

Chapter 2

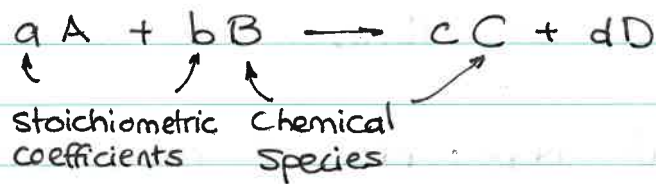
Conversion and reactor sizing

Notes on
Elements of chemical
reaction engineering, H.
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- Ranjeet Utikar

Conversion

- choose one of the reactants as the basis of calculation.
↳ usually the limiting reactant

Consider the general reaction



Let A be limiting reactant



conversion X_A

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

- For irreversible reactions maximum conversion is 1.0 → complete conversion
- For reversible reactions maximum conversion = equilibrium conversion X_e
 $X_{\max} = X_e$

Batch reactor design equations

- The longer a reactant stays in the reactor, the more the reactant is converted to product, until either the equilibrium is reached or the reactant is exhausted.
- Conversion X is a function of time

If N_{A0} : No. of moles of A initially present

$N_{A0}X(t)$: Total number of moles that have reacted after time t

$$\left[\begin{array}{l} \text{mols of A} \\ \text{reacted} \end{array} \right] = \left[\begin{array}{l} \text{mols of A} \\ \text{fed} \end{array} \right] \cdot \left[\frac{\text{mols of A reacted}}{\text{mols of A fed}} \right]$$
$$= N_{A0} \cdot X$$

$$\left[\begin{array}{l} \text{mols of A} \\ \text{in reactor at} \\ \text{any time } t \end{array} \right] = \left[\begin{array}{l} \text{mols of A} \\ \text{initially fed} \\ \text{to reactor} \\ \text{at } t=0 \end{array} \right] - \left[\begin{array}{l} \text{mols of A} \\ \text{reacted} \end{array} \right]$$

$$N_A = N_{A0} - N_{A0}X$$

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

when no spatial variation in reaction rate exists:

mole balance:

$$\frac{dN_A}{dt} = r_A V$$

$$-\frac{dN_A}{dt} = (-r_A) V$$

⇒ For batch reactor we are interested in determining how long to leave the reactants in the reactor to achieve a certain conversion x .

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

$$\frac{dN_A}{dt} = -N_{A0} \frac{dx}{dt}$$

$$\therefore \boxed{N_{A0} \frac{dx}{dt} = (-r_A) V}$$

differential form of the design equation

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

$$@ t=0 \quad x=0$$

$$@ t=t \quad x=x$$

$$t = N_{A0} \int_0^x \frac{dx}{-r_A V}$$

Batch
design
Equation

Design equations for flow reactors

- ⇒ Conversion increases with time spent in the reactor
- ⇒ For continuous flow reactors higher volume ⇒ more time spent
- ⇒ Conversion x is a function of reactor volume V

If F_{A0} is molar flow rate of species A fed to a system operated at steady state, molar rate at which species A is reacting within the entire system will be $F_{A0} X$

$$F_{A0} X = \frac{\text{mols of A fed}}{\text{time}} \cdot \frac{\text{mols of A reacted}}{\text{mols of A fed}}$$

$$= \frac{\text{mols of A reacted}}{\text{time}}$$

molar flow rate at which A is fed to the system = molar rate at which A is consumed within the system = molar flow rate at which A leaves the system

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

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

⇒ Entering molar flowrate is a product of concentration (molarity for liq.) and volumetric flow rate

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

For gas systems, C_{A0} can be calculated from mole fraction y_{A0} , temperature T_0 , and pressure P_0 using ideal gas law

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

CSTR

consider



CSTR mole balance:

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

$$F_A = F_{A0} (1 - X_A)$$

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

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

Design equation
for CSTR

⇒ Because the reactor is perfectly mixed, the exit composition from the reactor is identical to the composition inside the reactor.

⇒ rate of reaction is evaluated at the exit concentration.

Tubular flow reactor (PFR)

mole balance

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

for flow systems

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

$$dF_A = -F_{A0} dX$$

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

$$\textcircled{a} V=0 \quad X=0$$

$$\textcircled{b} V=V \quad X=X$$

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

design equation
for PFR

Packed bed reactor (PBR)

Similar to PFR we can show that for PBR

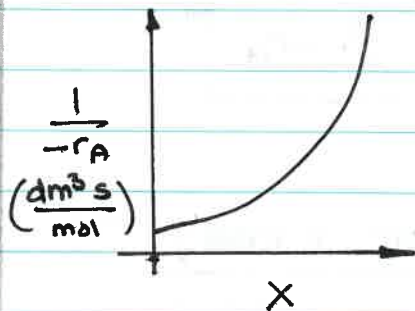
$$F_{A0} \frac{dX}{dW} = -r'_A \Rightarrow W = F_{A0} \int_0^X \frac{dX}{-r'_A}$$

design equation for PBR

Sizing continuous flow reactors

- ⇒ By sizing we mean either
- determine the reactor volume for specified conversion or
 - determine the conversion for specified volume.

- For all irreversible reactions of order greater than 0, as we approach complete conversion, the reciprocal rate approaches infinity



$$\text{As } X \rightarrow 1 ; -r_A \rightarrow 0$$

$$\Rightarrow \frac{1}{-r_A} \rightarrow \infty \therefore V \rightarrow \infty$$

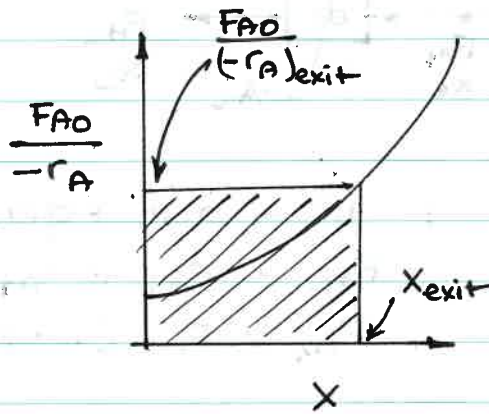
⇒ Infinite reactor volume is necessary to reach complete conversion.

For reversible reaction

$$\text{As } X \rightarrow X_e ; -r_A \rightarrow 0$$

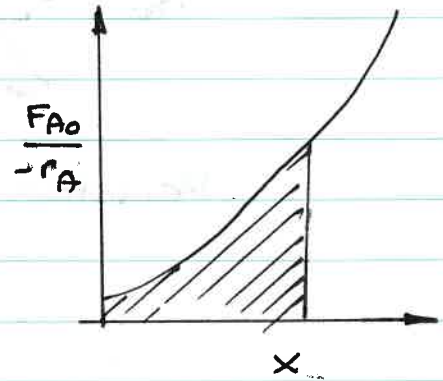
$$\Rightarrow \frac{1}{-r_A} \rightarrow \infty \Rightarrow V \rightarrow \infty$$

Levenspiel plot



CSTR volume
= Area under
rectangle.

$$V = \left(\frac{F_{A0}}{(-r_A)_{exit}} \right) \cdot X$$



PFR volume
= Area under
the curve

$$V = \int_0^X \left(\frac{F_{A0}}{(-r_A)} \right) dx$$

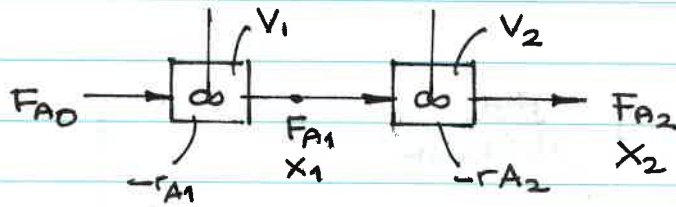
Reactors in series

$X_i = \frac{\text{Total mols of A reacted up to point } i}{\text{Moles of A fed to the first reactor}}$

$$F_{A_i} = F_{A0} (1 - X_i)$$

↑ True only for
Systems with
no side streams

CSTR in series



Reactor 1 : In - out + generation = 0

$$F_{A0} - F_{A1} + r_{A1} V_1 = 0$$

$$F_{A1} = F_{A0} (1 - X_1)$$

$$V_1 = \frac{F_{A0} X_1}{-r_{A1}}$$

Reactor 2 : In - out + generation = 0

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

$$F_{A1} = F_{A0} (1 - X_1)$$

$$F_{A2} = F_{A0} (1 - X_2)$$

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

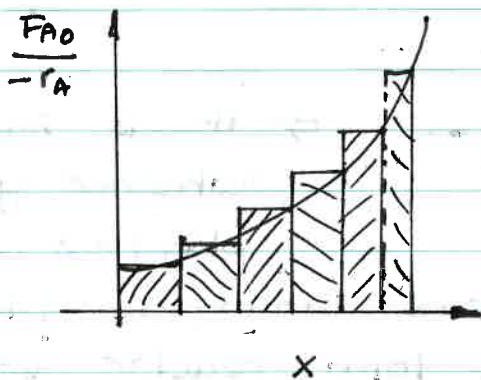
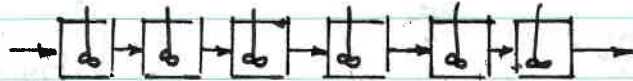
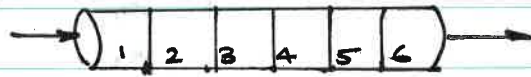
$$V_2 = \frac{F_{A0} (X_2 - X_1)}{-r_{A2}}$$

for i th reactor

$$V_i = \frac{F_{A0} (X_i - X_{i-1})}{-r_{Ai}}$$

$$X_0 = 0$$

Approximating a PFR by a large number of CSTRs in series



⇒ The total volume of CSTRs in series is 'roughly' same as the volume of PFR

⇒ As we make volume of each CSTR smaller and increase the

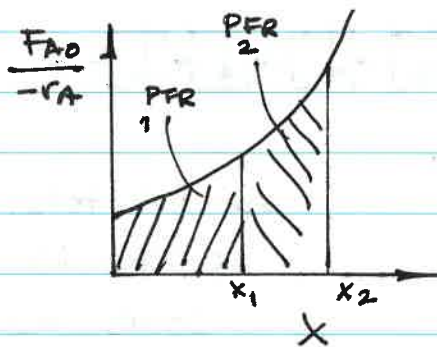
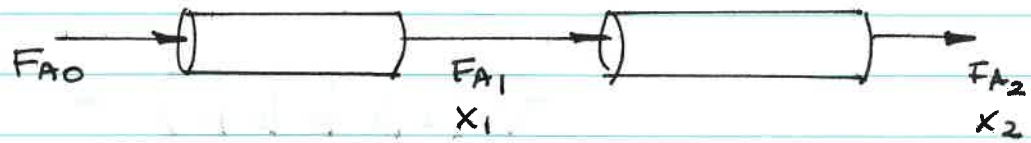
number of CSTRs, the ^{total} volume of the CSTRs and PFR will become equal.

⇒ The concept of using CSTRs in series to model PFR is used in large number of situations

⇒ Modeling catalyst decay in packed bed

⇒ Transient heat effects in PFR

PFRS in series



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

⇒ It is immaterial whether you put two plug flow reactors in

series or one continuous plug flow reactor; the total reactor volume required to achieve the same conversion is identical.

⇒ If the reaction rate is available or can be obtained solely as a function of X , or it can be generated by some intermediate calculation, one can design a variety of reactors and combinations of reactors.

Space time / holding time / mean residence time

obtained by dividing the reactor volume by volumetric flow rate entering the reactor

$$\tau = \frac{V}{\dot{V}_0}$$

⇒ Time necessary to process one reactor volume of fluid based on entrance conditions

Typical space time for industrial reactors

Batch	15 min - 20 h
CSTR	10 min - 4 h
Tubular	0.5 s - 1 h

space velocity $SV = 1/\tau \equiv \dot{V}_0/V$

$$LHSV = \frac{\dot{V}_0 | \text{liquid}}{V}$$

liquid hourly space velocity

$$GHSV = \frac{\dot{V}_0 | \text{gas}}{V}$$

gas hourly space velocity.

↳ usually @ STP