C_0 - C_8}{C_0} = \underline{\underline{0.9322}}$$

MFR in Series



Zero order rxn

$$\frac{k\tau}{C_0} = \frac{C_0 - C}{C_0} = X$$

re-arranging

$$C = C_0 - k\tau$$

For reactor 1

$$C_1 = C_0 - k\tau_1$$

For reactor 2

$$C_2 = C_1 - k\tau_2 = C_0 - k\tau_1 - k\tau_2$$

For reactor 3

$$C_3 = C_2 - k\tau_3 = C_1 - k\tau_2 - k\tau_3 = C_0 - k\tau_1 - k\tau_2 - k\tau_3$$

In general

$$C_n = C_0 - \Sigma k\tau_i$$

If τ all the same,

$$C_n = C_0 - nk\tau$$

MFR in Series

1^{st} order rxn

$$k\tau = \frac{C_0 - C}{C} \Rightarrow C = \frac{C_0}{1+k\tau}$$

So,

$$C_1 = \frac{C_0}{1+k\tau_1}$$

$$C_2 = \frac{C_1}{1+k\tau_2} = \frac{C_0}{(1+k\tau_1)(1+k\tau_2)}$$

$$C_3 = \frac{C_2}{1+k\tau_3} = \frac{C_0}{(1+k\tau_1)(1+k\tau_2)(1+k\tau_3)}$$

In general,

$$C_n = \frac{C_0}{\Pi(1+k\tau_i)}$$

If all τ are the same

$$C_n = \frac{C_0}{(1+k\tau)^n}$$

mfr

2nd order $r = -kC^2$ equal volume $\Rightarrow \tau$

$$\tau = \frac{C_0 - C_1}{kC_1^2} \Rightarrow k\tau C_1^2 + C_1 - C_0 = 0$$

$$C_1 = \frac{-1 + \sqrt{1 + 4\tau k C_0}}{2\tau k}$$

$$= \frac{1}{4\tau k}\left(-2 + 2\sqrt{1 + 4\tau k C_0}\right)$$

$$\tau = \frac{C_1 - C_2}{kC_2^2} \Rightarrow C_2 = \frac{1}{4\tau k}\left(-2 + 2\sqrt{1 + 4\tau k C_1}\right)$$

$$C_2 = \frac{1}{4\tau k}\left(-2 + 2\sqrt{1 + 4\tau k\left(\frac{1}{4\tau k}\left(-2 + 2\sqrt{1 + 4\tau k C_0}\right)\right)}\right)$$

$$= \frac{1}{4\tau k}\left(-2 + 2\sqrt{-1 + 2\sqrt{1 + 4\tau k C_0}}\right)$$

$$C_3 = \frac{1}{4\tau k}\left(-2 + 2\sqrt{1 + 4\tau k C_2}\right)$$

$$= \frac{1}{4\tau k}\left(-2 + 2\sqrt{1 + \left(-2 + 2\sqrt{-1 + 2\sqrt{1 + 4\tau k C_0}}\right)}\right)$$

$$= \frac{1}{4\tau k}\left(-2 + 2\sqrt{-1 + 2\sqrt{-1 + 2\sqrt{1 + 4\tau k C_0}}}\right)$$

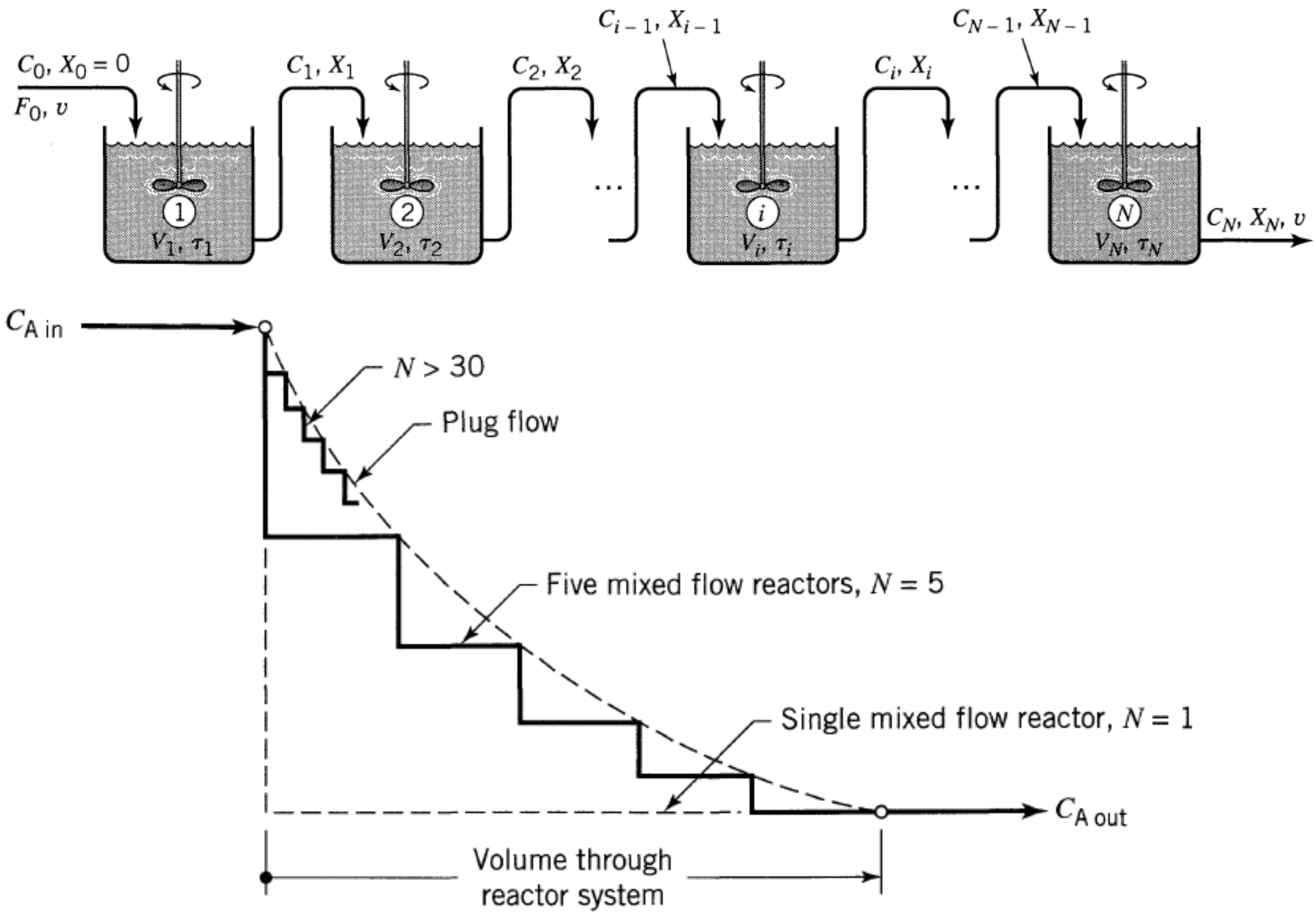


Figure 6.3 Concentration profile through an N-stage mixed flow reactor system compared with single flow reactors.

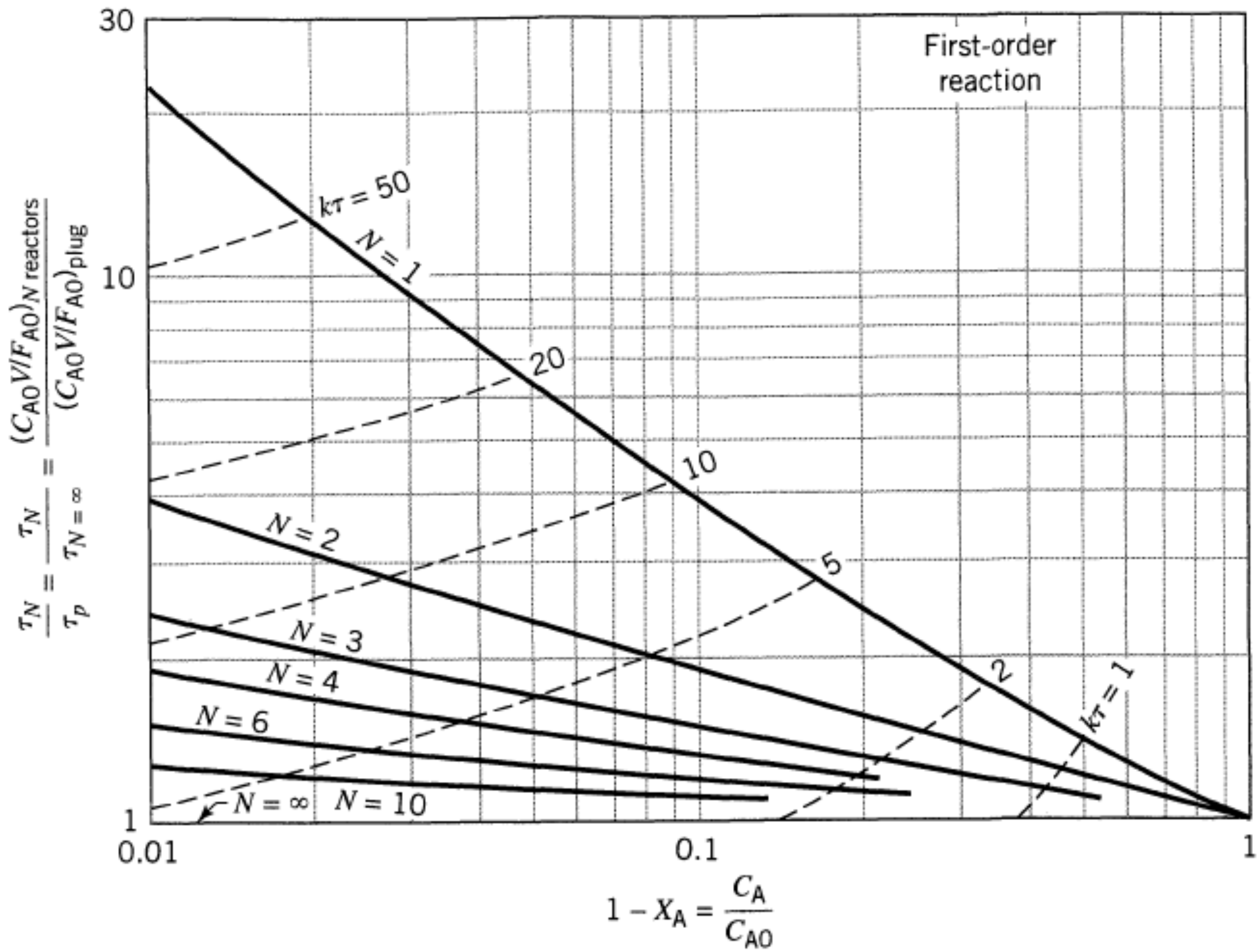


Figure 6.5 Comparison of performance of a series of N equal-size mixed flow reactors with a plug flow reactor for the first-order reaction

$$A \rightarrow R, \qquad \varepsilon = 0$$