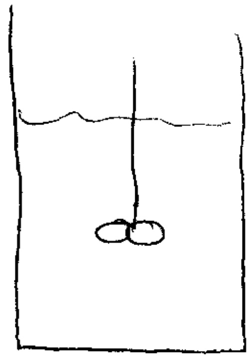
1/24/00

1/

Batch Reactor

a) Draw Picture
b) fluid flow
c) what is changing
— graph
d) assumptions



Show encyclopedia & Chem Tech

1) Assume contents are well-mixed

2) At ($t=0$) start A is added where A

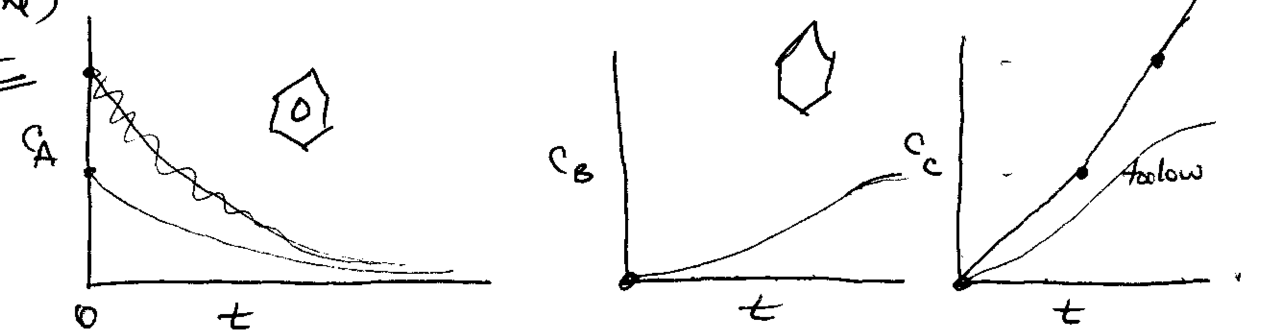
$+ 3H_2$ dehydrogenation

A → B + 3C

~~Benzene~~ Cyclo → ~~cyclohexane~~ Benzene + Hydrogen

(quick one)

Plot



How do we capture this in engineering?

Control Volume?

Mass Balance: M_R total mass of fluid in reactor

chem principles
heat T.
mass T.
(Eq stage)

$$\frac{dM_R}{dt} = 0 - 0$$

accumulation = in − out

∴ the mass in the reactor does not change with time

We need a mole balance < total / component

$$A: \quad \frac{dN_A}{dt} = 0 - 0 + \underline{\qquad}$$

New term — what is it?

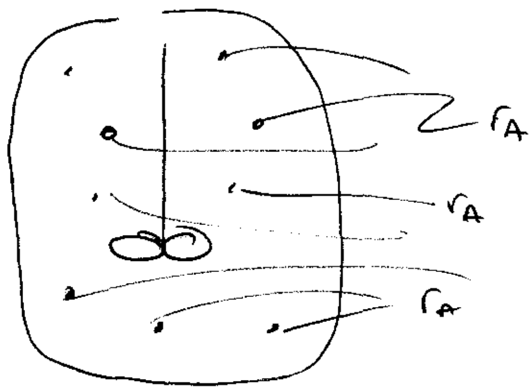
Since it is a reactor I hope a reaction occurs!

1/24/00 ch 1 - Batch 2/

Reaction term : $r_A V$

$$\left(\frac{\text{mol A generated (formed)}}{\text{s m}^3}\right)\left(\text{m}^3\right)$$

Since reactor is well-mixed, then the rate of reaction is the same anywhere in the reactor (at a given time



Well-mixed Assumption

what do reaction rates look like?

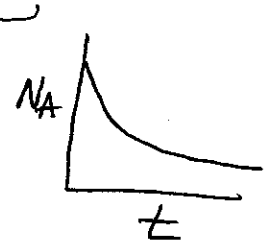
$r_A = -k C_A$ (Book has $-r_A = k C_A$)

k: always positive

C_A: concentration of A is always positive (this is the real world)

A: $\frac{dN_A}{dt} = r_A V = -k C_A V$ ← Volume is always positive

$\therefore \frac{dN_A}{dt} < 0$



1/24/00 Ch 1 – Batch 3

B: $\frac{dN_B}{dt} = r_B V$

always keep subscripts the same in the initial balance

$r_B = kC_A$ (rate of generation of B is positive)

$$\frac{dN_B}{dt} = r_B V = kC_A V$$

C: $\frac{dN_C}{dt} = r_C V$ Very easy!

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

$$r_C = -\frac{c}{a} r_A = \frac{3 \text{ mol } H_2}{-1 \text{ mol Ben}} \frac{\text{mol Ben}}{\text{s m}^3}$$

$$r_C = 3 \frac{\text{mol C}}{\text{mol A}} r_A$$

$$r_C = 3kC_A$$

$$\frac{dN_C}{dt} = 3kC_A V$$

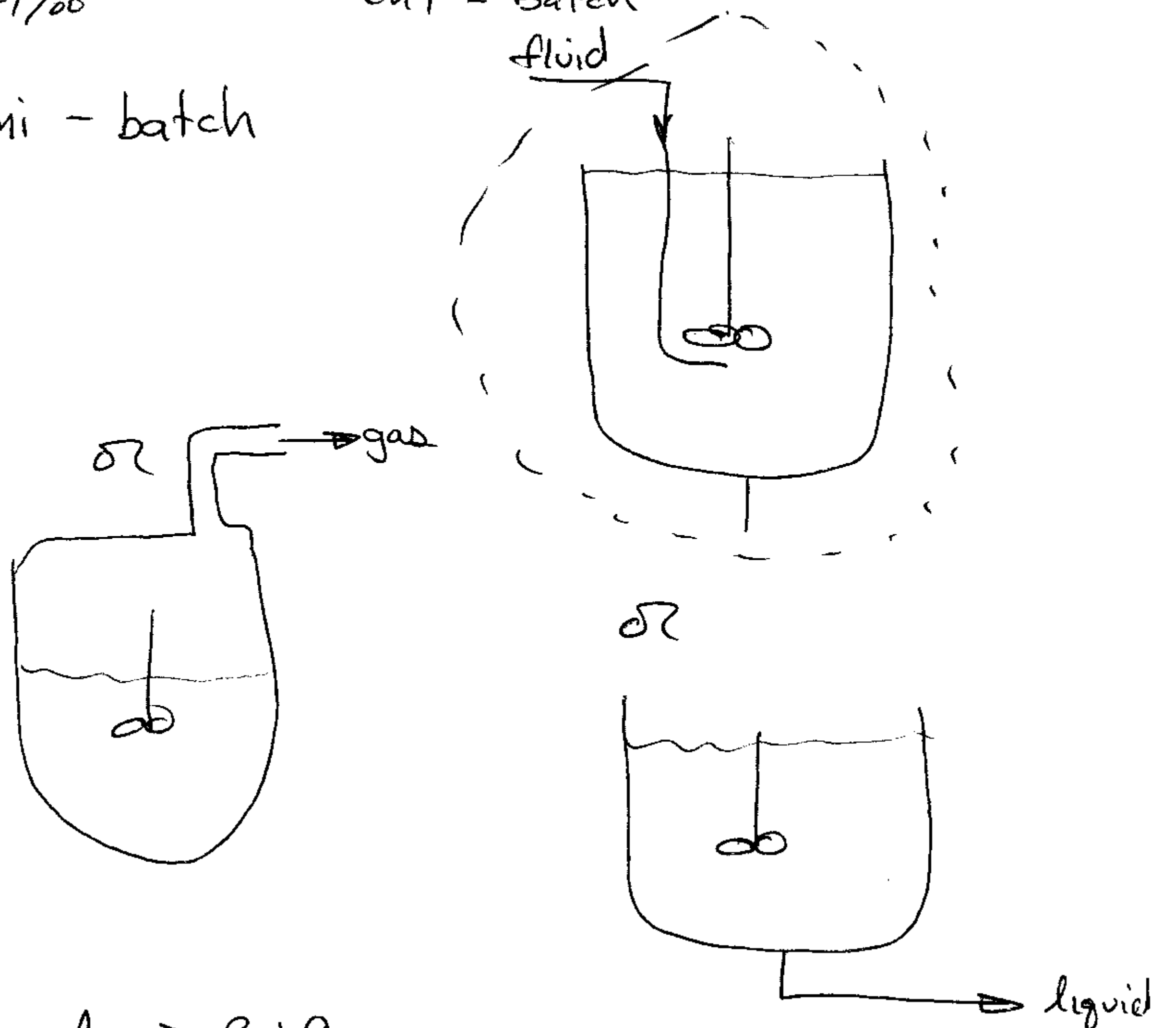
Total Mole balance $N_T = N_A + N_B + N_C$

$$\frac{dN_T}{dt} = \frac{dN_A}{dt} + \frac{dN_B}{dt} + \frac{dN_C}{dt} = -kC_A + kC_A + 3kC_A$$

$$\frac{dN_T}{dt} = 3kC_A V$$

1/24/00 CH1 - Batch 4

Semi - batch



$A \rightarrow B + C$

A is being added to a fluid X

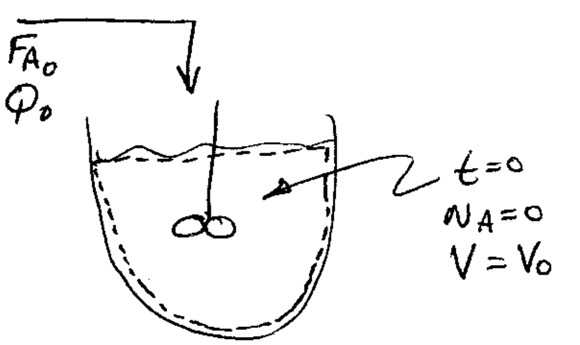
at $t=0$ $\quad N_A = 0$ in tank $\quad$ eg. tank is filled only with fluid X

Component mole bal 1) C.V. 2) well mixed

$$A: \quad \frac{dN_A}{dt} = F_{A_0} + 0 + r_A V$$

accum = in − out + gen

where $r_A = -kC_A$



<u>mass balance ?</u> team quick one

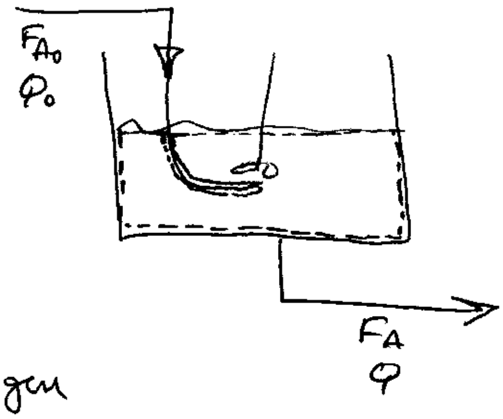
$$\frac{dm_T}{dt} = \rho_0 \varphi_0 - 0$$

1/24/00 Ch 1 – CSTR 5

Now add fluid and remove fluid

1) C.V. [ ]

2) Still assume well-mixed



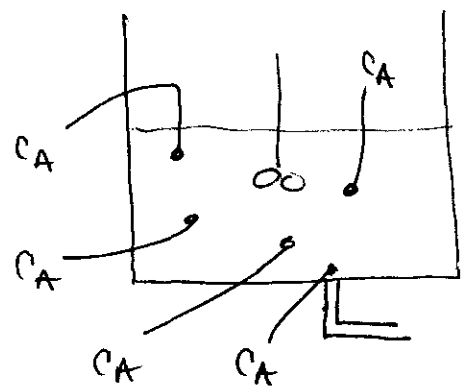
$A \Rightarrow B + C$

accum = in – out + gen

$$\frac{dN_A}{dt} = F_{A0} - F_A + r_A V$$ done! very easy!!

<u>What does well mixed mean?</u>

All C_A's are the same?

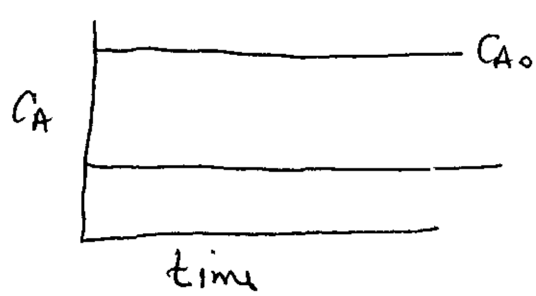


Called a continuous stirred tank reactor (CSTR)

at steady-state $dN_A/dt = 0$

$$\frac{F_A - F_{A0}}{r_A} = V$$ ← find the size of the reactor

Draw a plot of C_A vs t for a CSTR at S.S.



1/31/00

Review: M.B.

Batch
Semi batch
CSTR

C.V – fluid
Assumption – well mixed

accum = in – out + gen

$$\frac{d}{dt}(C_A V) = 0 - 0 + r_A V \quad \text{Batch}$$

$$\left.\begin{aligned} &= F_{A0} - 0 + r_A V \\ &= 0 - F_A + r_A V \end{aligned}\right\} \text{semi batch}$$

$$\frac{d}{dt}(C_A V) = F_{A0} - F_A + r_A V \quad \underline{\underline{\text{CSTR}}}$$

objectives

1) Derive M.B. for 4 types of reactors

2) State assumptions

Discuss <u>Reactor Design Probs</u>

Assign <u>Homework</u> 2-6

Tubular Reactors Section 1.4.2 9/1/94 - 6

continuous flow of fluid

F_{A0}
F_{B0}

F_A
F_B

How do we model – ask a student to derive the equation

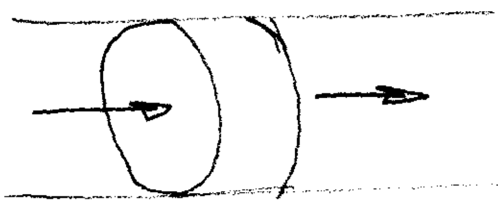
$$0 = F_{A_0} \cancel{- F_A + r_A V} \ ?$$

How can a long tube be perfectly mixed ?

What do we hope will happen in this Reactor? $A + B \rightarrow C$

Show Transparency PFR

Define a control Volume of a stationary

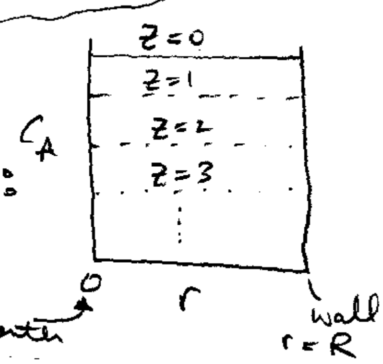


dV
or
A dz (if area is constant)

Assume that there are no radial or axial gradients, or within plug the fluid is perfectly mixed

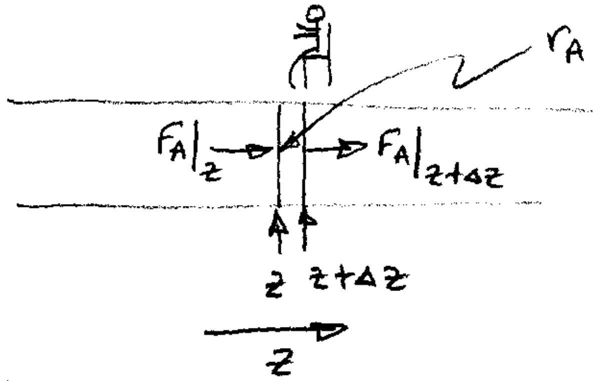
Plug Flow
and no mixing
or dispersion
or diffusion
in z direction

So with respect to Radial position:



9/1/94-7

fluid flows as a plug

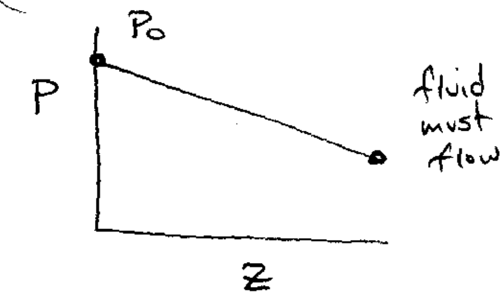


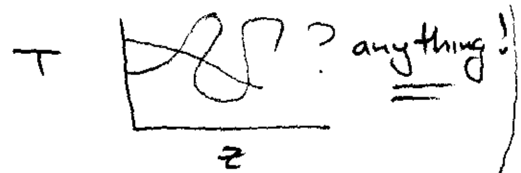
$r_A = f(c_i, T \text{ and } P)$

Skip 7

$$\left\{ \begin{array}{ll} \frac{dc_i}{dr} = 0 & \frac{\partial c}{\partial \theta} = 0 \\ \frac{\partial T}{\partial r} = 0 & \frac{\partial T}{\partial \theta} = 0 \\ \frac{\partial P}{\partial r} = 0 & \frac{\partial P}{\partial r} = 0 \end{array} \right\}$$

But





accum = in - out + gen

$$\Delta V \frac{dc_A}{dt} = F_A|_z - F_A|_{z+\Delta z} + r_A \Delta V$$

in with respect to z

out with respect to z

$$\frac{dc_A}{\partial t} = \frac{F_A|_z - F_A|_{z+\Delta z}}{\Delta V} + r_A$$

$$A\Delta z = \Delta V$$

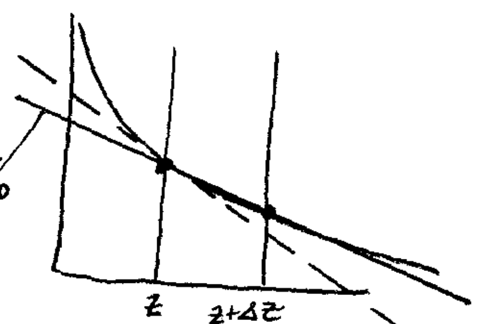
$$\frac{\partial c_A}{\partial t} = \frac{F_A|_z - F_A|_{z+\Delta z}}{A\Delta z} + r_A$$

$$= \frac{F_A|_z - F_A|_{z+\Delta z}}{A(\Delta z + z - z)}$$

$$\frac{\partial c_A}{\partial t} = -\boxed{\frac{\left(F_A|_{z+\Delta z} - F_A|_z\right)}{z+\Delta z - z}} + r_A$$

Before limit $\Delta z \to 0$

definition of a derivitive



Slope at z which is $\frac{dc_A}{dz}$ or $\frac{1}{\varphi}\frac{dF_A}{dz}$

take limit $\Delta z \to 0$

$$\frac{\partial c_A}{\partial t} = -\frac{\partial F_A}{A\partial z} + r_A$$

At steady state:

$$\frac{dF_A}{A\,dz} = r_A$$

if $V = Az$

$dV = d(Az) = A\,dz$ if A is constant

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

$$V = \int \frac{dF_A}{r_A}$$

Read Section 1.4.3 Packed-Bed Reactors : $\frac{dF_A}{dW} = r_A'$

is this a Fraternity Sorority thing?

Read section on industrial reactors 1.5

Nice examples of

size – in jacuzzis!

cost

flowrates

# of tubes (2050!) 5cm ID
12 m long