

## Chapt. 1 Mole Balances

Chemical Reaction Engineering

- Chemical kinetics
  - rates
  - mechanisms
- reactor design

applications: production (need purification, separation....)  
living systems  
waste treatment  
air & water pollution control  
....

### Chemical kinetics

1. reaction rate
2. mechanism (detail of process)
3. rate-limiting step

### thermodynamics

1. equilibrium
2. extent of reaction
3. properties of compounds

reactor design: to achieve production goal  
(time, temp, reactor size and type,  
conversion, production rate)

## 1.1 Rate of Reaction, $-r_A$

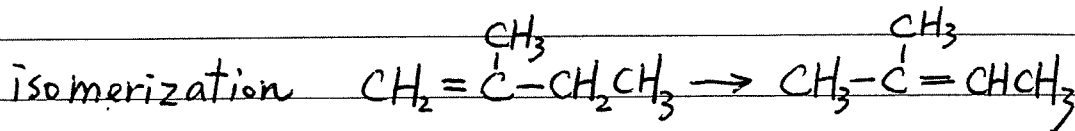
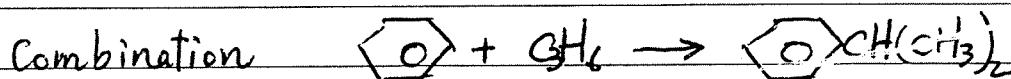
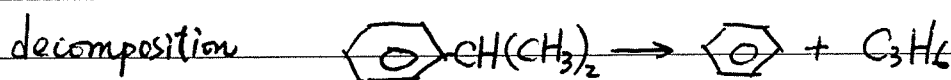
A: chemical species — identical <sup>chemical</sup> physical properties

Chemical reaction: chemical species produced and lost

- total mass constant, but individual changes
- caused by changing in structure and configuration of molecules, i.e. lose chemical identity

$-r_A$ : the no. of moles disappearing per unit time per unit volume,  $[\text{mol}/\text{dm}^3 \cdot \text{s}]$

"disappearance" of a species



heterogeneous

$-r_A'$ : no. of moles disappearing per unit time per unit mass of catalyst (or solid),  $[\text{mol}/\text{s} \cdot \text{g catalyst}]$



## Rate Law

Chemical rxn rate = func. (temp, conc.)  
i.e. rate equation or rate law.

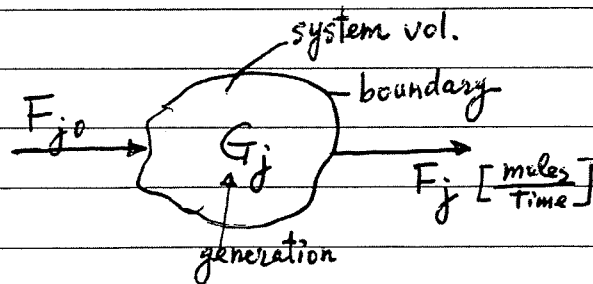
determined from experimental observation

for ex.

$$-r_A = k C_A, \quad k C_A^2, \quad \frac{k_1 C_A}{1 + k_2 C_A}, \dots$$

independent of reactor type

## 1.2 General Mole Balance Equation



for species  $j$

mole balance

in + generation - out = accumulation

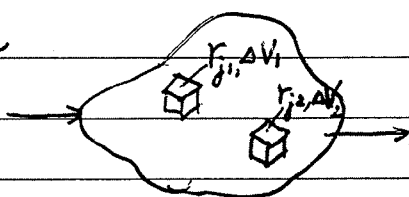
$$F_{j0} + G_j - F_j = \frac{dN_j}{dt}$$

spatially uniform throughout the system vol.

$$G_j = r_j \cdot V$$

$$\left[ \frac{\text{mol}}{t} \right] \quad \left[ \frac{\text{mol}}{t \cdot \text{vol}} \right] [\text{vol}]$$

or not uniform



$$G_j = \sum r_{j1} \Delta V_1 + r_{j2} \Delta V_2 + \dots \quad , \quad \text{let } \Delta V \rightarrow 0$$

$$= \int^V r_j dV$$

$$\therefore \boxed{F_{j0} + \int^V r_j dV - F_j = \frac{dN_j}{dt}} \quad \text{design equation of reactors}$$

$$F_j = C_j \cdot v$$

$$F_j : \text{moles/time}$$

$$C_j : \text{moles/vol.}$$

$$v : \text{vol./time}$$

## 1.3 Batch Reactors



No in and out  $\Rightarrow F_{j0} = F_j = 0$

$$\therefore \frac{dN_j}{dt} = \int^V r_j dV$$

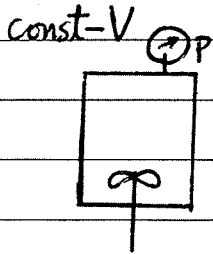
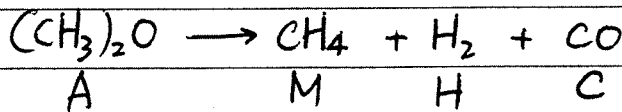
if perfectly mixed (ideal BR)

$$\boxed{\frac{dN_j}{dt} = r_j V} \quad \text{or} \quad \frac{1}{V} \frac{dN_j}{dt} = r_j$$

$V$  usually constant for liquid phase

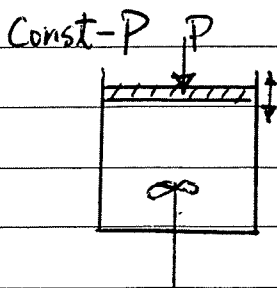
For gas phase

Ex 1-2



$p \neq \text{const.}$

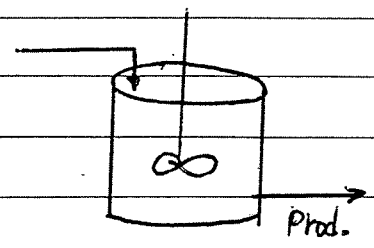
$$\frac{1}{V} \frac{dN_A}{dt} = \frac{d(N_A/V)}{dt} = \frac{dC_A}{dt} = r_A$$



$$\begin{aligned} \frac{1}{V} \frac{dN_A}{dt} &= \frac{1}{V} \frac{d(C_A V)}{dt} = \frac{dC_A}{dt} + C_A \frac{d \ln V}{dt} \\ &= r_A \end{aligned}$$

# 1.4 Continuous-Flow Reactors

## Continuous-Stirred Tank Reactor (CSTR)



perfectly mixed, steady state  
 same temp and conc. everywhere

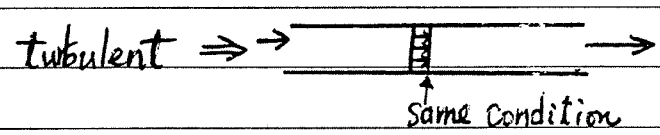
prod. 的 conc., temp. ...  
 每 vessel 內 - 一樣

$$\int_V r_j dV = r_j V, \quad \frac{dN_j}{dt} = 0$$

$$\Rightarrow \boxed{V = \frac{F_{j0} - F_j}{-r_j}}$$

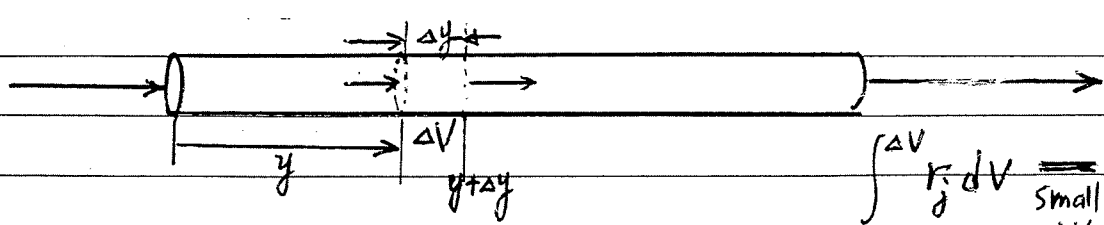
Design eq. for a CSTR

## Tubular Reactor



plug-flow reactor (PFR)

steady state,  $\frac{dN_j}{dt} = 0$



$$\int_{\Delta V} r_j dV \approx r_j \Delta V$$

small  $\Delta V$

$$\therefore F_j(y) - F_j(y + \Delta y) + r_j \Delta V = 0$$

$$\Delta V = A \Delta y$$

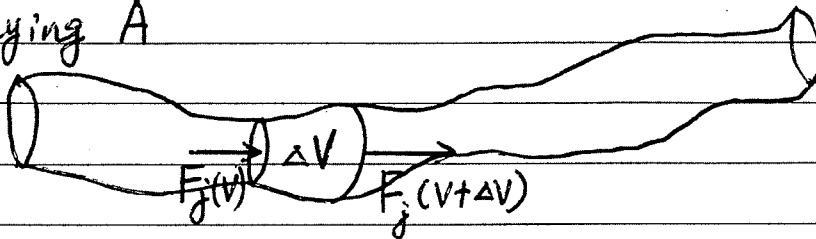
$$-\left[ \frac{F_j(y + \Delta y) - F_j(y)}{\Delta y} \right] = -r_j A$$

↑  
 same cross-sectional area

$$\Delta y \rightarrow 0 \quad - \frac{dF_j}{dy} = -r_j A$$

$$\text{or} \quad \frac{dF_j}{dV} = r_j$$

For varying A



$$F_j(V) - F_j(V+\Delta V) + r_j \Delta V = 0$$

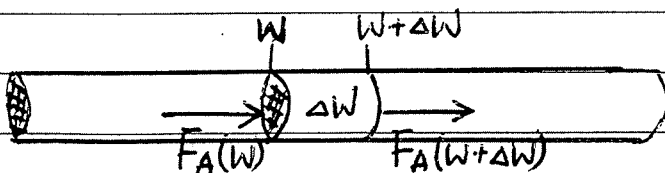
$$\frac{F_j(V+\Delta V) - F_j(V)}{\Delta V} = r_j$$

$\Delta V \rightarrow 0$

$$\boxed{\frac{dF_j}{dV} = r_j}$$

design eq. for a PFR

packed-Bed Reactor (PBR)

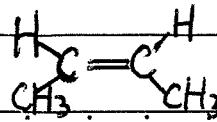


design eq.

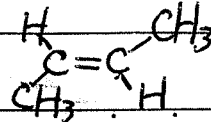
$$\frac{dF_A}{dW} = r'_A \left[ \frac{\text{mol A reacted}}{\text{s} \cdot \text{g cat.}} \right]$$



cis-2-butene



trans-2-butene

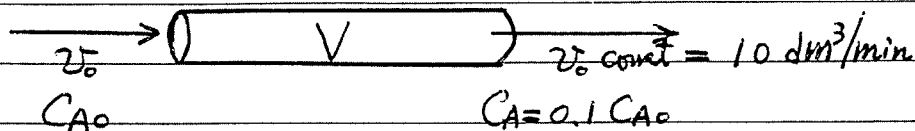


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Ex 1-1 find reactor size from design eqs.

1st-order reaction  $A \longrightarrow B$   $-r_A = k C_A$

a tubular reactor used  $k = 0.23 \text{ min}^{-1}$



$$V = ?$$

Sol.

$$\frac{dF_A}{dV} = r_A \quad -r_A = k C_A$$

$$\therefore \frac{dF_A}{dV} = \frac{d(C_A v)}{dV} = v_0 \frac{dC_A}{dV} = r_A = -k C_A$$

$$\Rightarrow -\frac{v_0}{k} \frac{dC_A}{C_A} = dV$$

$$-\frac{v_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^V dV$$

$$-\frac{v_0}{k} \ln \frac{C_A}{C_{A0}} = V$$

$$\therefore V = -\frac{10 \text{ dm}^3/\text{min}}{0.23 \text{ min}^{-1}} \ln \frac{0.1 C_{A0}}{C_{A0}}$$

$$= 100 \text{ dm}^3 = 100 \text{ liters}$$

## 1.5 Industrial Reactors

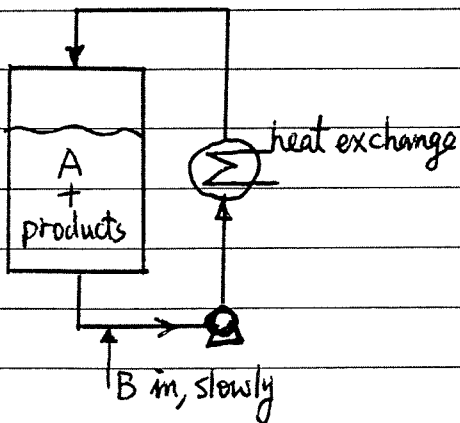
Small-scale operation  
 testing new process  
 need high conversion  
 hard to operate continuously

⇒ Batch reactor

- disadvantage
- high labor cost
  - difficult for large-scale production

## Liquid-Phase Reactions.

### Semibatch reactor



disadvantage

- same as BR

advantage

- good temperature control
- maintain low conc. of B

HW#2

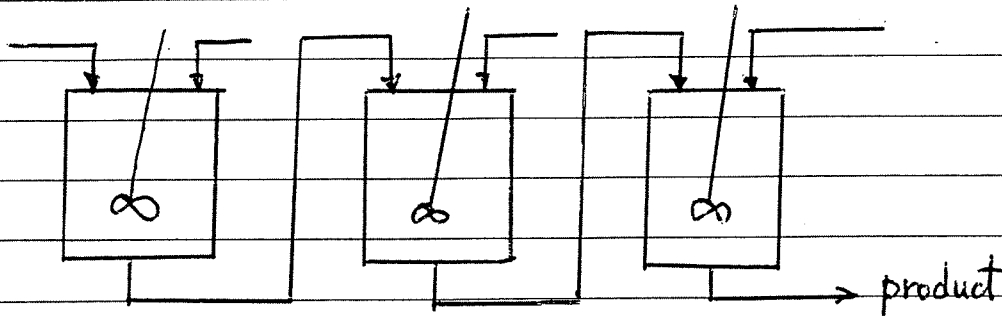
1-2

1-11

1-12

~~1-13~~

### CSTR



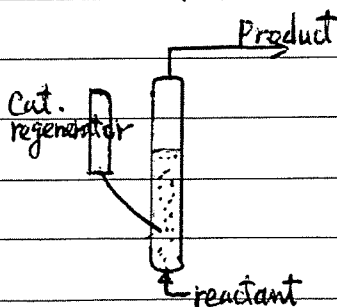
advantage : good temp. control (因 tank 內 temp 一致) 只要控一個 temp 即可  
 disadv. : low conversion/volume

### Gas-Phase Reactions

#### PFR or PBR

advantage : easy to maintain, high conversion/vol.  
 disadv. : difficult to control temp. (Temp 各處都不同) 須控制 temp.  
 hard to replace catalyst } PBR  
 channeling of flows }

#### Fluidized-Bed reactor



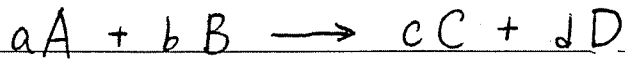
analogous to CSTR

advantage : good temp control  
 easy to replace catalyst  
 regenerate

disadv. : high cost

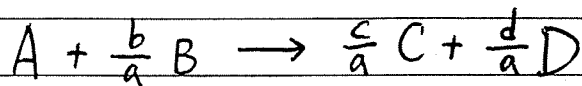
## Chapter 2 Conversion and Reactor Sizing

### 2.1 Definition of Conversion



choose the limiting reactant for calculating conversion

take A as the basis for calculation ↙ 有可能完全反应着



"How far the rxn has progressed?" → 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.

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

↖  $N_{A0} - N_{A0}X$

∴  $N_{A0} \frac{dX}{dt} = -r_A \cdot V$       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  $-r_A = -\frac{1}{V} \frac{dN_A}{dt} \Rightarrow -r_A = -\frac{dC_A}{dt}$  --- Const-V R  
 or  
 $-r_A = C_{A0} \frac{dX}{dt}$  ---

varying-V BR

X vs. t

if  $V = V(t)$

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

or

if  $V = V(X)$

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

} integral form of design eq.

### 2.3 Design Equations for Flow Reactors

[mole rate leaving the system]	[mole rate fed]	[mole rate consumed in system]
$F_A$	$= F_{A0}$	$- F_{A0} X$
$= F_{A0} (1 - X)$		

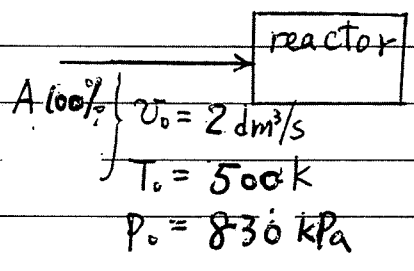
$$F_{A0} = C_{A0} v_0, \quad F_A = C_A \cdot v$$

$P_A v = F_A RT$  for ideal gas flow  $\frac{F_A}{v} = \frac{P_A}{RT}$  mole fraction / total P

$$\therefore C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0} P_0}{RT_0}$$

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

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  $C_{A0}, F_{A0}$

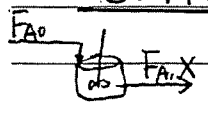
Sol.

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

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

2.3.1.

CSTR (or Vat / or Backmix R)



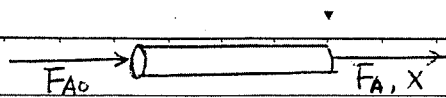
$$V = \frac{F_{A0} - F_A}{-r_A}$$

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

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

2.3.2.

PFR



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

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

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

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

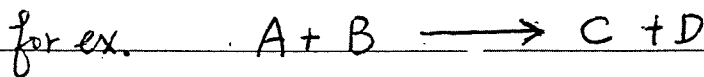
2.3.3. PBR

similar to PFR

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

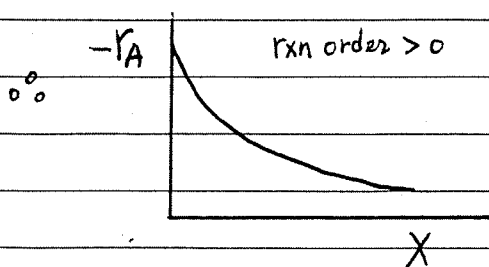
$$W = F_{A0} \int_0^X \frac{dX}{-r_A'}$$

## 2-4 Applications of Design Equations

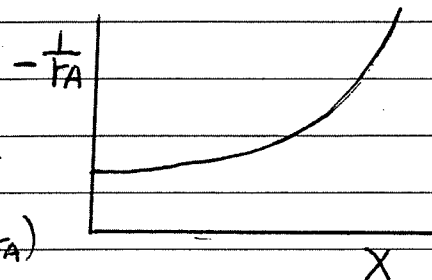


at specified  $C_{A0}, C_{B0}, \dots$

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



$\Rightarrow$   
because of  
design eqs  
(need  $-1/r_A$ )



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

### Ex 2-2 Sizing a CSTR

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

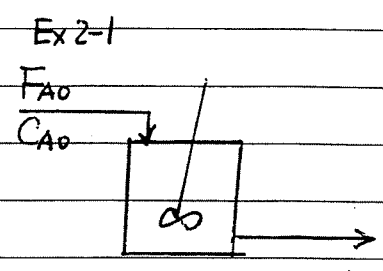
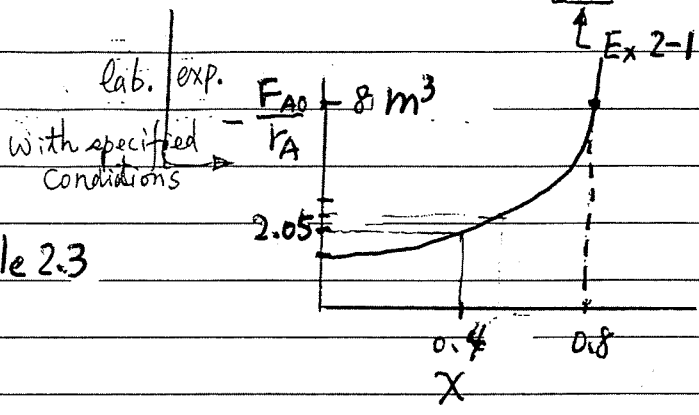


Figure 2-2

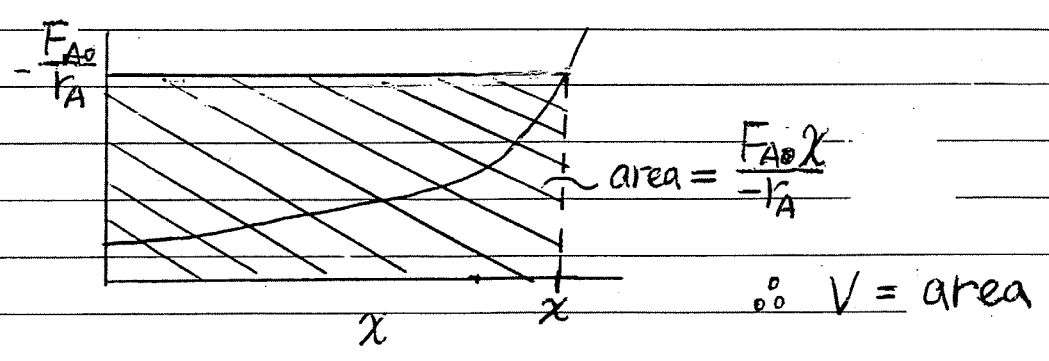
to achieve 80% conversion in a CSTR,  $V = ?$

Sol.

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

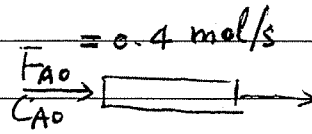
$$= [8 \text{ m}^3][0.8] = 6.4 \text{ m}^3$$

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





Ex 2-3 sizing a PFR

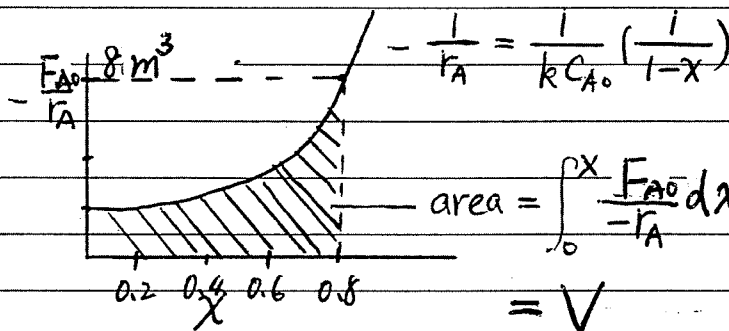


Same rxn in Ex 2-2

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

Sol.

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

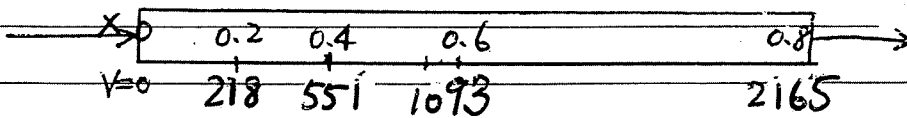


area =  $\int_0^X \frac{F_{A0}}{-r_A} dx \approx 2.165 \text{ m}^3 = 2165 \text{ dm}^3$  (numerical)

$= V$

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

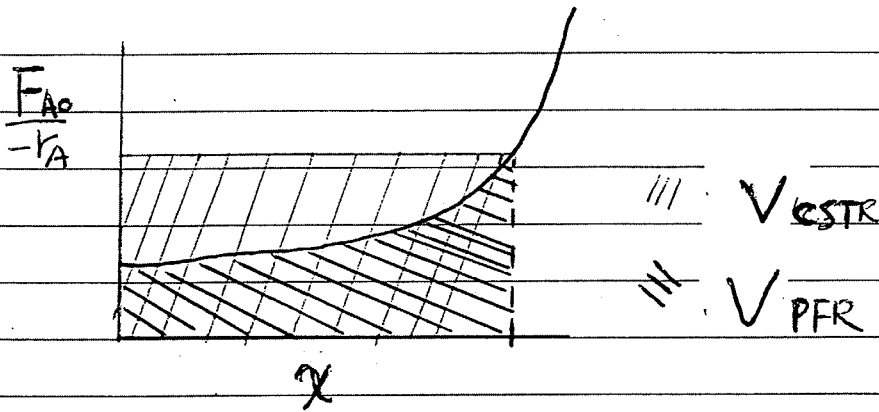
$X =$	0	0.2	0.4	0.6	0.8
$V(\text{dm}^3)$	0	218	551	1093	2165



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

## Ex 2-4 Comparing CSTR and PFR sizes

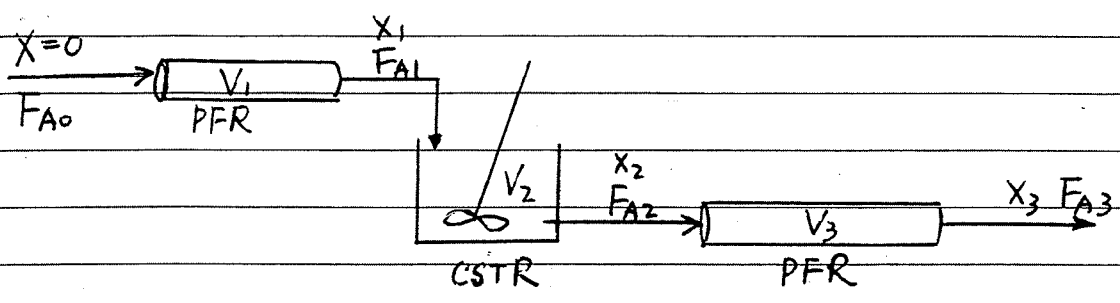
在相同的 feed conditions, 且到達某一 Conversion 時



∴ 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

$$\frac{-dF_A}{dV} = -r_A \Rightarrow F_{A0} \frac{dX}{dV} = -r_A \Rightarrow \boxed{V_1 = F_{A0} \int_0^{X_1} \frac{dX}{-r_A}}$$

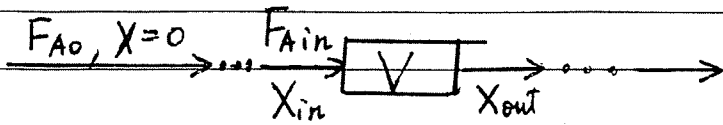
Reactor 2

mol bal.  $F_{A1} + r_{A2}V_2 - F_{A2} = 0$   
 $\Rightarrow V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} \Rightarrow \boxed{V_2 = \frac{F_{A0}(X_2 - X_1)}{-r_{A2}}}$

Reactor 3

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

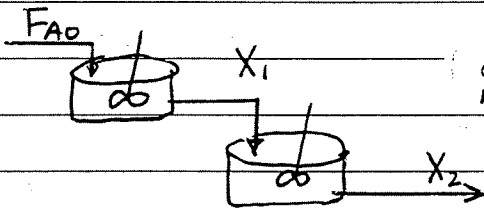
General Cases for reactors in series



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

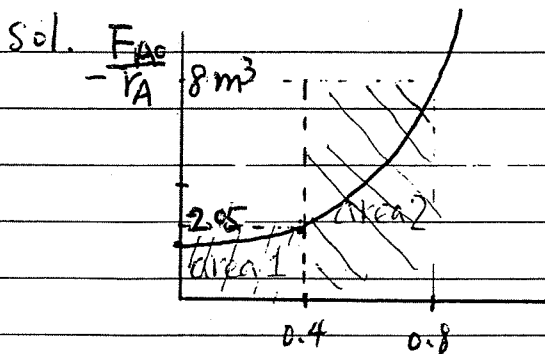
$$V = F_{A0} \int_{X_{in}}^{X_{out}} \frac{dX}{-r_A} \quad \text{for PFR}$$

Ex 2-5



$\frac{C_{A0}}{r_{X1}} = \frac{F_{A0}}{r_{X1}}$  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

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

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

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

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

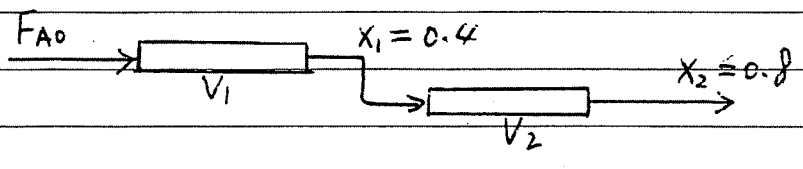
$$= (8.0)(0.8) = 6.4 \text{ m}^3$$

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

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

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

Ex 2-6  
for two PFRs in series



$$V_1 = F_{A0} \int_0^{X_1=0.4} \frac{dx}{-r_A} = 551 \text{ dm}^3$$

$$V_2 = F_{A0} \int_{X_1=0.4}^{X_2=0.8} \frac{dx}{-r_A} = 1614 \text{ dm}^3$$

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

Simpson's rule

(numerical method)  
Appendix A.4

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

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

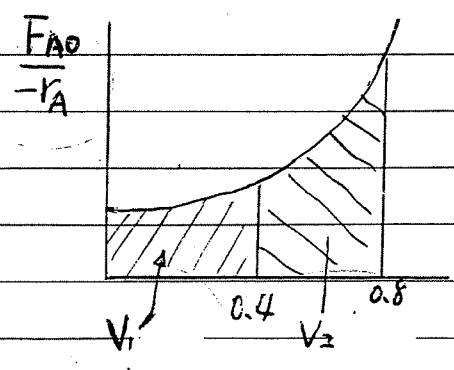
$$\Delta X = \frac{x_2 - x_0}{2}$$

$$x_1 = x_0 + \Delta X$$

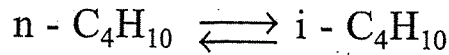
as a matter of fact

$$F_{A0} \int_0^{X_1} \frac{dx}{-r_A} + F_{A0} \int_{X_1}^{X_2} \frac{dx}{-r_A} = F_{A0} \int_0^{X_2} \frac{dx}{-r_A}$$

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 <sup>3</sup> · 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.

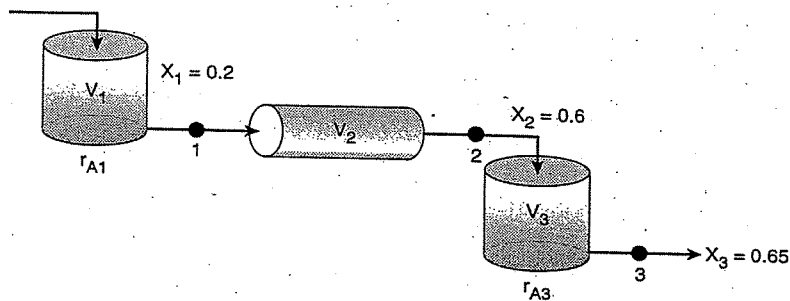


Figure E2-7.1 Reactors in series.

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 <sup>3</sup> · h)	39	53	59	38	25
$[F_{A0}/-r_A]$ (m <sup>3</sup> )	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.

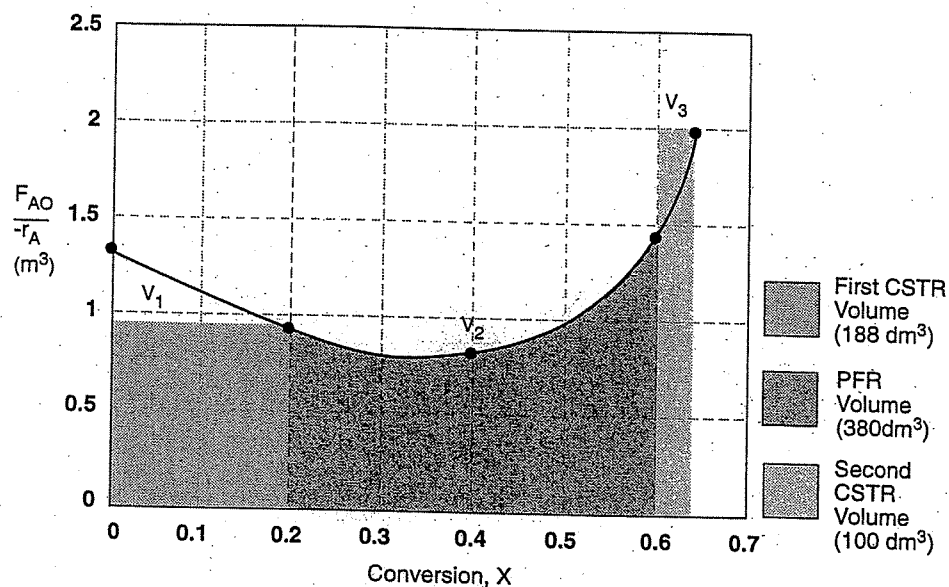


Figure E2-7.2 Levenspiel plot for adiabatic reactors in series.

### 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.

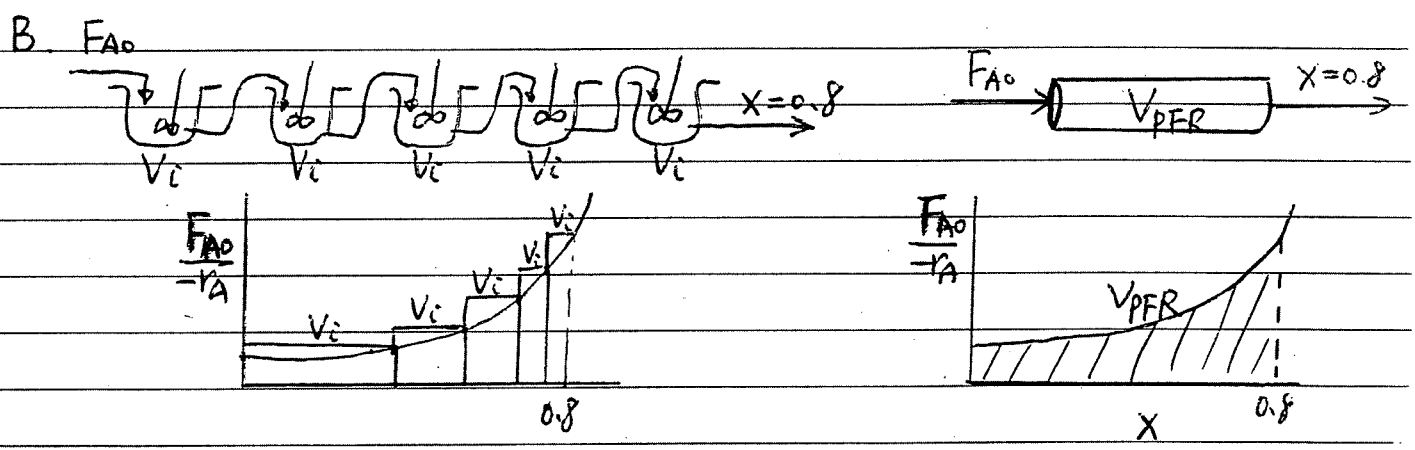
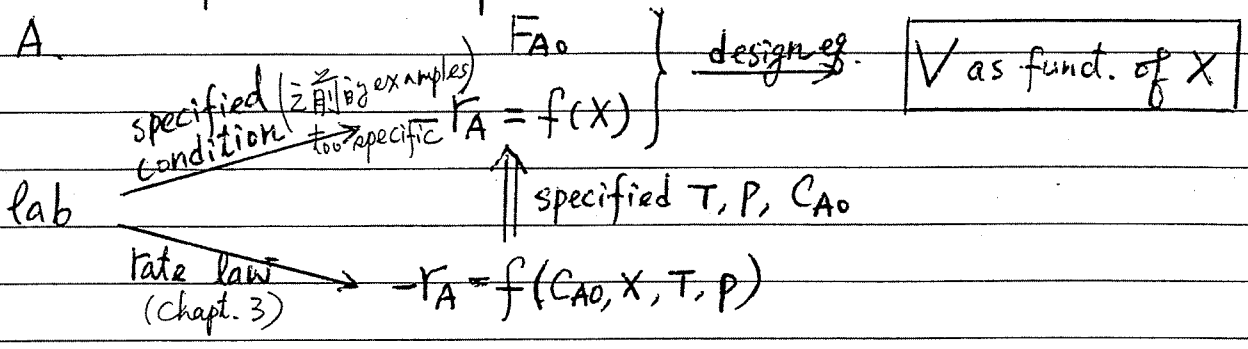
➤ In the *sequencing of reactors* one is often asked, "Which reactor should go first to give the highest overall conversion? Should it be a PFR followed by a CSTR, or two CSTRs, then a PFR, or ...?" The answer is "**It depends.**" It depends not only on the shape of the Levenspiel plots ( $F_{A0}/-r_A$ ) 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<sub>B</sub>.

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, $\tau$

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

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

↑ 剛進入 reactor 的時間

DER

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

### 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  $v = v_0$ .

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

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

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

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

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

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

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

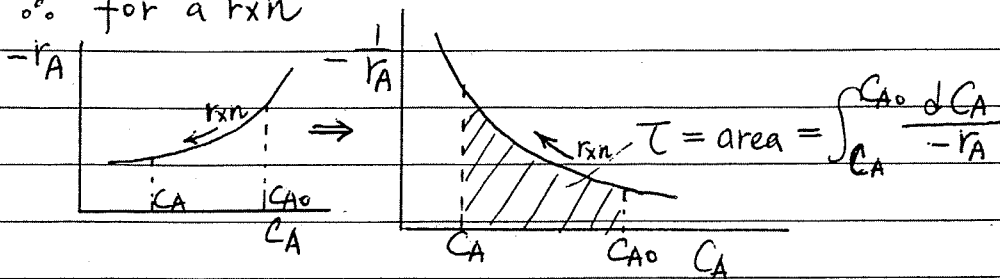
太麻烦; 可改写

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

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

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

$\therefore$  for a rxn



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