BITS, PILANI – K. K. BIRLA GOA CAMPUS

KINETICS & REACTOR DESIGN

PROF. SRINIVAS KRISHNASWAMY
PROF. & HEAD OF DEPARTMENT
DEPARTMENT OF CHEMICAL ENGINEERING
BITS PILANI, K. K. BIRLA GOA CAMPUS

Time to move ahead…

You never know what is enough, until you know what is more than enough.

William Blake

Conversion

Consider the general equation

$$aA + bB \longrightarrow cC + dD$$

We will choose A as our basis of calculation

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

The basis of calculation is most always the limiting reactant.

The conversion of species A in a reaction is equal to the number of moles of A reacted per mole of A fed.

Conversion

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

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

Batch reactor   Flow reactor

For irreversible reactions, the maximum value of conversion, X, is that for complete conversion, i.e. X=1.0

For reversible reactions, the maximum value of conversion, X, is the equilibrium conversion, i.e. $X=X_e$

Design Equations (Batch Reactor)

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

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

$$dN_A = 0 - N_{Ao}dX$$

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

$$\boxed{N_{Ao}\frac{dX}{dt} = -r_A V}$$ Diff. form

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

$$t = 0 \quad X = 0$$

$$\boxed{t = N_{Ao}\int_0^X \frac{dx}{-r_A V}}$$ Integral form
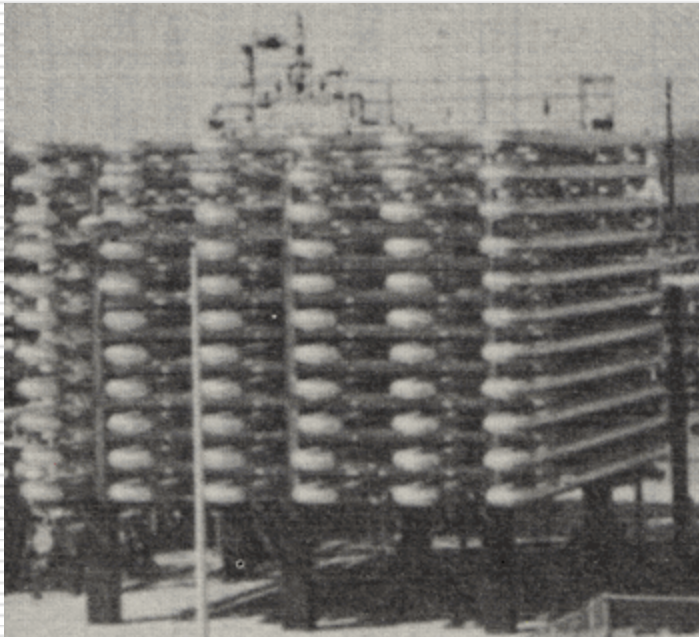
Design Equations (Flow Reactors : CSTR)

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

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

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

Backmix reactor

Design Equations (Flow Reactors : PFR)

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

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

$$dF_A = 0 - F_{Ao}\,dX$$

$$-F_{Ao}\frac{dX}{dV} = r_A$$

$$\boxed{F_{Ao}\frac{dX}{dV} = -r_A} \quad \Longleftarrow \quad \text{Diff. form}$$

$$\frac{F_{Ao}\,dX}{-r_A} = dV$$

$$V = 0 \,,\, X = 0$$

$$\boxed{V = F_{Ao}\int_0^X \frac{dX}{-r_A}} \quad \Longleftarrow \quad \text{Integral form}$$

Design Equations (Flow Reactors : PBR)
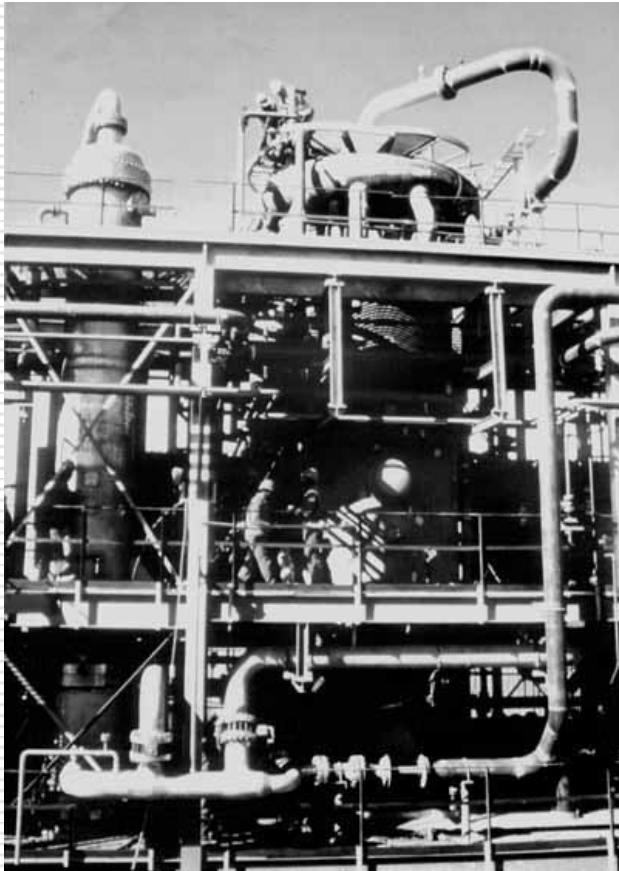
DIY (Do it yourself)

$$\frac{dF_A}{dW} = r_A'$$

⬇

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

⬇

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

Some more work to do!!!

$$C_{Ao} = N_{Ao} / V$$

$$F_{Ao} = C_{Ao} \, v$$

(v = volumetric flowrate)

$$P_{Ao}V = N_{Ao}RT$$

$$C_{Ao} = P_{Ao} / RT$$

$$C_{Ao} = y_{Ao}P_o / RT$$

Get cracking!!!

A gas of pure A at 830 kPa enters a reactor with a volumetric flowrate of 2 litres /s at 500 K. Calculate the entering concentration of A and molar flowrate
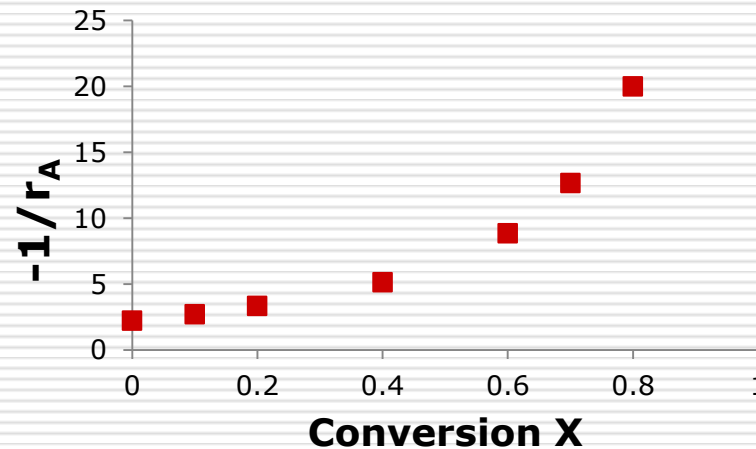
The size of the reactor will depend on the flowrate, reactor kinetics, reactor conditions and desired conversion.
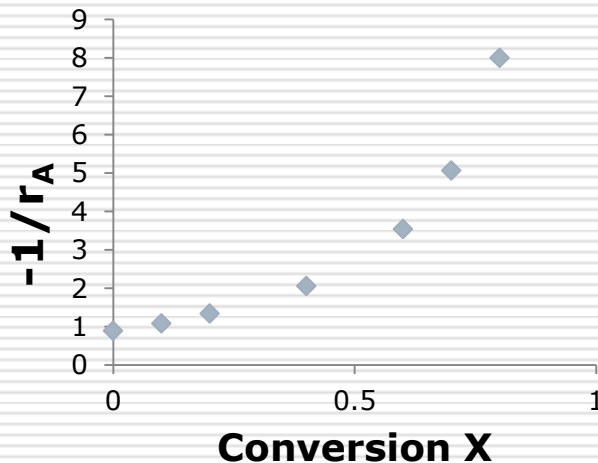
Application of Design equations (CSTR)

For a single reaction $-r_A$ if a function of $C_A \to X$?

For all irreversible reaction of order > 0, as $X \to 1$, $-1/-r_A \to \infty$

For all reversible reaction as $X \to X_e$, $-1/-r_A \to \infty$

Application of Design equations (CSTR volume)

F_{Ao} = 0.4 mol/s

$V = F_{Ao} X / (-r_A)_{exit}$
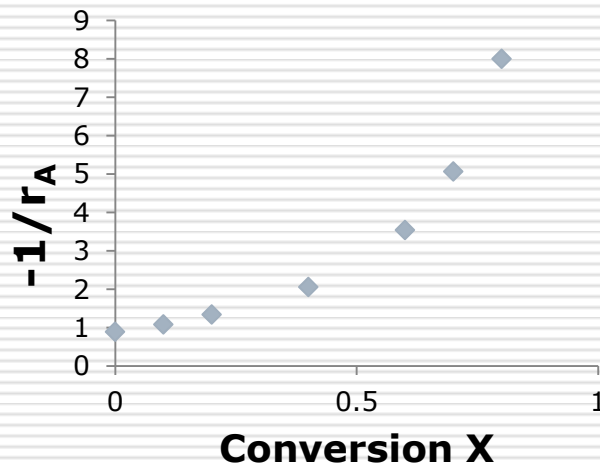
V = 6400 litres

A little too large for comfort!!! Why?

Probably because it is a gas phase reaction

Graphically it is the area of rectangle with height = $F_{Ao} / -r_A$ and base = X

LEVENSPIEL PLOT

Application of Design equations (PFR volume)

$F_{Ao} = 0.4$ mol/s

$V = F_{Ao} \int dX / -r_A$

$V = 2165$ litres

 Compare with CSTR
$V = 6400$ Litres

Numerical techniques to evaluate integral:
1. Trapezoidal rule
2. Simpson's $1/3^{rd}$ rule
3. Simpson $3/8^{th}$ rule
4. Five point Quadrature

Graphically it is the area under the curve

CSTR vs. PFR volume comparison

For isothermal reactions of order greater than zero, the CSTR volume is always greater than PFR volume since CSTR is always operating at the lowest reaction rate.

The PFR on the other hand starts at a high rate at the entrance and gradually decreases to the exit rate, thereby requiring less volume because volume and rate are inversely proportional.

This conclusion may not applicable for autocatalytic reactions, product inhibited reactions and non-isothermal exothermic reactions

Trapezoidal rule

General info

Reactor volume (DIY)

Consider the liquid phase reaction which is to take place in a PFR. A → Products

X	0	0.4	0.8
$-r_A$ (mol/dm^3·s)	0.01	0.008	0.002

The following data was obtained in a batch reactor.

If the molar feed of A to the PFR is 2 mol/s, what PFR volume is necessary to achieve 80% conversion under identical conditions as those under which the batch data was obtained?

Reactor in Series

Given $-r_A$ as a function of conversion, one can also design any sequence of reactors:

Only valid if there are no side streams

$$X_i = \frac{\text{moles of A reacted up to point } i}{\text{moles of A fed to first reactor}}$$

$$F_{Ai} = F_{Ao} - F_{Ao}X_i$$

Reactor in Series (2 CSTR's): DIY

1. Starting with a mole balance, derive expressions for volume of each reactor in terms of conversion

2. For two CSTR's in series 40% conversion is expected in the first reactor. What is the volume of each of the two reactors to achieve 80% conversion overall of entering species A?

X	0	0.1	0.2	0.4	0.6	0.7	0.8
$F_{A0}/-r_A$	0.89	1.09	1.33	2.05	3.54	5.06	8

To achieve the same conversion, the sum of 2 reactor volumes in series is less than volume of 1 CSTR

What would happen if we have n CSTR's in series???

Reactor in Series (2 PFR's): DIY

1. Starting with a mole balance, derive expressions for volume of each reactor in terms of conversion

2. For two PFR's in series 40% conversion is expected in the first reactor. What is the volume of each of the two reactors to achieve 80% conversion overall of entering species A? F_{A0} = 0.4 mol/s

X	0	0.1	0.2	0.4	0.6	0.7	0.8
$F_{A0}/-r_A$	0.89	1.09	1.33	2.05	3.54	5.06	8

To achieve the same conversion, it is immaterial whether you place 2 PFR's in series or use 1 PFR

Reactor Sequencing (Combination)

Consider a PFR between two CSTRs
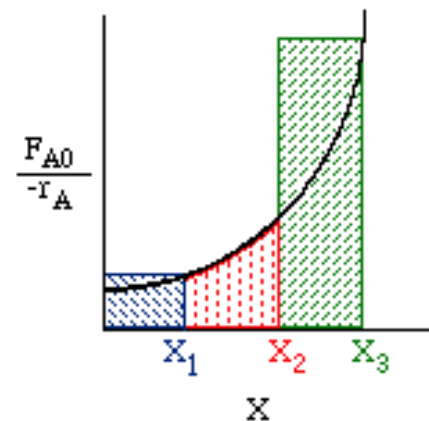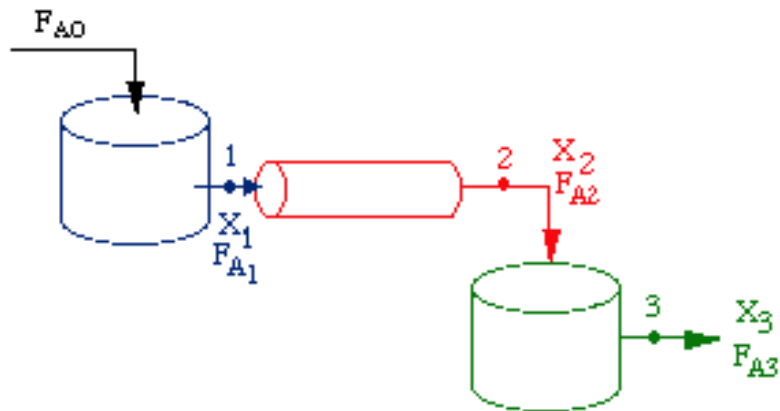
$$V_1 = \frac{F_{A0}X_1}{-r_{A_1}}$$

$$V_2 = \int_{X_1}^{X_2} \frac{F_{A0}}{-r_{A_2}} dX$$

$$V_3 = \frac{F_{A0}(X_3 - X_2)}{-r_{A_3}}$$

Reactor Sequencing (Isomerization)

The isomerization of butane n $C_4H_{10} = i. C_4H_{10}$ was carried our adiabatically in the liquid phase (CSTR – PFR – CSTR) and the following data was obtained

| X	0	0.1	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m^3.hr)	0.89	1.09	1.33	2.05	3.54	5.06

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

So which is the best sequencing option? Any ideas.

Space / Holding / Mean Residence time

The **Space time,** τ, is obtained by dividing the reactor volume by the volumetric flow rate entering the reactor: V/v_o

Space time is the time necessary to process one volume of reactor fluid at the entrance conditions. This is the time it takes for the amount of fluid that takes up the entire volume of the reactor to either completely enter or completely exit the reactor.

V = 0.2 m³   a   b

0.01 m³/s

20 m   20 m
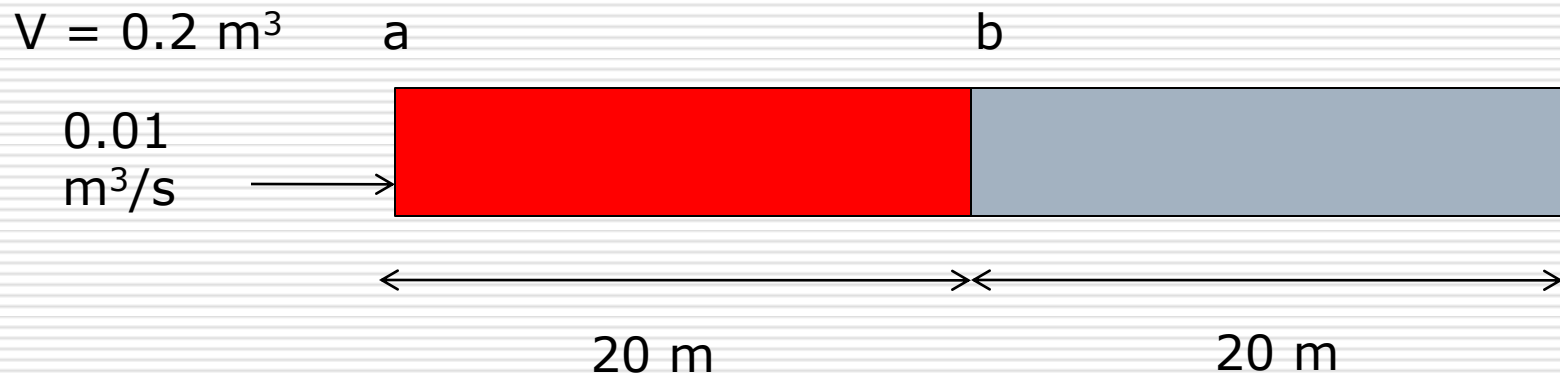
Space Velocity

Space velocity = reciprocal of space time = $1 / \tau$

There is a subtle difference (Beware!!!)

Space time is evaluated at entrance conditions while SV is evaluated at other conditions

LHSV (entrance flowrate measured at liquid feed rate at 60 or 75 ^{o}F) EVEN IF FEED IS VAPOUR AT HIGHER TEMPERATURE

GHSV (entering flowrate is measured at standard temperature and pressure (STP)

Modeling the Digestive System of a Hippopotamus[*]

Matthew Robertson, Fredrik Persson, Brian Vicente, Professor H. Scott Fogler

"Even hippo's like Chemical Reaction Engineering."

Objective Assessment of Chapter

- ➢ Define conversion and space time
- ➢ Write the mole balances in terms of conversion for a batch reactor, CSTR, PFR, and PBR
- ➢ Size reactors either alone or in series once given the molar flow rate of A, and the rate of reaction, - r_A, as a function of conversion X
- ➢ Understand concept of space time and space velocity

I think that everything is possible as long as you put your mind to it and you put the work and time into it. I think your mind really controls everything.