Introduction to Chemical Reactors

August 2013

2. Design of Isothermal Reactors

René Bañares-Alcántara

room: 8239

tel: 73-9530

rene.banares@eng.ox.ac.uk

Objectives and sources

- Develop the mole balance / design equations for
  - Batch reactors
  - CSTR (continuous stirred tank reactors)
  - PFR (plug flow reactors) / PFTR (plug flow tubular reactors)
  - PBR (packed bed reactors)
- Size different types of reactors (volume and/or residence time)
- Design reactor systems (series of reactors)
- Compare and select between CSTR and PFR

Sources for isothermal reactors
- Schmidt: chapters 2 and 3
- Fogler: sections 1.2-1.4, 2.2-2.5

We start by modelling the simplest type of reaction system:
- one reaction
- isothermal
- occurring in one fluid phase
- inside a single idealised reactor.

We will relax each of these constraints in the next lectures.

The design of a reactor (through the development of a *model*) depends on the combination of
(a) the type of reactor,
(b) the kinetics, and
(c) the stoichiometry of the reaction.

As a result there is a *huge* number of possible models.

Attempting to memorise them would be a wrong strategy.

Thankfully, there is a *systematic and general procedure* to design reactors …

Types of reactors

Chemical reactors

    Batch

    Continuous flow

        Continuous Stirred Tank Reactor (CSTR)

        Plug Flow Reactor (PFR)

        Packed Bed Reactor (PBR)

photographs of real reactors:
`http://www.engin.umich.edu/~cre/01chap/html/reactors/`
`    photos.htm`

▶

Algorithm for isothermal reactor design

1. Design Equation

2. Rate Law

3. Stoichiometry

$$\text{Design eqn} = \text{fn}\,(\mathbf{r})$$

$$\mathbf{r} = \text{fn}\,(C_A, C_B, ...)$$

$$C_J = \text{fn}\,(X) = \text{fn}\,(\text{stoichiometry})$$

4. Combine 1, 2 & 3
5. Evaluate/Solve
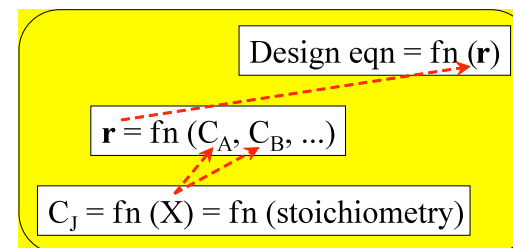
2.1 Reactor design equations

The **General Mole Balance equation** (GMB) is a material balance around a reactor, in fact, around any item of equipment.

When the **GMB** is specialised for a type of reactor we obtain its **design equation**, which is nothing more than its material balance. A design equation is generally a *differential equation.*

Designing a reactor is synonymous to solving its design equation.

General Mole Balance equation (GMB)

ACCUMULATION = IN - OUT + GENERATION   [mol/T]

$$\frac{dN_J}{dt} = F_{J0} - F_J + G_J$$

Generation term:

- in a spatially uniform system: $G_J = \nu_j r V$

- when properties (C_J, T) are a function of position:

$$G_J = \int_V \nu_j r \, dV$$

We will derive the design equations for
  – Batch
  – CSTR
  – PFR
  – PBR
and solve them for 1st and 2nd order reactions.

(remember that we are assuming one reaction, a single fluid phase, and isothermal conditions)
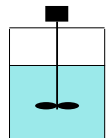

Batch reactors

Batch reactor stirring apparatus
(from [Fogler 05])

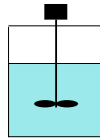Batch reactor
(from [Fogler 05])

Batch reactors (1)

1. Fundamentally _unsteady_, all variables change in time.

2. Mixture is assumed to be perfectly mixed,
    i.e. _uniform_ (in space) C_J and T

from GMB equation

$$\frac{dN_j}{dt} = F_{j0} - F_j + V\nu_j r \quad \Rightarrow \quad \boxed{\frac{dN_j}{dt} = V\nu_j r}$$

$$F_{j0} = F_j = 0$$

Batch reactors (2)

$$\frac{dN_j}{dt} = V\nu_j r$$

$$\frac{dN_j}{dt} = \frac{d(VC_j)}{dt} = V\frac{d(C_j)}{dt} + C_j\frac{d(V)}{dt} = V\nu_j r \quad \Rightarrow \quad \frac{dC_j}{dt} = \nu_j r$$

V constant

$N_j = VC_j$ | V constant

$C_j = C_{j0}(1-X)$
$\therefore \quad dC_j = -C_{j0}dX$

$$\frac{dN_j}{dt} = -N_{j0}\frac{dX}{dt} = V\nu_j r \quad \Rightarrow \quad t = -N_{j0}\int_0^X \frac{dX}{V\nu_j r(X)} = -C_{j0}\int_0^X \frac{dX}{\nu_j r(X)}$$

$N_j = N_{j0}(1-X)$ | V constant

Batch reactors - solutions
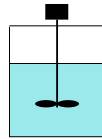
1st order reaction

$$A \rightarrow B \qquad r = kC_A$$

into design eqn:

$$\frac{dC_A}{dt} = -kC_A$$

$$BC: C_A = C_{A0} \quad @\ t = 0$$

separate

integrate

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^t -kdt$$

$$\ln\frac{C_A}{C_{A0}} = -kt$$

solve

$$C_A = C_{A0}e^{-kt}$$

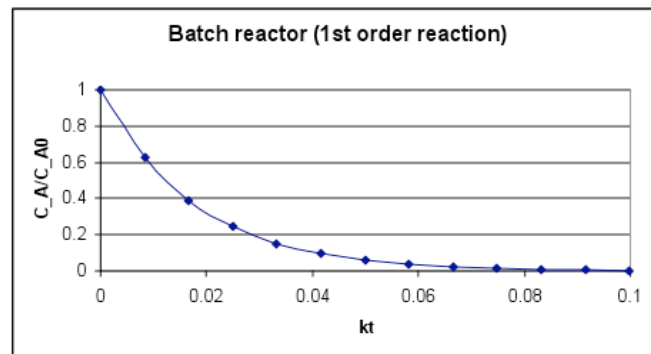### 2nd order reaction

$$A \rightarrow B \qquad r = kC_A^2$$

into design eqn:

$$\frac{dC_A}{dt} = -kC_A^2$$

$$BC: C_A = C_{A0} \quad @\ t = 0$$

separate

integrate

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^t -kdt$$

$$\left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right] = kt$$

solve

$$C_A = \frac{C_{A0}}{1 + kt\,C_{A0}}$$

Batch reactors

The typical behaviour of a first order reaction in a batch reactor is (plotting C_A/C_{A0} vs kt):

Batch reactor (1st order reaction)

The idea is always the same:

1. Start from the **GMB**.
2. **Specialise it** according to the type of reactor.
3. Substitute in the expression for **reaction rate**.
4. **Solve it**, i.e. integrate a differential equation.

The solution is an expression of how the product/ reactant concentration varies as a function of time (or residence time, or reactor volume or length)

Alternatively, it allows to predict the required reaction time (or residence time, or reactor volume or length) given a required product/reactant concentration.
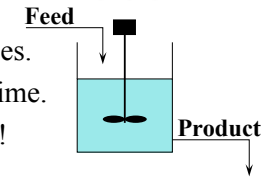
Continuous Stirred Tank Reactor (CSTR)

Feed

Product
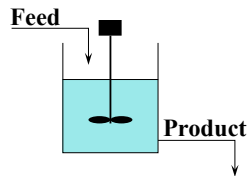
Cutaway view of CSTR
(from [Fogler 05])

Continuous Stirred Tank Reactor (CSTR) (1)

Feed

Product

1. Assume perfect mixing, i.e. _uniform_ properties.
2. Assume _steady state_, i.e. props. constant in time.
3. Note: discontinuity where feed is introduced!

from GMB equation

$$\frac{dN_j}{dt} = F_{j0} - F_j + V\nu_j r$$

$$\frac{d(VC_j)}{dt} = V\frac{d(C_j)}{dt} + C_j\frac{d(V)}{dt} \qquad v(C_{j0} - C_j) + V\nu_j r$$

$N_j = VC_j$ V constant

$$V\frac{dC_j}{dt} = v(C_{j0} - C_j) + V\nu_j r$$

Continuous Stirred Tank Reactor (CSTR) (2)

Feed

Product

$$V\frac{dC_j}{dt} = v(C_{j0} - C_j) + V\nu_j r$$

$$\tau = \frac{V}{v}$$

$$\frac{dC_j}{dt} = \frac{1}{\tau}(C_{j0} - C_j) + \nu_j r \qquad \Rightarrow \qquad C_{j0} - C_j = -\tau\nu_j r$$

non steady state   steady state
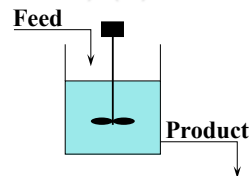
Continuous Stirred Tank Reactor (CSTR) (3)

Feed

Product

steady state

$$C_{j0} - C_j = -\tau\nu_j r \qquad \Rightarrow \qquad V = \frac{-F_{j0}X}{\nu_j r}$$

$\times$ v

$$F_{j0} - F_j = -V\nu_j r$$

$$X = \frac{F_{j0} - F_j}{F_{j0}} \qquad F_{j0}X = -V\nu_j r$$

CSTR –solution 1st order reaction

1st order reaction

$$A \rightarrow B \qquad r = kC_A$$

into steady state design eqn:

$$C_{A0} - C_A = \tau\, kC_A$$

solve

$$C_A = \frac{C_{A0}}{1 + k\tau}$$

this is a constant value! (not a function of time)

$\dfrac{C_A}{C_{A0}}$

$\dfrac{1}{1+k\tau}$

t
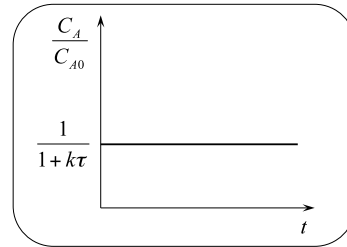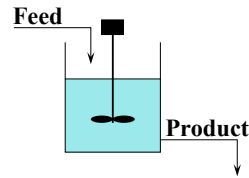
CSTR –solution 2nd order reaction

2nd order reaction

$$A \rightarrow B \qquad r = kC_A^2$$
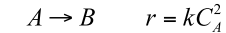
into steady state design eqn:

$$C_{A0} - C_A = \tau\, kC_A^2$$

solve

$$\tau\, kC_A^2 + C_A - C_{A0} = 0$$

$$C_A = \frac{-1 \pm \sqrt{4\tau\, kC_{A0} + 1}}{2\tau\, k}$$

only +ve root makes sense; also sqrt(4kτC_{A0}+1) > 1

$$C_A = \frac{-1 + \sqrt{4\tau\, kC_{A0} + 1}}{2\tau\, k}$$

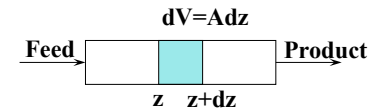*also constant! (not fn(t))*
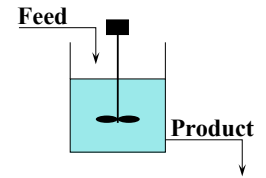
The PFR design equation is going to be derived as an analogy to the Batch reactor design equation this time (rather than from first principles, i.e. the GMB).

The result is, of course, the same.

Plug Flow Reactor (PFR)

aka Plug Flow Tubular Reactor (PFTR)

1. Assume velocity profile of plug or piston flow (high turbulence; true at high flow rates, i.e. Re > 10^4)
   – *uniform* F_J and uniform properties over cross-section normal to flow
   – no axial mixing (not true in turbulent flow!!!)
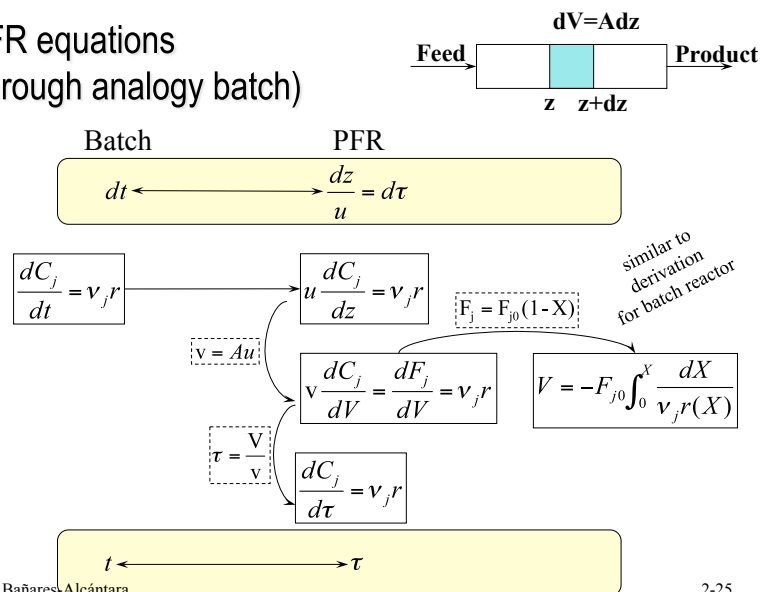2. *Steady state* operation (but properties change along the PFR!).

Note that, *for constant density*, a volume element in a PFR behaves as a batch reactor moving along *z*, i.e. there is a correspondence between
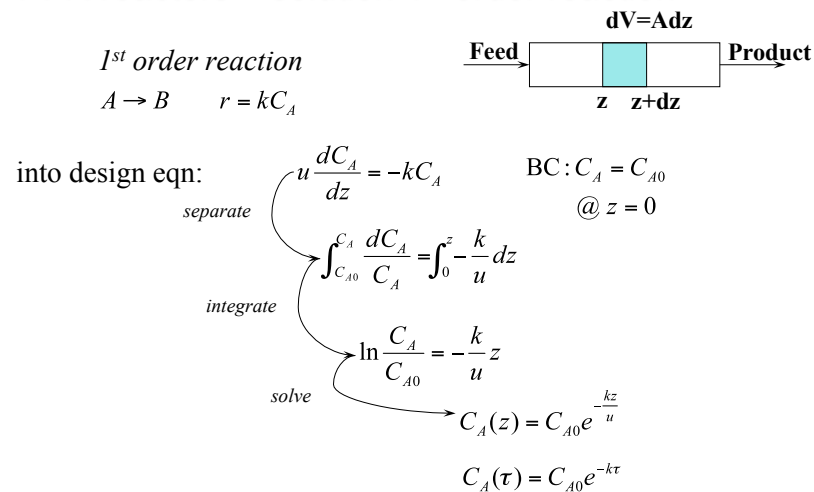- time in a batch reactor and
- position in a PFR.

PFR equations (through analogy batch)

dV=Adz

Feed → | z | z+dz | → Product

Batch	PFR

$$dt \longleftrightarrow \frac{dz}{u} = d\tau$$

$$\frac{dC_j}{dt} = \nu_j r \longrightarrow u\frac{dC_j}{dz} = \nu_j r$$

$$F_j = F_{j0}(1-X)$$

similar to derivation for batch reactor

$$v = Au$$

$$v\frac{dC_j}{dV} = \frac{dF_j}{dV} = \nu_j r \qquad V = -F_{j0}\int_0^X \frac{dX}{\nu_j r(X)}$$

$$\tau = \frac{V}{v}$$

$$\frac{dC_j}{d\tau} = \nu_j r$$

$$t \longleftrightarrow \tau$$

PFR reactors – solution 1st order reaction

dV=Adz

Feed → | z | z+dz | → Product

1st order reaction

$$A \to B \qquad r = kC_A$$

into design eqn:

separate
$$u\frac{dC_A}{dz} = -kC_A \qquad BC: C_A = C_{A0}$$
$$@ \ z = 0$$

integrate
$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^z -\frac{k}{u}dz$$

$$\ln\frac{C_A}{C_{A0}} = -\frac{k}{u}z$$
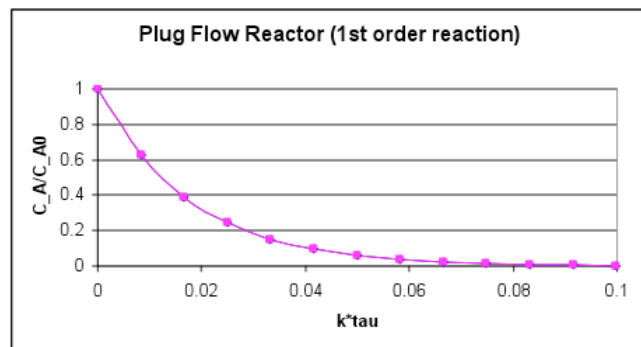
solve
$$C_A(z) = C_{A0}e^{-\frac{kz}{u}}$$

$$C_A(\tau) = C_{A0}e^{-k\tau}$$

Plug flow reactors

The typical behaviour of a first order reaction in a PFR is (plotting C_A/C_{A0} vs $k\tau$):
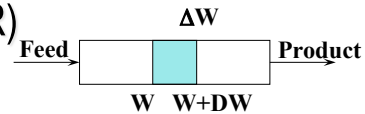

Plug Flow Reactor (1st order reaction)

PFR reactors – solution 2nd order reaction

dV=Adz

Feed → | z | z+dz | → Product

2nd order reaction

$$A \to B \qquad r = kC_A^2$$

into design eqn:

separate
$$u\frac{dC_A}{dz} = -kC_A^2 \qquad BC: C_A = C_{A0}$$
$$@ \ z = 0$$

integrate
$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^z -\frac{k}{u}dz$$

$$\frac{1}{C_{A0}} - \frac{1}{C_A} = -\frac{k}{u}z$$

solve
$$\frac{1}{C_A} = \frac{1}{C_{A0}} + \frac{k}{u}z = \frac{u + kC_{A0}z}{uC_{A0}}$$

$$C_A(z) = \frac{uC_{A0}}{u + kC_{A0}z} \qquad C_A(\tau) = \frac{C_{A0}}{1 + k\tau C_{A0}}$$

Packed Bed Reactor (PBR)

ΔW

Feed → [W W+DW] → Product
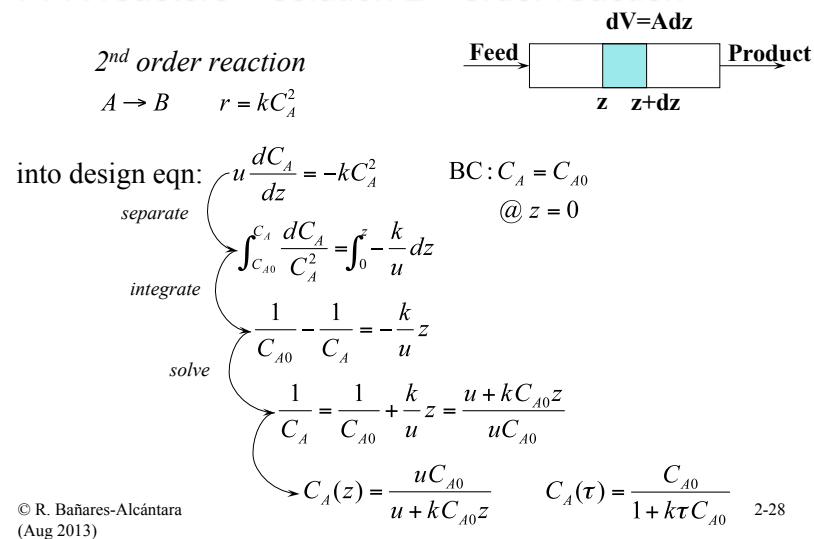
1. Involves fluid-solid heterogeneous reactions, i.e. catalysed.

2. Reaction rate, r_A' [mole s^{-1} kgcat^{-1}], based on mass of catalyst, W, rather than on reactor volume, V.
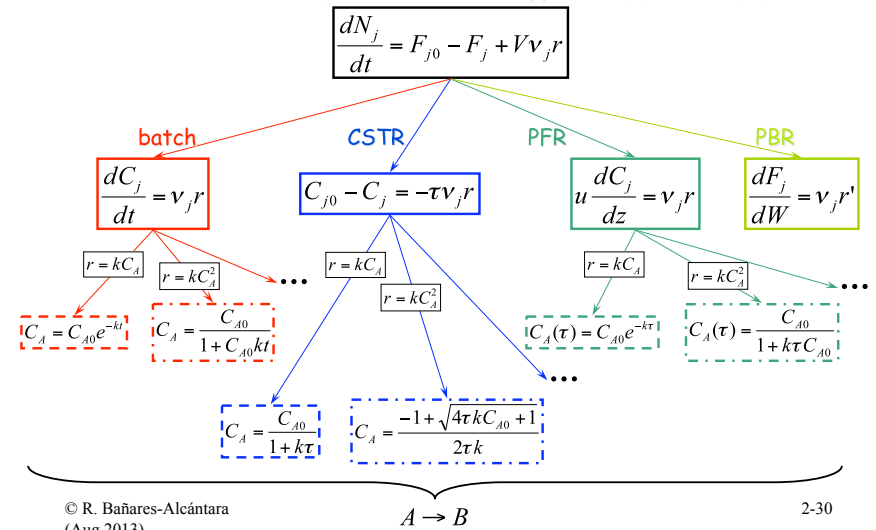
Derivation of design equation similar to PFR, but in terms of W:

$$\frac{dF_j}{dV} = \nu_j r \quad \rightarrow \quad \frac{dF_j}{dW} = \nu_j r' \quad \rightarrow \quad F_j = F_{j0}(1-X)$$

in terms of X: $\quad \nu_j r' = -F_{j0}\dfrac{dX}{dW}$

integrating (X = 0 @ W = 0): $\quad W = -F_{j0}\displaystyle\int_0^X \frac{dX}{\nu_j r'(X)}$

… all sorts of equations for C_A = fn(t) or fn(τ)

$$\frac{dN_j}{dt} = F_{j0} - F_j + V\nu_j r$$

batch
$$\frac{dC_j}{dt} = \nu_j r$$

$r = kC_A$ → $C_A = C_{A0}e^{-kt}$

$r = kC_A^2$ → $C_A = \dfrac{C_{A0}}{1 + C_{A0}kt}$ …

CSTR
$$C_{j0} - C_j = -\tau \nu_j r$$

$r = kC_A$
$r = kC_A^2$

$C_A = \dfrac{C_{A0}}{1 + k\tau}$

$C_A = \dfrac{-1 + \sqrt{4\tau kC_{A0} + 1}}{2\tau k}$ …

PFR
$$u\frac{dC_j}{dz} = \nu_j r$$

$r = kC_A$ → $C_A(\tau) = C_{A0}e^{-k\tau}$

$r = kC_A^2$ → $C_A(\tau) = \dfrac{C_{A0}}{1 + k\tau C_{A0}}$ …

PBR
$$\frac{dF_j}{dW} = \nu_j r'$$

$A \rightarrow B$

Summary of reactor design equations

	differential form	algebraic form	integral form
Batch	$\dfrac{dC_j}{dt} = \nu_j r$		$t = -C_{j0}\displaystyle\int_0^X \frac{dX}{\nu_j r(X)}$
CSTR	$\dfrac{dC_j}{dt} = \dfrac{1}{\tau}\left(C_{j0} - C_j\right) + \nu_j r$	$C_{j0} - C_j = -\tau \nu_j r$ $V = \dfrac{-F_{j0}X}{\nu_j r}$	
PFR	$\dfrac{dC_j}{d\tau} = \nu_j r$		$V = -F_{j0}\displaystyle\int_0^X \frac{dX}{\nu_j r(X)}$
PBR	$\dfrac{dF_j}{dW} = \nu_j r'$		$W = -F_{j0}\displaystyle\int_0^X \frac{dX}{\nu_j r'(X)}$

2.2 Examples of isothermal reactor design

Two examples of reactor design:

- calculation of the required CSTR volume to achieve an 80% conversion with a 3rd order reaction.

- calculation of the required PFR volume (and number of tubes) to achieve an 80% conversion with a 1st order reaction. A plot of conversion as a function of reactor length is also produced.

Algorithm for Isothermal Reactor Design

1. Obtain **Design Equation**

2. Determine **Rate Law**

3. Determine **Stoichiometry**

> Design eqn = fn (**r**)
>
> **r** = fn (C_A, C_B, ...)
>
> C_J = fn (X) = fn (stoichiometry)

4. Combine 1, 2 and 3
5. Evaluate to calculate

V = fn(X) or X = fn(V) or C_j = fn(t) or = $fn(\tau)$ or = fn(V) …

  a. Graphically (1/r_A vs. X ; see ahead Levenspiel plots)
  b. Numerically
  c. Analytically
  d. Use computer-based solvers
     (e.g. MATLAB, Polymath, Maple, Mathematica, ...)
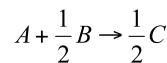

Example - size a CSTR

Gas phase rxn @ T_0=50 C; P_0=10 atm; F_0=8 mole/s (equimolar in A and B).

$$2\,A + B \rightarrow C \qquad\qquad k = 5 \text{ mol dm}^{-3}\text{ s}^{-1}$$

What should be the CSTR volume to achieve a conversion of 0.8?

$F_0 = 8$ mol/s
(50% A,
50% B)

2A + B → C
k = 5 mol/lt/s

V = ?

X = 0.8
50 C, 10 atm

Example - size a CSTR (2)

$F_0 = 8$ mol/s
(50% A,
50% B)

2A + B → C
k = 5 mol/lt/s

V = ?

X = 0.8
50 C, 10 atm

$$A + \frac{1}{2}B \rightarrow \frac{1}{2}C$$
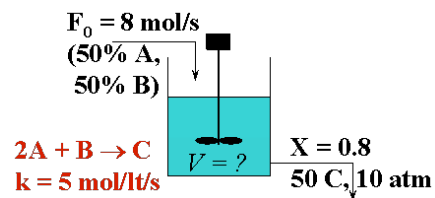
1. Design Equation:

$$V = \frac{-F_{A0}X}{\nu_A r}$$

2. Rate Law:

$$r = kC_A^2 C_B$$

3. Stoichiometry:

$$\nu_A = -1 \qquad \nu_B = -1/2 \qquad \nu_C = 1/2$$

$$\delta = 0.5 - 1 - 0.5 = -1$$

$$\varepsilon = y_{A0}\delta = (0.5)(-1) = -0.5$$

Conc for variable V systems

$$C_A = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right) = C_{A0}\frac{(1-X)}{(1-0.5X)}$$

$$C_B = C_{A0}\frac{\left(\Theta_B - \frac{\nu_B}{\nu_A}X\right)}{(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right) = C_{A0}$$

$$\Theta_B = 1$$

$$C_{A0} = \frac{y_{A0}P_0}{RT_0} = \frac{0.5 \times 10}{0.082 \times (50+273)}$$

$$= 0.1888\left[\frac{mol}{lt}\right]$$

Example - size a CSTR (3)

$F_0 = 8$ mol/s
(50% A, 50% B)

$2A + B \rightarrow C$
$k = 5$ mol/lt/s

$V = ?$

$X = 0.8$
50 C, 10 atm
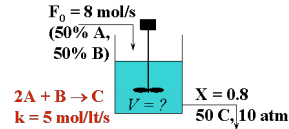
4. *Combine*

$$V = \frac{-F_{A0}X}{\nu_A r} = \frac{-F_0 y_{A0} X}{\nu_A k \left[C_{A0}^2 \dfrac{(1-X)^2}{(1-0.5X)^2} \cdot C_{A0} \right]} =$$

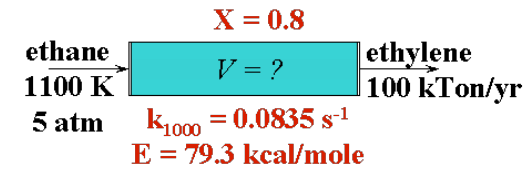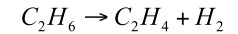$$= \frac{-(8)(0.5)(0.8)}{(-2)(5)\left[(0.1888)^3 \dfrac{0.2^2}{(1-0.5(0.8))^2}\right]} = 428.1 \left[dm^3\right]$$

$$V = 0.428 \left[m^3\right]$$

Example - size a PFR

Calculate V_{PFR} to produce 100 kTon/yr of ethylene from pure ethane@ T_0=1100 K and P_0 = 5 atm. Assume a conversion of 80%.

$k_{1000\ K} = 0.0835\ s^{-1}$; $E = 79.3$ kcal/gmole

$C_2H_6 \rightarrow C_2H_4 + H_2$

X = 0.8

ethane
1100 K
5 atm

$V = ?$

$k_{1000} = 0.0835\ s^{-1}$
E = 79.3 kcal/mole

ethylene
100 kTon/yr

Example - size a PFR (2)

X = 0.8

ethane 1100 K 5 atm — $V = ?$ — ethylene 100 kTon/yr
$k_{1000} = 0.0835\ s^{-1}$
E = 79.3 kcal/mole

$$C_2H_6 \rightarrow C_2H_4 + H_2$$
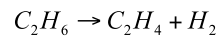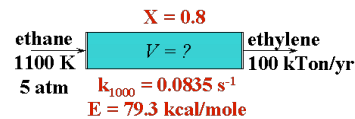
1. *Design Eqn:* $\quad V = -F_{A0}\displaystyle\int_0^X \frac{dX}{\nu_A r}$

2. *Rate Law:* $\quad r = kC_A$

3. *Stoichiometry:* $\nu_A = -1$ $\quad \varepsilon = y_{A0}\delta = (1)(1) = 1$
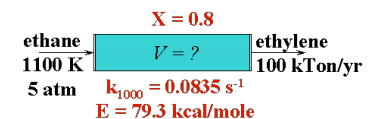
$$C_A = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\left(\frac{T_0}{T}\right)\left(\frac{P}{P_0}\right) = C_{A0}\frac{(1-X)}{(1+X)}$$

$$C_B = C_C = \left(C_{A0} - C_A\right) = C_{A0}\frac{2X}{(1+X)}$$

$$C_{A0} = \frac{y_{A0}P_0}{RT_0} = \frac{(1)(5)}{0.082(1100)} = 0.05543\left[\frac{mol}{lt}\right]$$

$$k_{1100\,K} = k_{1000\,K}\exp\left(\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right) = 3.142\left[s^{-1}\right]$$

Example - size a PFR (3)

X = 0.8

ethane 1100 K 5 atm — $V = ?$ — ethylene 100 kTon/yr
$k_{1000} = 0.0835\ s^{-1}$
E = 79.3 kcal/mole

4. *Combine*

$$F_{A0} = \frac{F_B}{X}$$

$$V = -F_{A0}\int_0^X \frac{(1+\varepsilon X)}{-k\big|_{1100\,K}C_{A0}(1-X)}dX = \frac{F_{A0}}{kC_{A0}}\left[(1+\varepsilon)\ln\frac{1}{1-X} - \varepsilon X\right]$$

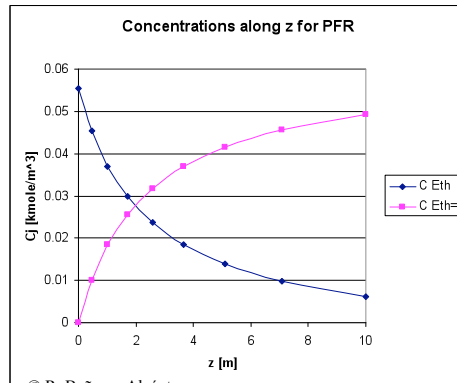$$= \frac{0.1416}{(3.142)(0.05543)}\left[\frac{1m^3}{1000lt}\right]\left[(1+1)\ln\frac{1}{1-0.8} - 0.8\right] = 1.97\left[m^3\right]$$

$$F_{A0} = 100\frac{kTon\,C_2H_4}{yr}\times\frac{1\times10^6\,kg}{1\,kTon}\times\frac{1000\,mole}{28\,kg\,C_2H_4}\times\frac{1\,year}{31.536\times10^6\,s}\times\frac{1}{0.8} = 0.1416\left[\frac{mole}{s}\right]$$

for pipes of D = 5 cm and L = 10 m

$$n_{tubes} = \frac{V}{V_{tube}} = \frac{1.97}{L\frac{\pi D^2}{4}} \approx 100\ tubes$$

Example - size a PFR (4)

To plot: $X \rightarrow V \rightarrow z = \dfrac{V}{A_t\, n_t}$ $C_{Eth} \rightarrow C_{Eth=}$

Conversion vs. z for PFR reactor

Concentrations along z for PFR
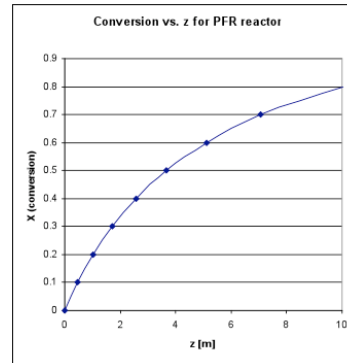
2.3 Comparison between CSTR and PFR

Are CSTR and PFR equivalent?

For positive order reactions PFRs are more efficient than CSTRs, i.e.

- PFRs require a smaller volume to achieve the same conversion, or
- PFRs achieve a larger conversion given a fixed volume.

There are, however, advantages of CSTRs over PFRs, but we will see them in future lectures.

Comparison between CSTRs and PFRs

For a 1st order reaction: $A \rightarrow B$ $r = kC_A$

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

Design Eqns.

CSTR

$$C_{A0} - C_A = \tau\, r$$

$$\tau_{CSTR} = \frac{C_{A0} - C_A}{kC_A}$$

PFR

$$\frac{dC_A}{d\tau} = -r$$

$$\tau_{PFR} = \frac{1}{k}\ln\frac{C_{A0}}{C_A}$$

$$\frac{\tau_{CSTR}}{\tau_{PFR}} = \left(\frac{C_{A0} - C_A}{kC_A}\right)\frac{k}{\ln\dfrac{C_{A0}}{C_A}} = \frac{X}{(1-X)\ln\left(\dfrac{1}{1-X}\right)}$$

X	0	0.2	0.8	0.9	0.99	0.999
τ_{CSTR}/τ_{PFR}	1.0	1.1	2.5	3.9	21.5	144.6
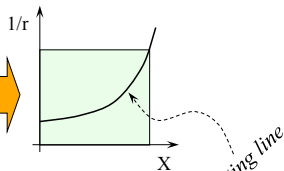
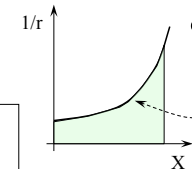## Reactor sizing: {1/r vs. X} or Levenspiel plots

To size a reactor (get its V or τ) we need F_{A0} and $r = fn(X)$

- for CSTR:

$$V = \frac{-F_{A0}X}{\nu_A r} \quad\Rightarrow\quad \frac{V}{F_{A0}} = \left[\frac{1}{r}\right][X] \quad \left[\frac{m^3 s}{mole}\right] \quad\Rightarrow$$

- for PFR:

$$\nu_A r = -F_{A0}\frac{dX}{dV} \quad\Rightarrow\quad \frac{V}{F_{A0}} = \int_{X_{in}}^{X_{out}} \frac{dX}{r} \quad\Rightarrow$$

$$Area \times F_{A0} \Rightarrow V \quad [m^3]$$

$$Area \times \frac{F_{A0}}{\nu_0} \Rightarrow Area \times \frac{\rho}{MW} \Rightarrow \tau \quad [s]$$

operating line

Comparing CSTRs vs. PFRs revisited

For the same F_{A0}, the PFR requires a smaller volume (V) than the CSTR to achieve the same conversion (X).

Note: observation valid for isothermal reactions of order greater than zero.

CSTR   PFR $\Delta\left(\dfrac{V}{F_{A0}}\right)$
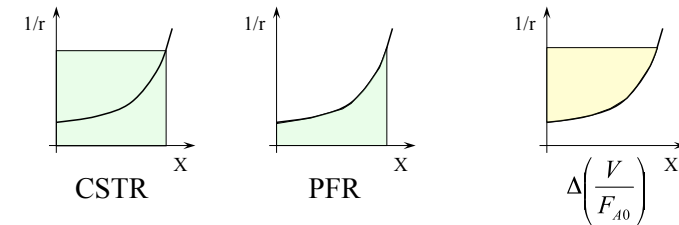
This is because the fresh feed to the CSTR is immediately diluted to exit concentration, hence there is a lower **r**, hence larger volumes or longer residence times are necessary.

2.4 Reactors in series

Reactors can, of course, be connected in series to form a ***system of reactors***.

CSTRs and PFRs behave quite differently when interconnected.

An interesting insight is derived from this analysis:
an infinite number of CSTRs connected in series (each with an infinitesimal volume) is equivalent to a PFR.
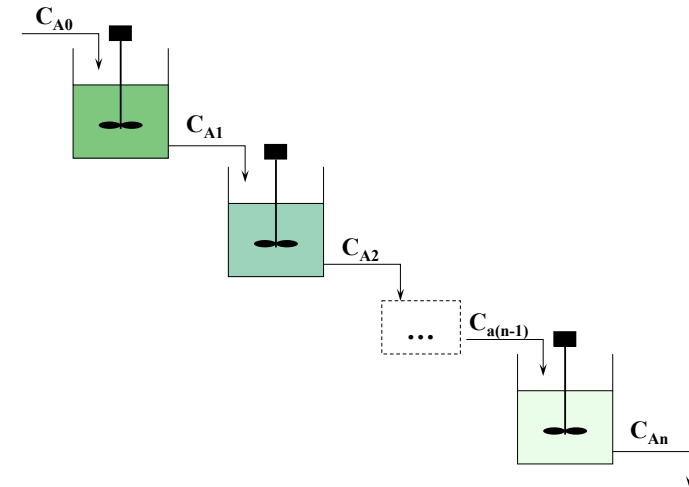
Reactors in series

Spherical reactors
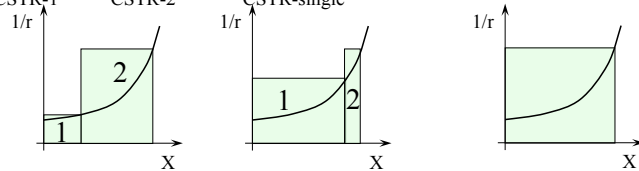connected in series
(from [Fogler 05])

CSTRs in series

Reactors in series - no sidestreams (1)
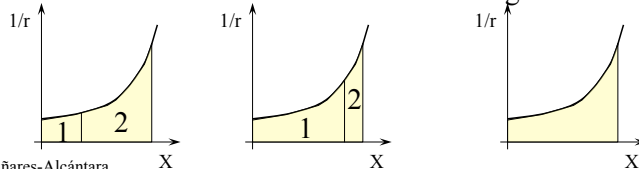
Conversion in each reactor is based on X up to a specified point.

To achieve the same conversion:

- $V_{CSTR-1} + V_{CSTR-2} < V_{CSTR-single}$

- it is immaterial to use 2 PFR in series or a single PFR

Reactors in series - no sidestreams (2)

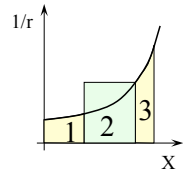We can model a PFR as a series of CSTRs, this is because we can
understand a PFR as $PFR = \sum_{\infty} d(CSTR)$

CSTRs

PFR

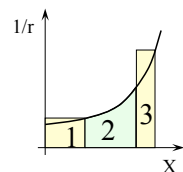## Reactors in series - no sidestreams (3)

CSTRs and PFRs can, of course, be connected in series:

PFR$_1$ + CSTR + PFR$_2$

CSTR$_1$ + PFR + CSTR$_2$

Summary

- General Mole Balance Equation

$$\frac{dN_j}{dt} = F_{j0} - F_j + \int_V \nu_j r\, dV$$

- Batch reactors

$$\frac{dC_j}{dt} = \nu_j r$$

- CSTR

$$C_{j0} - C_j = -\tau \nu_j r$$
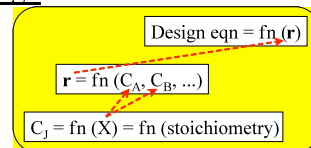
- PFR

$$\frac{dC_j}{d\tau} = \nu_j r$$

- PBR

$$\frac{dF_j}{dW} = \nu_j r'$$

Summary (2)

Algorithm for isothermal reactor design

1. **Design Equation**
2. **Rate Law**
3. **Stoichiometry**
4. Combine 1, 2 and 3
5. Evaluate

Design eqn = fn (**r**)

r = fn (C$_A$, C$_B$, ...)

C$_J$ = fn (X) = fn (stoichiometry)

Reactor sizing: {1/rA vs. X} plots

- CSTRs vs. PFRs
- reactors in series