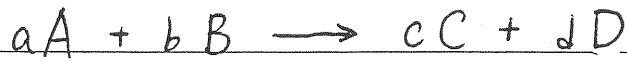


Chapter 2 Conversion and Reactor Sizing

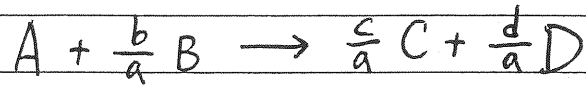
2.1 Definition of Conversion



choose the limiting reactant for calculating conversion

take A as the basis for calculation

有可能完全反应者



"How far the rxn has progressed?" $\xrightarrow{\text{answer}}$ Conversion

define

$$X_A \equiv \frac{\text{moles of A reacted}}{\text{moles of A fed}} \quad (\equiv X)$$

2.2 Design Equations for Batch Reactors

[moles of A at time t] [initial] [reacted]

$$\begin{aligned} N_A &= N_{A0} - N_{A0}X \\ &= N_{A0}(1-X) \end{aligned}$$

design eq.

$$\frac{dN_A}{dt} = r_A V \quad \text{or} \quad -\frac{dN_A}{dt} = -r_A V$$

\swarrow $N_{A0} - N_{A0}X$

$$\therefore \boxed{N_{A0} \frac{dX}{dt} = -r_A \cdot V} \quad \text{differential form of design eq.}$$

special case

Const-V BR

$$N_A = N_{A0}(1-X)$$

$$\Rightarrow \frac{N_A}{V} = \frac{N_{A0}}{V}(1-X)$$

$$\Rightarrow C_A = C_{A0}(1-X) \text{ --- --- ---}$$

also $-r_A = -\frac{1}{V} \frac{dN_A}{dt} \Rightarrow -r_A = -\frac{dC_A}{dt} \text{ --- --- ---}$ } Const-V F

or

$$-r_A = C_{A0} \frac{dX}{dt} \text{ ---}$$

varying-V BR

X vs. t

if $V = V(t)$

$$V dt = N_{A0} \frac{dX}{-r_A} \Rightarrow$$

$$\int_0^t V dt = N_{A0} \int_0^X \frac{dX}{-r_A}$$

integral form of
design eq.

or

if $V = V(X)$

$$dt = N_{A0} \frac{dX}{-r_A \cdot V} \Rightarrow$$

$$t = N_{A0} \int_0^X \frac{dX}{-r_A \cdot V}$$

2.3 Design Equations for Flow Reactors

$$\begin{array}{l} \text{[mole rate} \\ \text{leaving the system]} \end{array} = \begin{array}{l} \text{[mole rate]} \\ \text{[fed]} \end{array} - \begin{array}{l} \text{[mole rate} \\ \text{consumed in system]} \end{array}$$

$$F_A = F_{A0} - F_{A0}X$$

$$= F_{A0}(1-X)$$

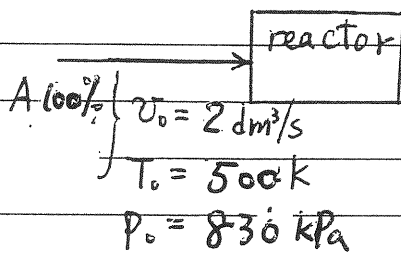
$$F_{A0} = C_{A0} v_0, \quad F_A = C_A \cdot v$$

$$P_A v = F_A RT \quad \text{for ideal gas flow} \quad \frac{F_A}{v} = \frac{P_A}{RT} \quad \text{mole fraction}$$

$$\therefore C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0} P_0}{RT_0} \quad \text{total } P$$

$$F_{A0} = v_0 \frac{y_{A0} P_0}{RT_0}$$

Ex 2-1



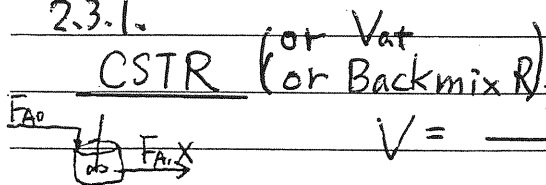
$$R = 0.082 \text{ dm}^3 \cdot \text{atm} / \text{mol} \cdot \text{K} \\ = 8.314 \text{ dm}^3 \text{ kPa} / \text{mol} \cdot \text{K}$$

calculate C_{A0} , F_{A0}

$$\text{Sol.} \quad C_{A0} = \frac{\frac{F_{A0}}{v_0} y_{A0} P_0}{RT_0} = \frac{(1)(830 \text{ kPa})}{(8.314 \frac{\text{dm}^3 \text{ kPa}}{\text{mol K}})(500 \text{ K})} = 0.20 \frac{\text{mol}}{\text{dm}^3}$$

$$F_{A0} = C_{A0} \cdot v_0 = (0.20)(2) = 0.4 \text{ mol/s} \quad *$$

2.3.1.

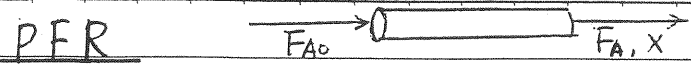


$$V = \frac{F_{A0} - F_A}{-r_A}$$

$$F_A = F_{A0} - F_{A0} X$$

$$\rightarrow \quad V = \frac{F_{A0} X}{(-r_A)_{\text{exit}}}$$

2.3.2.



$$-\frac{dF_A}{dV} = -r_A \quad F_A = F_{A0} - F_{A0}X$$

$$\therefore F_{A0} \frac{dX}{dV} = -r_A$$

$$\Rightarrow V = F_{A0} \int_0^X \frac{dX}{-r_A}$$

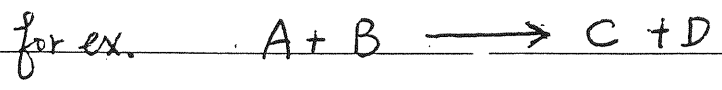
2.3.3. PBR

similar to PFR

$$F_{A0} \frac{dX}{dW} = -r_A'$$

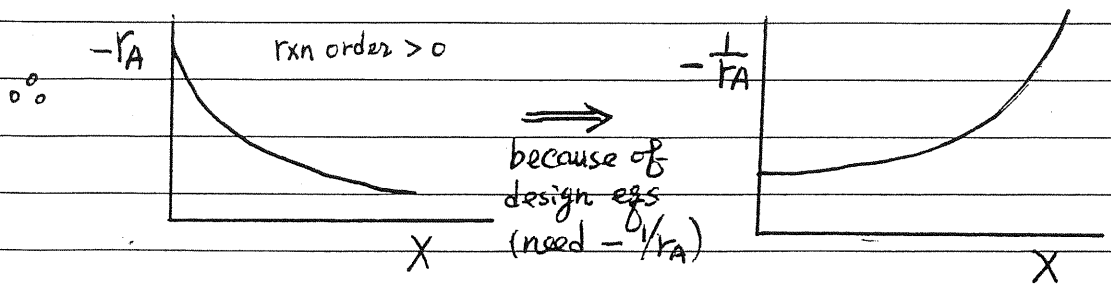
$$W = F_{A0} \int_0^X \frac{dX}{-r_A'}$$

2.4 Applications of Design Equations



at specified C_{A0}, C_{B0}, \dots

$$-r_A = f(C_A, C_B, \dots, T, P) \text{ or } -r_A = f(X, T, P)$$



$$-\frac{1}{r_A} \rightarrow \infty \text{ as } X \rightarrow 1$$

Ex 2-2 Sizing a CSTR

a rxn $\rightarrow = f(X)$ at specified C_{A0}
 $-r_A \approx k C_{A0} (1-X)$

lab. exp.
 With specified conditions

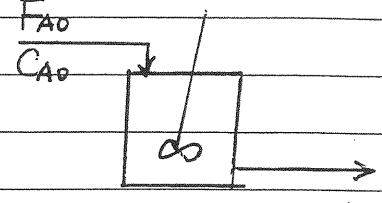
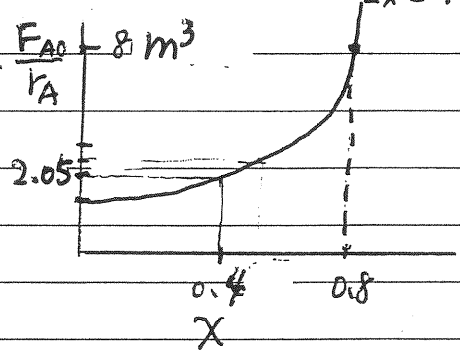


Figure 2-2

Table 2.3

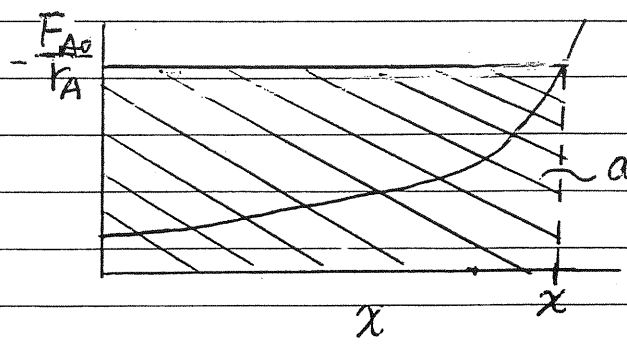
to achieve 80% conversion in a CSTR, $V = ?$

Sol.

$$V = \frac{F_{A0} X}{-r_A} = (0.4 \frac{\text{mol}}{\text{s}})(0.8) \cdot (20 \frac{\text{m}^3 \cdot \text{s}}{\text{mol}})$$

$$= [8 \text{ m}^3][0.8] = 6.4 \text{ m}^3$$

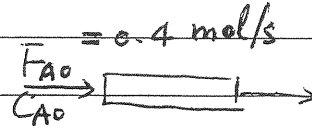
in fact, $V = (-\frac{F_{A0}}{r_A})(X)$



area = $\frac{F_{A0} X}{-r_A}$

$\therefore V = \text{area}$

Ex 2-3 sizing a PFR

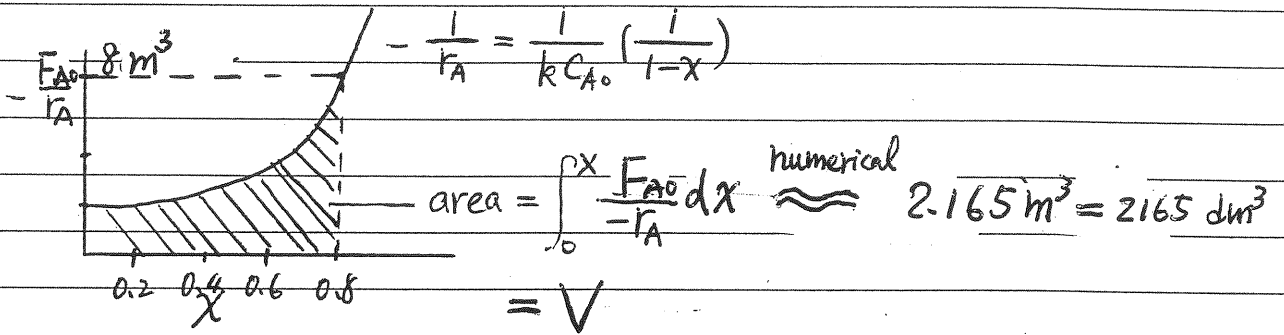


Same rxn in Ex 2-2

to achieve 80% conversion in a PFR, $V = ?$

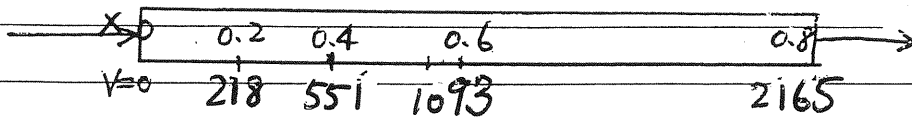
Sol.

$$V = F_{A0} \int_0^X \frac{dx}{-r_A}$$



可任意指定 Conv., find required V (由 shaded area or 積分式)

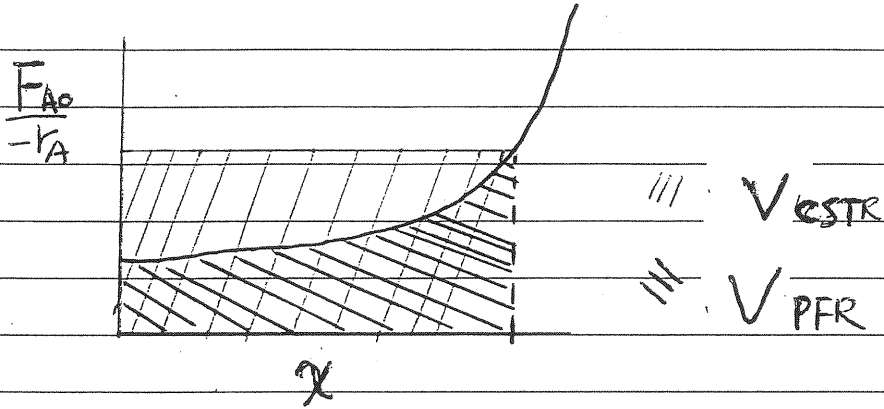
X =	0	0.2	0.4	0.6	0.8
V (dm ³)	0	218	551	1093	2165



$$C_A = C_{A0}(1-X)$$

Ex 2-4 Comparing CSTR and PFR sizes

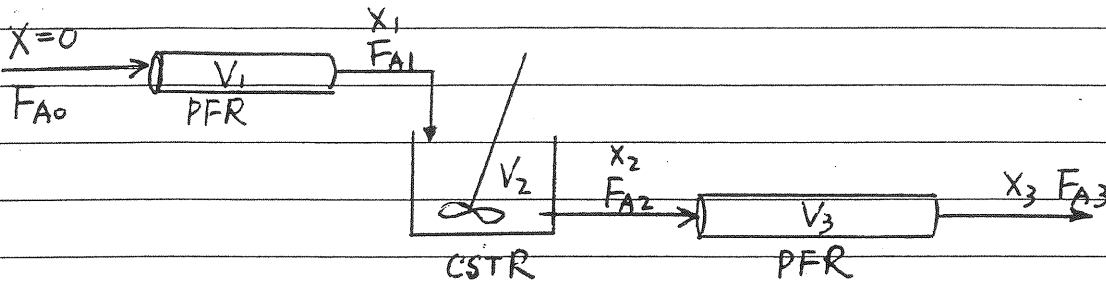
在相同的 feed conditions, 且到達某一 Conversion 時



∴ for isothermal rxns of greater than zero order,
to achieve the same conversion, $V_{PFR} < V_{CSTR}$

2.5 Reactors in Series (no side stream flows in or out)

ex.



Reactors in series 時, 全1st reactor 進料為 $X=0$ 較利於計算

∴ $X_1 =$ similar

$X_2 = \frac{\text{total moles of A reacted up to point 2}}{\text{moles of A fed to first reactor}}$

$X_3 =$ similar

∴ $F_{A1} = F_{A0} - F_{A0}X_1$

$F_{A2} = F_{A0} - F_{A0}X_2$

$F_{A3} = F_{A0} - F_{A0}X_3$

Reactor 1

$$\frac{-dF_A}{dV} = -r_A \Rightarrow F_{A0} \frac{dX}{dV} = -r_A \Rightarrow$$

$$V_1 = F_{A0} \int_0^{X_1} \frac{dX}{-r_A}$$

Reactor 2

mol bal. $F_{A1} + r_{A2}V_2 - F_{A2} = 0$

$$\Rightarrow V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} \Rightarrow$$

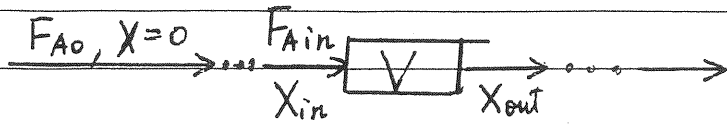
$$V_2 = \frac{F_{A0}(X_2 - X_1)}{-r_{A2}}$$

Reactor 3

$$F_{A0} \frac{dX}{dV} = -r_A \Rightarrow$$

$$V_3 = F_{A0} \int_{X_2}^{X_3} \frac{dX}{-r_A}$$

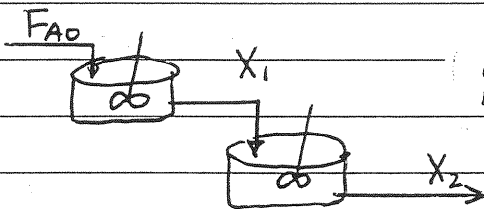
General Cases for reactors in series

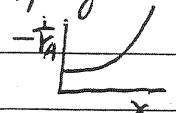


$$V = \frac{F_{A0}(X_{out} - X_{in})}{-r_{A,out}} \quad \text{for CSTR}$$

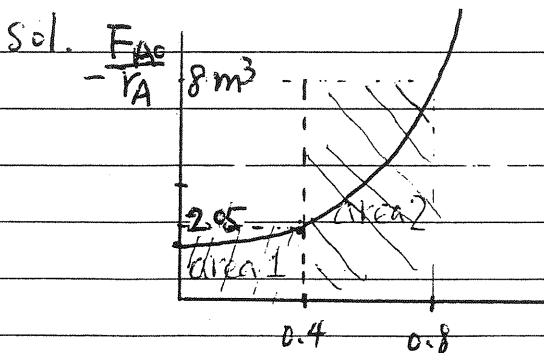
$$V = F_{A0} \int_{X_{in}}^{X_{out}} \frac{dX}{-r_A} \quad \text{for PFR}$$

Ex 2-5



$0.4 \text{ mol/s} = \frac{C_{A0}}{r_{X1}}$ } same as in Ex 2-1, Fig 2-1


if $X_1 = 0.4$, $X_2 = 0.8$, total volume of reactors = ?



$$V_1 = F_{A0} \cdot (X_1 - X_0) \cdot \frac{1}{-r_{A1}} = \text{(area 1)}$$

$$= (2.05)(0.4 - 0) = 0.82 \text{ m}^3$$

$$= 820 \text{ dm}^3$$

if one CSTR used

$$V_2 = F_{A0} \cdot (X_2 - X_1) \cdot \frac{1}{-r_{A2}} = \text{(area 2)}$$

$$= (8.0)(0.8 - 0.4) = 3.2 \text{ m}^3$$

$$= 3200 \text{ dm}^3$$

$$V = F_{A0}(X) \left(\frac{1}{-r_A} \right) = \text{(area of square)}_{0.8}$$

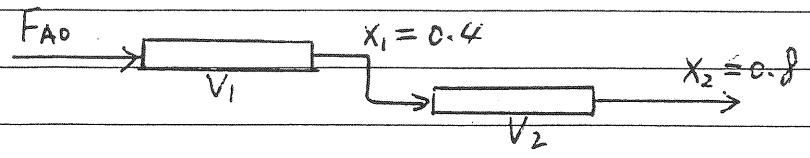
$$= (8.0)(0.8) = 6.4 \text{ m}^3$$

$$= 6400 \text{ dm}^3$$

$$V_1 + V_2 = V_{total} = 4020 \text{ dm}^3 = 4.02 \text{ m}^3$$

∴ to achieve same conv., $V_{\text{CSTR in series}} < V_{\text{one CSTR}}$.

Ex 2-6
for two PFRs in series



$$V_1 = F_{A0} \int_0^{x_1=0.4} \frac{dx}{-r_A} = 551 \text{ dm}^3$$

$$V_2 = F_{A0} \int_{x_1}^{x_2=0.8} \frac{dx}{-r_A} = 1614 \text{ dm}^3$$

Simpson's rule

(numerical method)
Appendix A.4

$$\int_{x_0}^{x_2} f(x) dx$$

$$\approx \frac{\Delta X}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$

$$\Delta X = \frac{x_2 - x_0}{2}$$

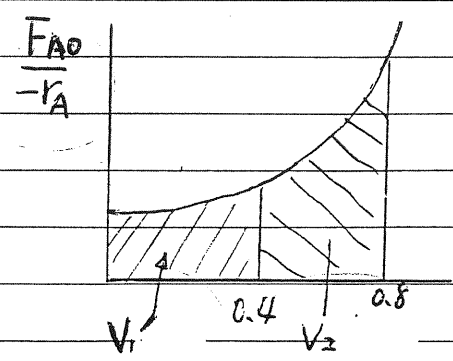
$$x_1 = x_0 + \Delta X$$

$$V_{\text{total}} = V_1 + V_2 = 2165 \text{ dm}^3$$

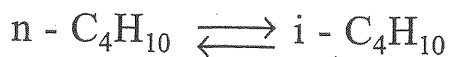
as a matter of fact

$$F_{A0} \int_0^{x_1} \frac{dx}{-r_A} + F_{A0} \int_{x_1}^{x_2} \frac{dx}{-r_A} = F_{A0} \int_0^{x_2} \frac{dx}{-r_A}$$

same as one PFR



The isomerization of butane



was carried out adiabatically in the liquid phase and the data in Table E2-7.1 were obtained. (Example 8.4 shows how the data in Table E2-7.1 were generated.)

TABLE E2-7.1 RAW DATA

X	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m ³ · h)	39	53	59	38	25

Don't worry how we got this data or why the $(1/-r_A)$ looks the way it does, we will see how to construct this table in Chapter 8. It is *real data* for a *real reaction* carried out adiabatically, and the reactor scheme shown in Figure E2-7.1 is used.

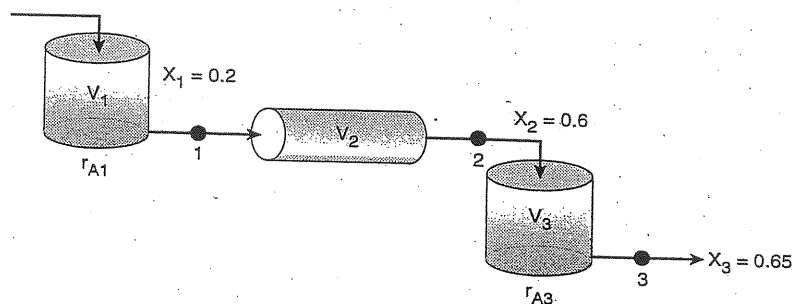


Figure E2-7.1 Reactors in series.

Calculate the volume of each of the reactors for an entering molar flow rate of n-butane of 50 kmol/hr.

Solution

Taking the reciprocal of $-r_A$ and multiplying by F_{A0} we obtain Table E2-7.2.

$$\text{E.g., at } X = 0: \frac{F_{A0}}{-r_A} = \frac{50 \text{ kmol/h}}{39 \text{ kmol/h} \cdot \text{m}^3} = 1.28 \text{ m}^3$$

TABLE E2-7.2 PROCESSED DATA

X	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m ³ · h)	39	53	59	38	25
$[F_{A0}/-r_A]$ (m ³)	1.28	0.94	0.85	1.32	2.0

(a) For the first CSTR,
when $X = 0.2$, then $\frac{F_{A0}}{-r_A} = 0.94 \text{ m}^3$

$$V_1 = \frac{F_{A0}}{-r_A} X_1 = (0.94 \text{ m}^3)(0.2) = 0.188 \text{ m}^3 \quad (\text{E2-7.1})$$

$$\boxed{V_1 = 0.188 \text{ m}^3 = 188 \text{ dm}^3} \quad (\text{E2-7.2})$$

(b) For the PFR,

$$V_2 = \int_{0.2}^{0.6} \left(\frac{F_{A0}}{-r_A} \right) dX$$

Using Simpson's three-point formula with $\Delta X = (0.6 - 0.2)/2 = 0.2$, and $X_1 = 0.2$, $X_2 = 0.4$, and $X_3 = 0.6$.

$$\begin{aligned} V_2 &= \int_{0.2}^{0.6} \frac{F_{A0}}{-r_A} dX = \frac{\Delta X}{3} \left[\left(\frac{F_{A0}}{-r_A} \right)_{X=0.2} + 4 \left(\frac{F_{A0}}{-r_A} \right)_{X=0.4} + \left(\frac{F_{A0}}{-r_A} \right)_{X=0.6} \right] \\ &= \frac{0.2}{3} [0.94 + 4(0.85) + 1.32] \text{m}^3 \end{aligned} \quad (\text{E2-7.3})$$

$$\boxed{V_2 = 0.38 \text{ m}^3 = 380 \text{ dm}^3} \quad (\text{E2-7.4})$$

(c) For the last reactor and the second CSTR, mole balance on A for the CSTR:

$$\text{In} - \text{Out} + \text{Generation} = 0$$

$$F_{A2} - F_{A3} + r_{A3} V_3 = 0 \quad (\text{E2-7.5})$$

Rearranging

$$V_3 = \frac{F_{A2} - F_{A3}}{-r_{A3}} \quad (\text{E2-7.6})$$

$$F_{A2} = F_{A0} - F_{A0} X_2$$

$$F_{A3} = F_{A0} - F_{A0} X_3$$

$$V_3 = \frac{(F_{A0} - F_{A0} X_2) - (F_{A0} - F_{A0} X_3)}{-r_{A3}}$$

Simplifying

$$\boxed{V_3 = \left(\frac{F_{A0}}{-r_{A3}} \right) (X_3 - X_2)} \quad (\text{E2-7.7})$$

We find from Table E2-7.2 that at $X_3 = 0.65$, then $\frac{F_{A0}}{-r_{A3}} = 2.0 \text{ m}^3$

$$V_3 = 2 \text{ m}^3 (0.65 - 0.6) = 0.1 \text{ m}^3$$

$$V_3 = 0.1 \text{ m}^3 = 100 \text{ dm}^3$$

(E2-7.8)

A Levenspiel plot of $(F_{A0}/-r_A)$ vs. X is shown in Figure E2-7.2.

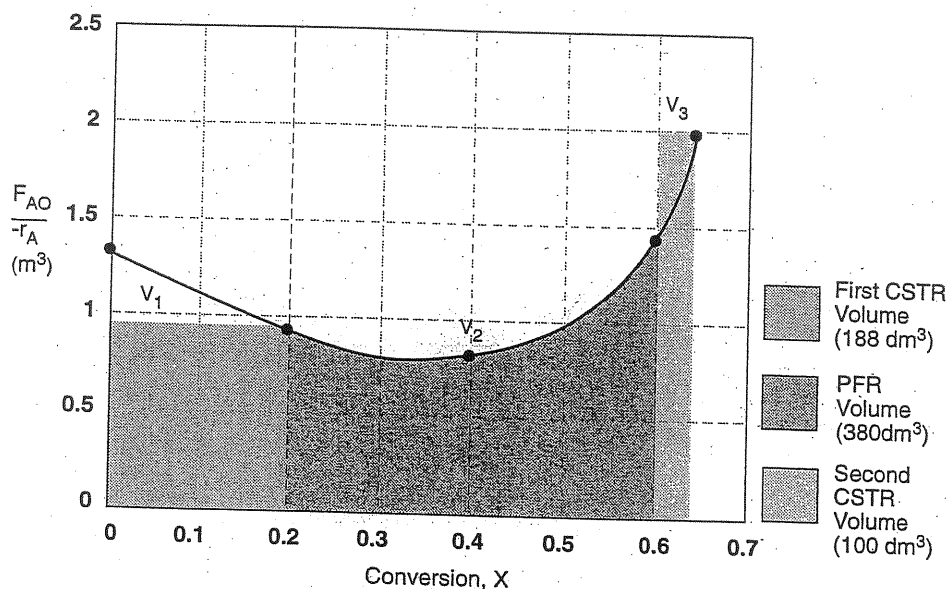


Figure E2-7.2 Levenspiel plot for adiabatic reactors in series.

2.5.4 Comparing the CSTR and PFR Reactor Volumes and Reactor Sequencing

If we look at Figure E2-7.2, the area under the curve (PFR volume) between $X = 0$ and $X = 0.2$, we see that the PFR area is greater than the rectangular area corresponding to the CSTR volume, i.e., $V_{\text{PFR}} > V_{\text{CSTR}}$. However, if we compare the areas under the curve between $X = 0.6$ and $X = 0.65$, we see that the

area under the curve (PFR volume) is smaller than the rectangular area corresponding to the CSTR volume, i.e., $V_{\text{CSTR}} > V_{\text{PFR}}$. This result often occurs when the reaction is carried out adiabatically, which is discussed when we look at heat effects in Chapter 8.

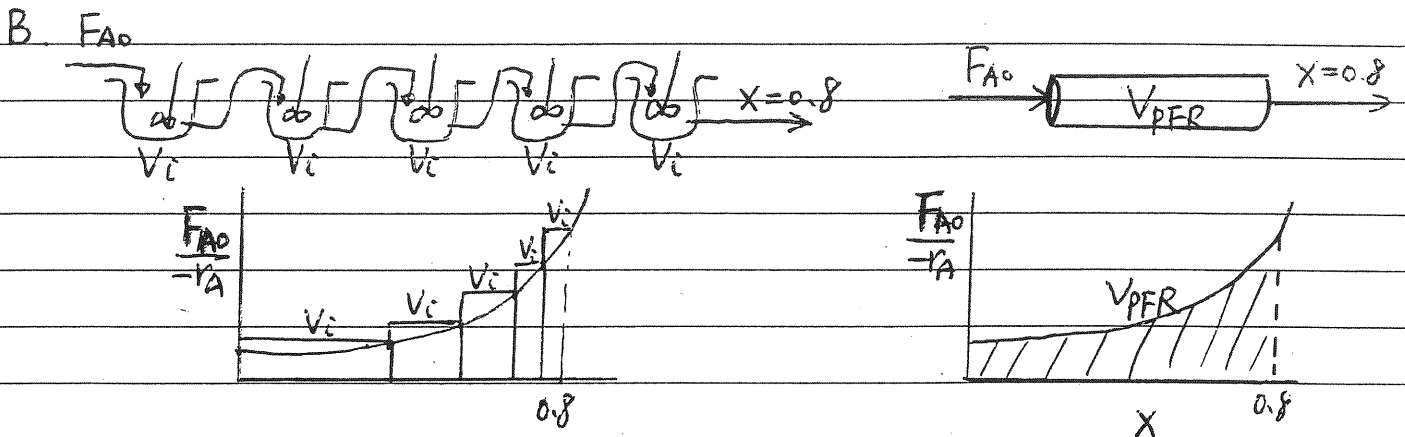
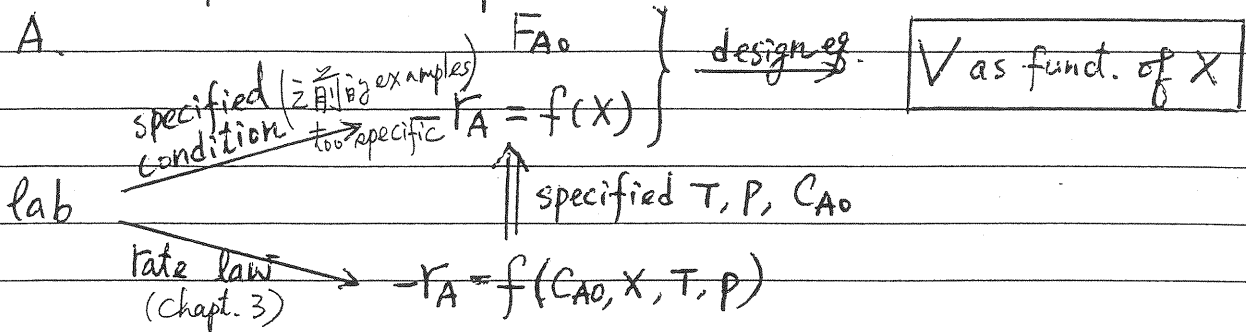
➤ In the *sequencing of reactors* one is often asked, "Which reactor should go first to give the highest overall conversion? Should it be a PFR followed by a CSTR, or two CSTRs, then a PFR, or ...?" The answer is "**It depends.**" It depends not only on the shape of the Levenspiel plots ($F_{A0}/-r_A$) versus X , but also on the relative reactor sizes. As an exercise, examine Figure E2-7.2 to learn if there is a better way to arrange the two CSTRs and one PFR. Suppose you were given a Levenspiel plot of ($F_{A0}/-r_A$) vs. X for three reactors in series along with their reactor volumes $V_{\text{CSTR1}} = 3 \text{ m}^3$, $V_{\text{CSTR2}} = 2 \text{ m}^3$, and $V_{\text{PFR}} = 1.2 \text{ m}^3$ and asked to find the highest possible conversion X . What would you do? The methods we used to calculate reactor volumes all apply, except the procedure is reversed and a trial-and-error solution is needed to find the exit overall conversion from each reactor. See Problem P2-5_B.

The previous examples show that *if* we know the molar flow rate to the reactor and the reaction rate as a function of conversion, *then* we can calculate the reactor volume necessary to achieve a specified conversion. The reaction rate does not depend on conversion alone, however. It is also affected by the initial concentrations of the reactants, the temperature, and the pressure. Consequently, the experimental data obtained in the laboratory and presented in Table 2-1 as $-r_A$ as a function of X are useful only in the design of full-scale reactors that are to be operated at the *identical conditions* as the laboratory experiments (temperature, pressure, initial reactant concentrations). However, such circumstances are **seldom** encountered and we must revert to the methods we describe in Chapter 3 to obtain $-r_A$ as a function of X .

It is important to understand that if the rate of reaction is available or can be obtained solely as a function of conversion, $-r_A = f(X)$, or if it can be generated by some intermediate calculations, one can design a variety of reactors or a combination of reactors.

Ordinarily, laboratory data are used to formulate a rate law, and then the reaction rate-conversion functional dependence is determined using the rate law. The preceding sections show that with the reaction rate-conversion relationship, different reactor schemes can readily be sized. In Chapter 3, we show how we obtain this relationship between reaction rate and conversion from rate law and reaction stoichiometry.

the previous examples show that:



$$\sum V_i \approx V_{PFR}$$

若 no. of CSTRs $\rightarrow \infty$

i.e. $V_i \rightarrow 0$

$$\Rightarrow \sum_{CSTR} V_i = V_{PFR}$$

∴ PFR 可視為無限多個 small CSTRs in series

2.5 Some Further Definitions

Relative Rates



$$\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}$$

Space time, τ

$$\tau \equiv \frac{V}{v_0} = \frac{\text{reactor volume } [dm^3]}{\text{Volumetric feed rate } [dm^3/min]} = [\text{min}]$$

= time necessary to process one reactor volume of fluid based on entrance conditions

↑ 剛進入 reactor 的時間

PFR

$$V = F_{A_0} \int_0^X \frac{dX}{-r_A} \implies \tau = \frac{V}{v_0} = C_{A_0} \int_0^X \frac{dX}{-r_A}$$

Space velocity, SV

$$SV \equiv \frac{v_0}{V} = \frac{1}{\tau}, \quad v_0 \text{ usually based on specific condition}$$

LHSV, liquid hourly SV measured at 60 or 75 °F

GHSV, gas hourly SV measured at STP.

單位時間內 (e.g. 1 hour) 處理多少個 reactor 體積的流体

If $-r_A$ depends on C_A only (not on C_B, C_D, \dots), usually convenient to use $-r_A = f(C_A)$, rather than $-r_A = f(C_{A0}, X)$

for PFR at special case $v = v_0$.

$$V = F_{A0} \int_0^X \frac{dX}{-r_A} \quad (*)$$

$$F_{A0} = v_0 C_{A0}$$

$$X = \frac{F_{A0} - F_A}{F_{A0}}$$

$$X = \frac{C_{A0} v_0 - C_A v}{C_{A0} v_0} = \frac{C_{A0} - C_A}{C_{A0}}$$

$$\therefore dX = \frac{-dC_A}{C_{A0}} \quad \text{代入 (*)}$$

$$\Rightarrow V = v_0 \int_{C_A}^{C_{A0}} \frac{-dC_A}{-r_A}$$

$$\Rightarrow \tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

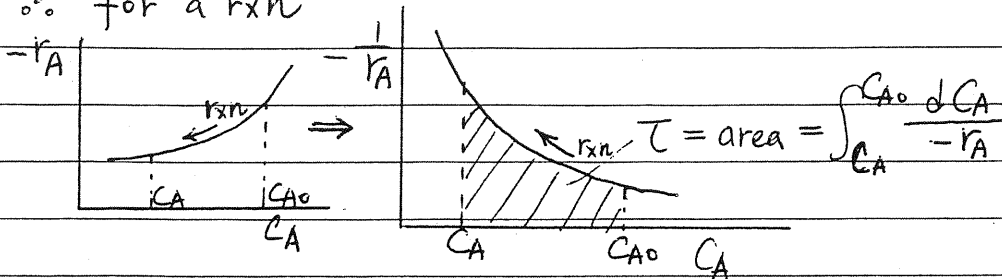
太麻烦; 可改为

$$\frac{-dF_A}{dV} = -r_A$$

$$\frac{-dC_A \cdot v_0}{dV} = -r_A$$

$$V = v_0 \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

∴ for a rxn



∴ 只要有 $-r_A$ vs. X or vs. C_A 即可 design reactors,
毋须 details of rate law.