CHEMICAL REACTION ENGINEERING (SKF3223)

Chapter 2: Conversion and Reactor Sizing

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Conversion, X

- To quantify how far a reaction has progressed
- How many moles of C are formed for every mole A consumed

Consider : $aA + bB \rightarrow cC + dD$

The basis of calculation is always the limiting reactant

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

- Irreversible reaction: $X_{max} = 1.0$ (complete conversion)
- Reversible reaction: $X_{max} = X_{equilibrium}$ (equilibrium conversion)

CONVERSION

X = moles of A reacted / consumed
moles of A fed

Batch system (X,t)

$$X_A = \frac{N_{A0} - N_A}{N_{A0}}$$

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

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

$N_{A0}X$= moles of A consumed / reacted

Flow system (X,V/W)

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

$$F_A(mol/s) = F_{A0} - F_{A0}X$$

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

$F_{A0}X$= molar flow rate at which A is consumed / reacted

BATCH REACTOR

- For batch reactor , we are interested in determining how long to leave the reactants in the reactor to achieve a certain conversion

From mole balance: $r_A V = \frac{dN_A}{dt}$ From the conversion: $N_A = N_{A0} - N_{A0} X$

- This is how the Design Equation derived from mole balance equation in terms of conversion

Differentiating with respect of time:

$$\frac{dN_A}{dt} = 0 - N_{A0}\frac{dX}{dt}$$

N_{A0} = 0 : constant with respect of time

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

GAS FLOW SYSTEM

- The entering molar flow rate, F_{A0} (mol/s)

$$F_{A0} = C_{A0}\upsilon_0$$

$$\frac{mol}{s} = \frac{mol}{dm^3} \cdot \frac{dm^3}{s}$$

C_{A0} for gas system

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

C_{A0}= entering concentration, mol/dm^3

Y_{a0}= entering mole fraction of A

P_0= entering total pressure, kPa

T_0=entering temperature, K

P_{a0}= entering partial pressure

R= ideal gas constant = 8.314k.Pa.dm^3/mol.K

CSTR

From mole balance:

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

From the conversion:

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

Design Equation:

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

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

➡

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

PFR

From mole balance:

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

From the conversion:

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

Design Equation:

Differentiating with respect of volume:

$$\frac{dF_A}{dV} = 0 - F_{A0}\frac{dX}{dV}$$

F_{A0} = 0 : constant with respect of volume

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

PBR

From mole balance:

$$\frac{dF_A}{dW} = r'_A$$

From the conversion:

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

Design Equation:

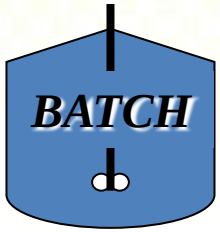
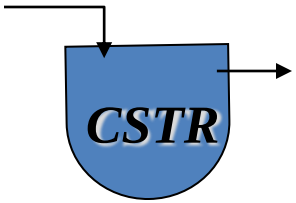
Differentiating with respect of weight of catalyst:

$$\frac{dF_A}{dW} = 0 - F_{A0}\frac{dX}{dW}$$

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

DESIGN EQUATIONS

Design Equations for Isothermal Reactors

REACTOR	DIFFERENETIAL FORM	ALGEBRAIC FORM	INTEGRAL FORM
	$N_{AO}\frac{dX}{dt}=(-r_A)V$		$t=N_{AO}\int_0^X\frac{dX}{-r_AV}$
		$V=\frac{F_{AO}(X)}{(-r_A)_{Exit}}$	
	$F_{AO}\frac{dX}{dV}=(-r_A)$		$V=F_{AO}\int_0^X\frac{dX}{-r_A}$
	$F_{AO}\frac{dX}{dW}=(-r'_A)$		$W=F_{AO}\int_0^X\frac{dX}{-r'_A}$

REACTOR SIZING

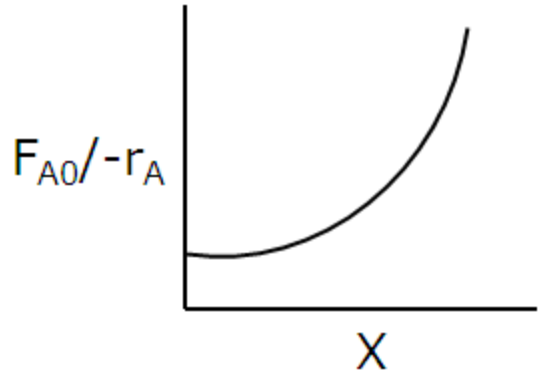
- By sizing a chemical reactor we mean we're either determine the reactor volume to achieve a given conversion or determine the conversion that can be achieved in a given reactor type and size.

- Normally, the process / experimental data will be given (X, $-r_A$)

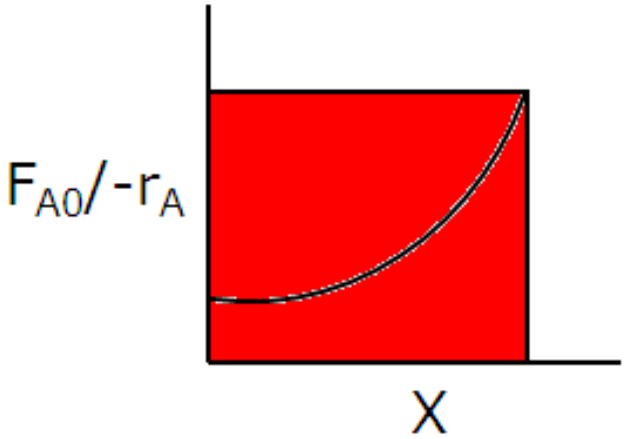
PFR

- Simpson's One-Third Rule is one of the more common numerical methods.
- Other numerical methods (see Appendix A.4, pp 1013-1015):
  - (i) Trapezoidal Rule (2 data points)
  - (ii) Simpson's Three-Eighth's Rule (4 data points)
  - (iii) Five-Point Quadrature Formula (5 data points)

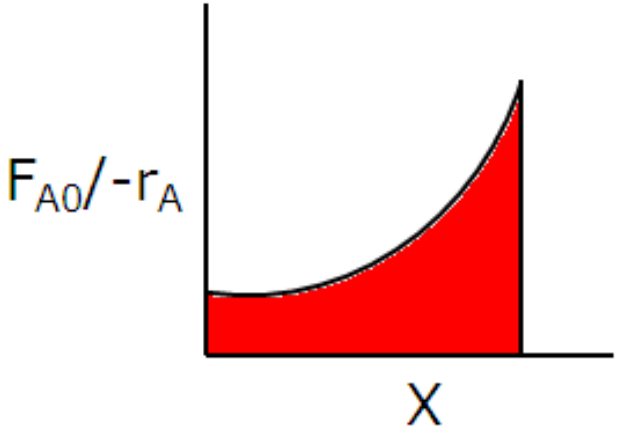
Reactor Sizing



Levenspiel Plot



CSTR



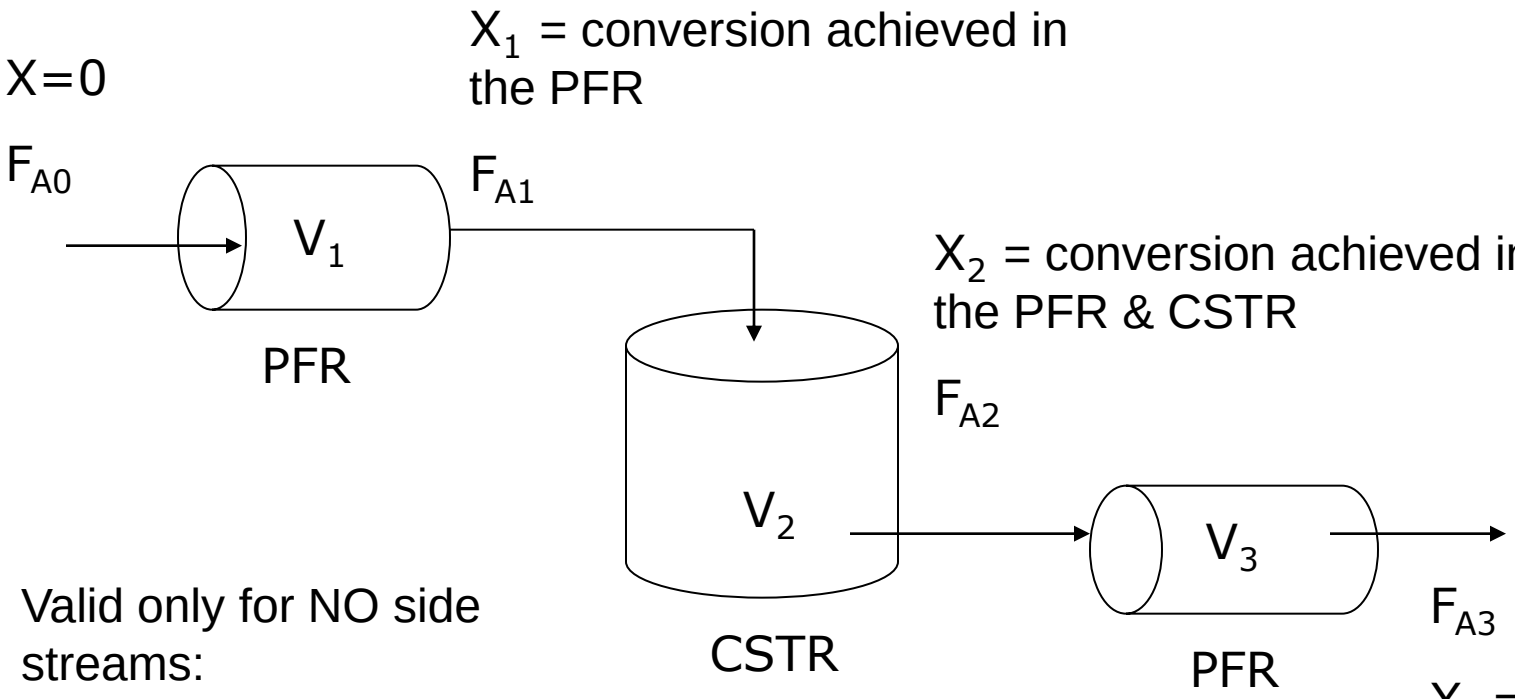
PFR

REACTORS IN SERIES

Why?

- Sometimes 2 CSTR reactor volumes in series is less than the volume of 1 CSTR to achieve the same conversion.
- Can model a PFR with a large number of CSTR in series.
- In the case of PFR, whether you place 2 PFR in series or have 1 PFR, the total reactor volume required to achieve the same conversion is identical.

REACTORS IN SERIES



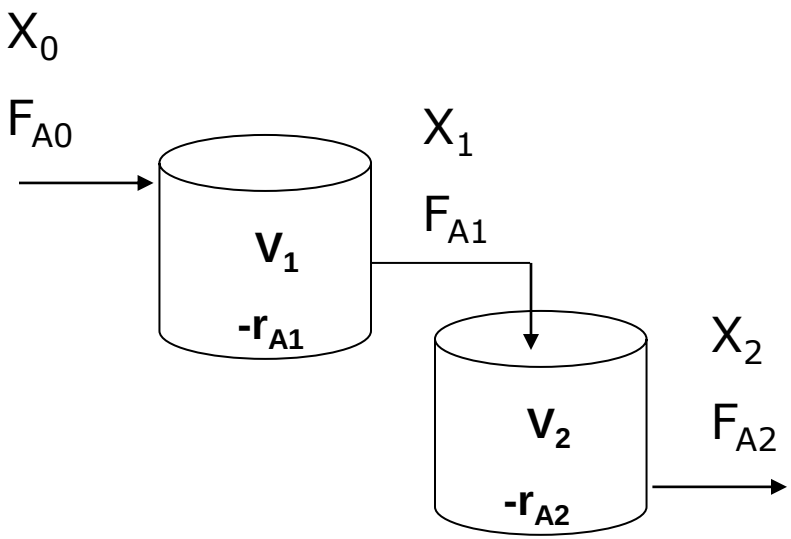
Valid only for NO side streams:

$$F_{A1} = F_{A0} - F_{A0}X_1$$

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

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

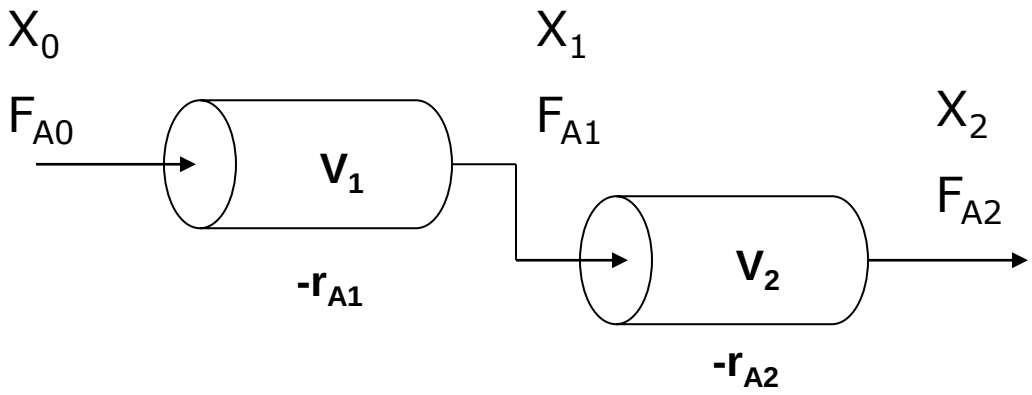
(i) CSTR in series:



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

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

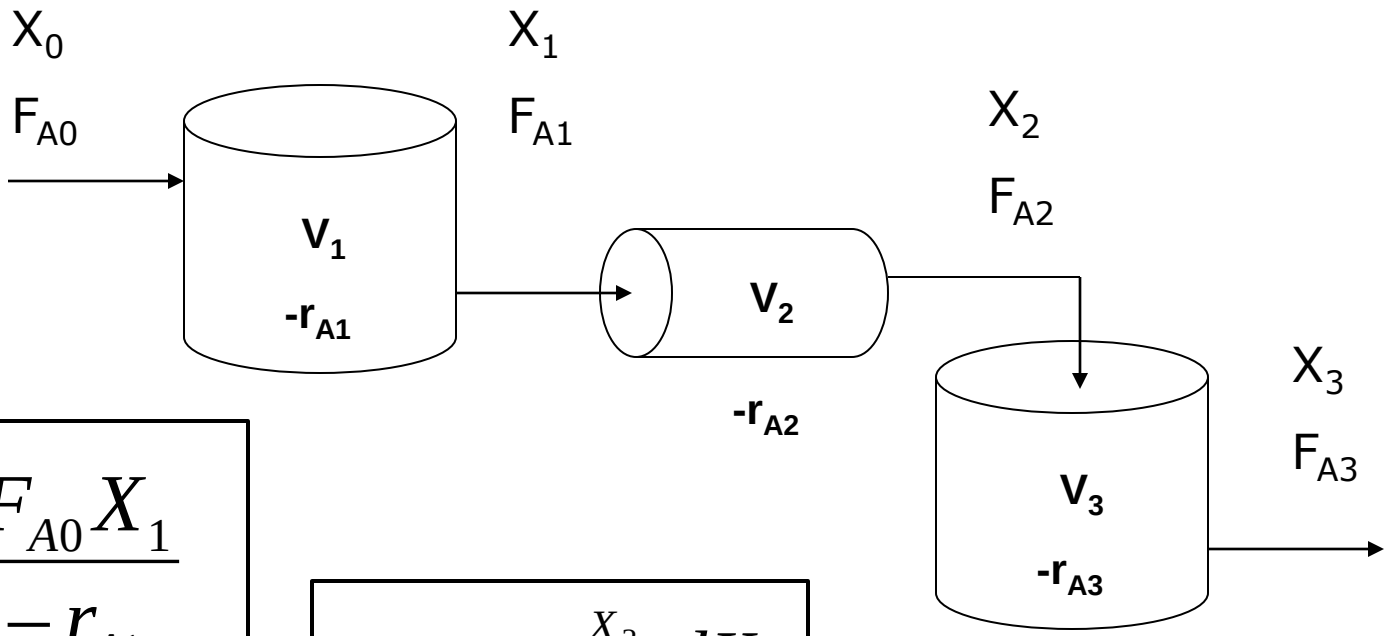
(ii) PFR in series:



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

$$V_2 = F_{A0} \int_{X_1}^{X_2} \frac{dX}{-r_A}$$

(iii) CSTR + PFR in series:



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

$$V_2 = F_{A0} \int_{X_1}^{X_2} \frac{dX}{-r_{A2}}$$

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

SPACE TIME, τ

- The time necessary to process one reactor volume by the volumetric rate entering the reactor

- Also called the *holding time* or *mean residence time*

$$\tau \equiv \frac{V}{\upsilon_0}$$

$$time = \frac{volume}{volume/time}$$

- *where* $\upsilon_{0\ is}$ *entrance volumetric rate*

SPACE VELOCITY (SV)

$$SV \equiv \frac{\upsilon_0}{V} = \frac{1}{\tau}$$

- Reciprocal of the space time, τ
- Two SV commonly used in industry:

GHSV	Gas Hourly Space Velocity, h^{-1} v_0 at STP (standard temp. and pressure)
LHSV	Liquid Hourly Space Velocity, h^{-1} v_0 at some reference temperature

REFERENCES

Main Reference:

1. Fogler,H.S., "*Elements of Chemical Reaction Engineering*", 4th Edition,Prentice Hall, New Jersey, 2006.

Other References:

1. Davis, M.E and Davis, R.J, *"Fundamentals of Chemical Reaction Engineering",* Mc-Graw-Hill, New York, 2003
2. Schmidt, L.D, "*The Engineering of Chemical Reactions"*, Oxford, New York, 1998
3. Levenspiel,O., "*Chemical Reaction Engineering*", 3rd Edition, Wiley,New York, 1998
4. Smith,J., "*Chemical Engineering Kinetics*", 3rd Edition, McGraw-Hill, New York, 1981