

CONVERSION AND REACTOR SIZING

- **Objectives:**

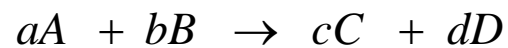
- Define conversion and space time.
- Write the mole balances in terms of conversion for a batch reactor, CSTR, PFR, and PBR.
- Size reactors either alone or in series once given the molar flow rate of A, and the rate of reaction, $-r_A$, as a function of conversion, X .

- **Conversion:** Choose one of the reactants as the basis of calculation and relate the other species involved in the rxn to this basis.
- **Space time:** the time necessary to process one reactor volume of fluid based on entrance conditions (holding time or mean residence time)

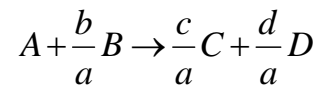
CONVERSION AND REACTOR SIZING

1. Conversion

Consider the general equation



We will choose A as our basis of calculation.



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.

$$X = \frac{\text{Batch}}{(N_{A0} - N_A)} \quad X = \frac{\text{Flow}}{(F_{A0} - F_A)}$$
$$X = \frac{(N_{A0} - N_A)}{N_{A0}} \quad X = \frac{(F_{A0} - F_A)}{F_{A0}}$$

$$X = \frac{\text{Moles of A reacted}}{\text{Moles of A fed}}$$

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.

2. Design Equations

Batch Reactor Design Equations:

$$\begin{aligned} \left[\begin{array}{c} \text{Moles of A} \\ \text{reacted} \\ \text{(consumed)} \end{array} \right] &= \left[\begin{array}{c} \text{Moles of A} \\ \text{fed} \end{array} \right] \cdot \left[\frac{\text{Moles of A reacted}}{\text{Moles of A fed}} \right] \\ &= [N_{A0}] \cdot [X] \end{aligned} \quad [1]$$

Now the # of moles of A that remain in the reactor after a time t , N_A can be expressed in terms of N_{A0} and X ;

$$\begin{aligned} [N_A] &= [N_{A0}] - [N_{A0} \cdot X] \\ N_A &= N_{A0} \cdot (1 - X) \end{aligned} \quad [2]$$

$$\frac{dN_A}{dt} = r_A \cdot V \quad (\text{perfect mixing}) \quad [3]$$

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

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

$$\frac{dN_A}{dt} = 0 - N_{A0} \cdot \frac{dX}{dt} \quad (\text{Since } N_{A0} \text{ is constant}) \quad [4]$$

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

$$N_{A0} \cdot \frac{dX}{dt} = -r_A \cdot V \quad \text{Batch reactor design eq'n} \quad [5]$$

(in differential form)

For a constant volume batch reactor: ($V = V_0$)

$$\frac{1}{V_0} \cdot \frac{dN_A}{dt} = \frac{d(N_A / V_0)}{dt} = \frac{dC_A}{dt}$$

From [3]

$$\frac{dC_A}{dt} = r_A$$

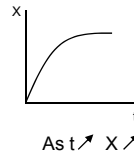
Constant volume batch reactor

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

From [5]

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

Batch time, t, required to achieve a conversion X.



Flow Reactor Design Equations:

For continuous-flow systems, time usually increases with increasing reactor volume.

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

$$\frac{F_{A0}}{\text{inlet molar flow rate}} - \frac{F_{A0} \cdot X}{\text{Molar flow rate at which A is consumed within the system}} = F_A \quad \left| \begin{array}{l} \text{Outlet flow rate} \end{array} \right.$$

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

$$F_{A0} = \underbrace{C_{A0}}_{\text{moles / volume}} \cdot \underbrace{v_0}_{\text{volume / time (volumetric flow rate, dm}^3\text{/s)}}$$

For liquid systems, C_{A0} is usually given in terms of molarity (mol/dm³)

For gas systems, C_{A0} can be calculated using gas laws.

$$C_{A0} = \frac{P_{A0}}{R \cdot T_0} = \frac{y_{A0} \cdot P_0}{R \cdot T_0}$$

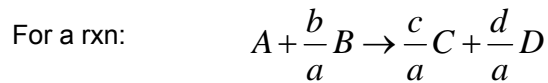
↖ Partial pressure

Entering molar flow rate is

$$F_{A0} = v_0 \cdot C_{A0} = v_0 \cdot \frac{y_{A0} \cdot P_0}{R \cdot T_0}$$

y_{A0} = entering mole fraction of A
 P_0 = entering total pressure (kPa)
 C_{A0} = entering conc'n (mol/dm³)
 R = 8.314 kPa dm³ / mol K
 T = T(K)

CSTR (Design Equation)



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

Substitute for F_A $F_A = F_{A0} - F_{A0} \cdot X$

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

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

PFR (Design Equation)

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

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

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

Substitute back:

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

Separate the variables $V = 0$ when $X = 0$

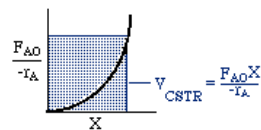
$$V = F_{A0} \cdot \int_0^X \frac{dX}{-r_A}$$

Applications of Design Equations for Continuous Flow Reactors

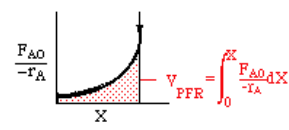
3. Reactor Sizing

Given $-r_A$ as a function of conversion, $-r_A = f(X)$, one can size any type of reactor. We do this by constructing a Levenspiel Plot. Here we plot either $F_{A0} / -r_A$ or $1 / -r_A$ as a function of X . For $F_{A0} / -r_A$ vs. X , the volume of a CSTR and the volume of a PFR can be represented as the shaded areas in the Levenspiel Plots shown below:

CSTR



PFR



Levenspiel Plots

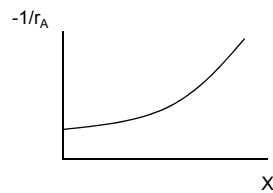
A particularly simple functional dependence is the first order dependence:

$$-r_A = k \cdot C_A = k \cdot C_{A0} \cdot (1 - X)$$

Specific rxn rate
(function of T)
initial conc'n

For this first order rxn, a plot of $1/-r_A$ as a function of X yields :

$$-\frac{1}{r_A} = \frac{1}{k \cdot C_{A0}} \cdot \left(\frac{1}{1 - X} \right)$$



Example: Let's consider the isothermal gas-phase isomerization:



X	$-r_A$ (mol/m ³ s)
0	0.45
0.1	0.37
0.2	0.30
0.4	0.195
0.6	0.113
0.7	0.079
0.8	0.05

[T = 500 K]

[P = 830 kPa = 8.2 atm]

initial charge was pure A

Example: Let's consider the isothermal gas-phase isomerization:



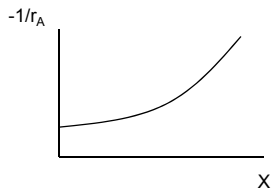
X	$-r_A(\text{mol/m}^3\text{s})$	$1 / -r_A$
0	0.45	2.22
0.1	0.37	2.70
0.2	0.30	3.33
0.4	0.195	5.13
0.6	0.113	8.85
0.7	0.079	12.7
0.8	0.05	20.0

[T = 500 K]

[P = 830 kPa = 8.2 atm]

initial charge was pure A

Draw $-1/r_A$ vs X:



We can use this figure to size flow reactors for different entering molar flow rates.

Keep in mind :

1. if a rxn is carried out isothermally, the rate is usually greatest at the start of the rxn, when the conc'n of reactant is greatest. (when $x \approx 0 \rightarrow -1/r_A$ is small)
2. As $x \rightarrow 1$, $-r_A \rightarrow 0$ thus $1/-r_A \rightarrow \infty$ & $V \rightarrow \infty$

→ An infinite reactor volume is needed to reach complete conversion.

For reversible reactions ($A \leftrightarrow B$), the max X is the equilibrium conversion X_e . At equilibrium, $r_A \approx 0$.

As $X \rightarrow X_e$, $-r_A \rightarrow 0$ thus $1/-r_A \rightarrow \infty$ & $V \rightarrow \infty$

→ An infinite reactor volume is needed to obtain X_e .

if $F_{A0} = 0.4 \text{ mol/s}$, we can calculate $[F_A/r_A](m^3)$

Plot F_{A0}/r_A vs X obtain Levenspiel Plot!

Example: Calculate volume to achieve 80 % conversion in CSTR.

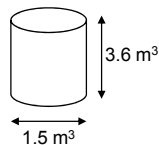
find $-r_A$ at $X = 0.8$

$$\left(-\frac{1}{r_A} \right)_{0.8} = 20 \frac{m^3}{mol \cdot s}$$

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

$$= 0.4 \frac{mol}{s} \cdot 20 \frac{m^3}{mol \cdot s} \cdot 0.8 = 6.4 m^3$$

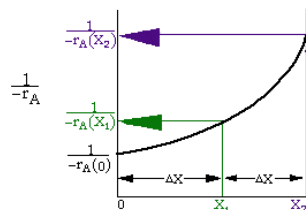
For instance:



CSTRs are usually used for liquid-phase rxns.

4. Numerical Evaluation of Integrals

The integral to calculate the PFR volume can be evaluated using a method such as Simpson's One-Third Rule.



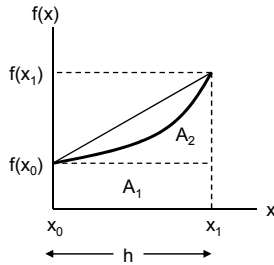
NOTE: The intervals (ΔX) shown in the sketch are not drawn to scale. They should be equal.

$$PFR: V = F_{A0} \int_0^X \frac{dX}{-r_A} = F_{A0} \frac{\Delta X}{3} \left[\frac{1}{-r_A(X=0)} + \frac{4}{-r_A(X_1)} + \frac{1}{-r_A(X_2)} \right]$$

Simpson's One-Third Rule is one of the most common numerical methods. It uses three data points. One numerical methods for evaluating integrals are:

1. Trapezoidal Rule (uses two data points)
2. Simpson's Three-Eighth's Rule (uses four data points)
3. Five-Point Quadrature Formula

Trapezoidal Rule



$$\int_{x_0}^{x_1} f(x) \cdot dx = \frac{1}{h} [f(x_0) + f(x_1)]$$

$$A_1 = f(x_0) \cdot h$$

$$A_2 = \frac{[f(x_1) - f(x_0)] \cdot h}{2}$$

$$A = A_1 + A_2$$

$$= h \cdot \left[f(x_0) + \frac{f(x_1) - f(x_0)}{2} \right]$$

$$= \frac{h}{2} \cdot [f(x_0) + f(x_1)]$$

Five Point Quadrature formula:

$$\int_{x_0}^{x_4} f(x) \cdot dx = \frac{h}{3} \cdot (f_0 + 4f_1 + 2f_2 + 4f_3 + f_4) \quad \text{where} \quad h = \frac{x_4 - x_0}{4}$$

$$\int_{x_0}^{x_N} f(x) \cdot dx = \frac{3h}{8} \cdot (f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \dots) \quad \Rightarrow \quad \begin{array}{l} \text{For } N+1 \text{ points, where} \\ N \text{ is an integer.} \end{array}$$

Example: Consider the liquid phase reaction;



which is to take place in a PFR. The following data was obtained in a batch reactor.

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

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?

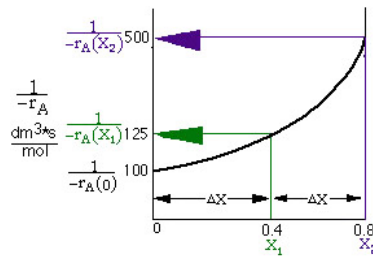
Hint :

$F_{A0} = 2 \text{ mol/s}$, fed to a plug flow reactor

$PFR \therefore V = F_{A0} \int_0^X \frac{1}{-r_A} dX$ Thus one needs $(1/-r_A)$ as a function of X .

X	0	0.4	0.8
$-r_A (\text{mol/dm}^3 \cdot \text{s})$	0.101	0.008	0.002
\downarrow			
$\frac{1}{-r_A} \left(\frac{\text{dm}^3 \cdot \text{s}}{\text{mol}} \right)$	100	125	500

Construct a
Levenspiel Plot
 $\frac{1}{-r_A}$ vs. X



For Simpson's three point formula we have:

$$PFR: V = F_{A0} \int_0^X \frac{dX}{-r_A} = F_{A0} \cdot \frac{\Delta X}{3} \left[\frac{1}{-r_A(X=0)} + \frac{4}{-r_A(X_1)} + \frac{1}{-r_A(X_2)} \right]$$

$$PFR: V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = 2 \frac{\text{mol}}{\text{s}} \cdot \left\{ \frac{0.4}{3} [100 + 4 \cdot (125) + 500] \frac{\text{dm}^3 \text{s}}{\text{mol}} \right\} = 293 \text{ dm}^3$$

To reach 80 % conversion, your PFR must be 293.3 dm³.

Sizing in PFR

Example: Determine the volume in PFR to achieve a 80 % conversion.

$$\text{For PFR: } F_{A0} \cdot \frac{dX}{dV} = -r_A$$

$$\text{Rearranging: } V = F_{A0} \cdot \int_0^{0.8} \frac{dX}{-r_A} = \int_0^{0.8} \frac{F_{A0}}{-r_A} \cdot dX$$

Let's numerically evaluate the integral with trapezoidal rule

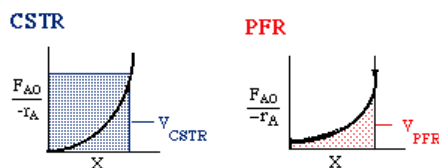
$$\int_0^{0.8} \frac{F_{A0}}{-r_A} \cdot dX \Rightarrow f(X) = \left. \frac{F_{A0}}{-r_A} \right|_{X=0} = 0.89$$

$$f(X) = \left. \frac{F_{A0}}{-r_A} \right|_{X=0.8} = 8.0$$

$$V = \frac{0.8}{2} \cdot (0.89 + 8.0) = 8.89 \cdot 0.4 = 3.556 \text{ m}^3$$

With five point quadrature $V = 2.165 \text{ m}^3$

Comparing CSTR & PFR Sizing



$V_{CSTR} > V_{PFR}$ for the same conversion and rxn conditions.

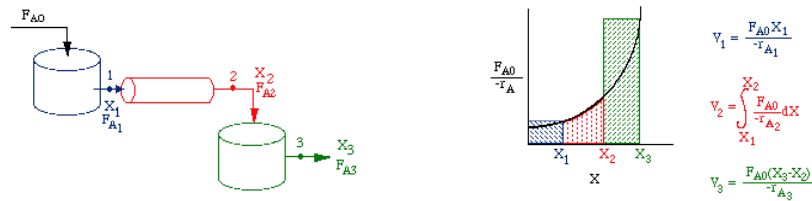
The reason is that CSTR always operates at lowest rxn rate. PFR starts at a high rate, then gradually decreases to the exit rate.

Reactors in Series: The exit of one reactor is fed to the next one.

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

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

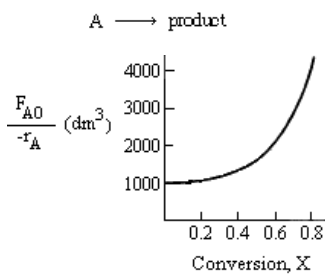
Only valid if there are no side streams.



$$F_{A_i} = F_{A0} - F_{A0} \cdot X_i$$

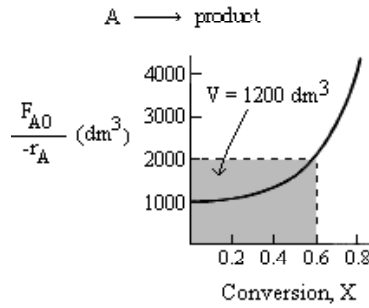
Example: Using Levenspiel plots to calculate conversion from known reactor volumes.

Pure A is fed at a volumetric flow rate $1000 \text{ dm}^3/\text{h}$ and at a concentration of 0.005 mol/dm^3 to an existing CSTR, which is connected in series to an existing tubular reactor. If the volume of the CSTR is 1200 dm^3 and the tubular reactor volume is 600 dm^3 , what are the intermediate and final conversions that can be achieved with the existing system? The reciprocal rate is plotted in the figure below as a function of conversion for the conditions at which the reaction is to be carried out.



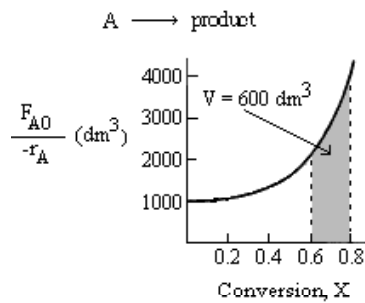
Solution:

By trial and error, we find that a conversion of 0.6 gives the appropriate CSTR volume of 1200 dm³.



Therefore, the intermediate conversion is $X = 0.6$

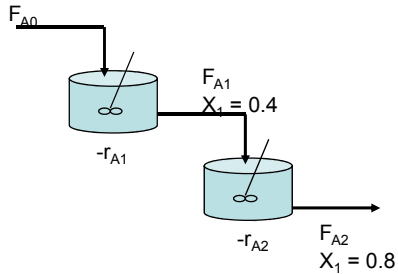
Similarly for the PFR, through trial and error, we find that a conversion of 0.8 gives the appropriate PFR volume of 600 dm³.



Therefore, the final conversion is $X = 0.8$

CSTRs in Series

Two CSTRs in series



Reactor 1:

$$\text{Mole Balance: } F_{A0} - F_{A1} + r_{A1} V_1 = 0 \quad [1]$$

$$F_{A1} = F_{A0} - F_{A0} X_1 \quad [2]$$

Combining [1] & [2]:

$$V_1 = F_{A0} (1 / -r_{A1}) X_1 \quad [3]$$

Reactor 2:

$$\text{Mole Balance: } F_{A1} - F_{A2} + r_{A2} V_2 = 0 \quad [4]$$

$$F_{A2} = F_{A0} - F_{A0} X_2 \quad [5]$$

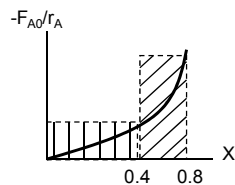
Combining [4] & [5]:

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} = \frac{(F_{A0} - F_{A0} \cdot X_1) - (F_{A0} - F_{A0} \cdot X_2)}{-r_{A2}} = \frac{F_{A0}}{-r_{A2}} (X_2 - X_1)$$

if we have the data:

$$X = 0.4 \quad \left(\frac{F_{A0}}{-r_{A1}} \right)_{X=0.4} = 2.05 m^3 \quad V_1 = \left(\frac{F_{A0}}{-r_{A1}} \right)_{0.4} \cdot X_1 = 0.82 m^3$$

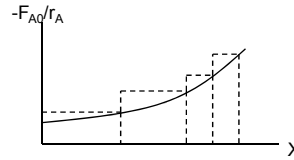
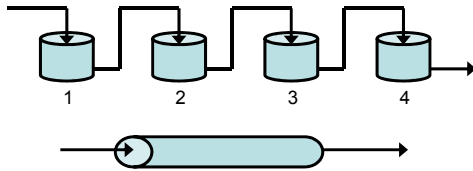
$$X = 0.8 \quad \left(\frac{F_{A0}}{-r_{A2}} \right)_{X=0.8} = 8.0 m^3 \quad V_2 = \left(\frac{F_{A0}}{-r_{A2}} \right) \cdot (X_2 - X_1) = 3.2 m^3$$



$$V_{\text{CSTR},2} > V_{\text{CSTR},1}$$

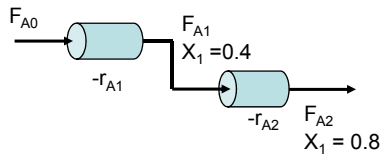
$$\text{Total } V = V_1 + V_2 = 4.02 m^3 < 6.4 m^3 \implies \text{volume necessary to get 80 \% conversion with one CSTR}$$

One can approximate a PFR by a large # of CSTRs in series:



$$V_{PFR} = \sum_{i=1}^n V_{CSTR,i}$$

PFRs in Series



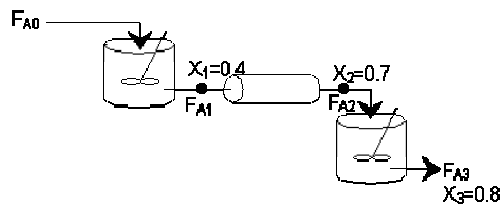
$$V_{TOTAL} = V_{PFR,1} + V_{PFR,2}$$

The overall conversion of two PFRs in series is the same as one PFR with the same total volume

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

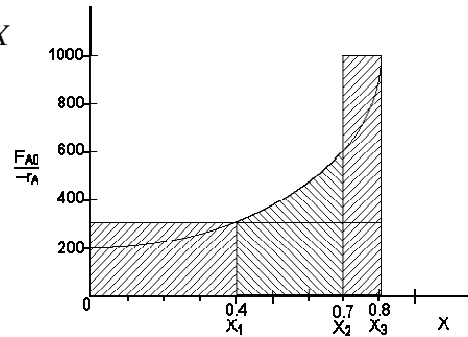
Reactors in Series: CSTR – PFR – CSTR

Using the data in the table, calculate the reactor volumes V_1 , V_2 and V_3 for the CSTR/PFR/CSTR reactors in series sequence along with the corresponding conversion.



X	0	0.2	0.4	0.6	0.8
$-r_A \left(\frac{\text{mol}}{\text{dm}^3 \cdot \text{s}} \right)$	0.010	0.0091	0.008	0.005	0.002
$(1/-r_A) \left(\frac{\text{dm}^3 \cdot \text{s}}{\text{mol}} \right)$	100	110	125	200	500
$F_{A0}/-r_A \left(\text{dm}^3 \right)$	200	220	250	400	1000

Use the plot of $\left(\frac{F_{A0}}{-r_A}\right)$ vs. X



(a) The CSTR design equation for Reactor 1 is:

$$V_1 = \left(\frac{F_{A0} \cdot X}{-r_{A1}} \right)$$

at $X = X_1 = 0.4$ the $(F_{A0} / -r_{A1}) = 300 \text{ dm}^3$

$$V_1 = (300 \text{ dm}^3) (0.4) = 120 \text{ dm}^3$$

The volume of the first CSTR is 120 dm^3

(b) Reactor 2: PFR The differential form of the PFR design is

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

Rearranging and intergrating with limits

when $V = 0$ $X = X_1 = 0.4$

when $V = V_2$ $X = X_2 = 0.7$

$$V = \int_{X_1}^{X_2} \left(\frac{F_{A0}}{-r_A} \right) \cdot dX = \int_{0.4}^{0.7} \left(\frac{F_{A0}}{-r_A} \right) \cdot dX$$

Choose three point quadrature formula with

$$\Delta X = \frac{X_2 - X_1}{2} = \frac{0.7 - 0.4}{2} = 0.15$$

$$V_2 = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(0.4)} + \frac{4 \cdot F_{A0}}{-r_A(0.55)} + \frac{F_{A0}}{-r_A(0.7)} \right]$$

Interpreting for $(F_{A0}/-r_A)$ at $X = 0.55$ we obtain

$$\left(\frac{F_{A0}}{-r_A} \right)_{X=0.55} = 370 \text{ dm}^3$$

$$V_2 = \frac{0.15}{3} [300 \text{ dm}^3 + 4 \cdot (370 \text{ dm}^3) + 600 \text{ dm}^3] = 119 \text{ dm}^3$$

The volume of the PFR is $V_2 = 119 \text{ dm}^3$

(c) Reactor 3: CSTR

Balance *in - out + generation*

$$F_{A2} - F_{A3} + r_{A3} \cdot V_3 = 0$$

$$V_3 = \frac{F_{A2} - F_{A3}}{-r_{A3}}$$

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

$$F_{A3} = F_{A0} \cdot (1 - X_3)$$

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

$$V_3 = 600 \text{ dm}^3 \cdot (0.7 - 0.4) = 180 \text{ dm}^3$$

The volume of last CSTR is 180 dm³

Summary:

CSTR $X_1 = 0.4$ $V_1 = 120 \text{ dm}^3$

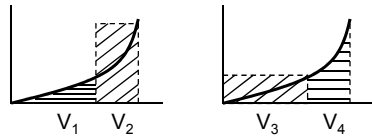
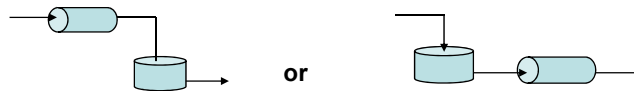
PFR $X_2 = 0.7$ $V_2 = 119 \text{ dm}^3$

CSTR $X_3 = 0.8$ $V_3 = 180 \text{ dm}^3$

Total volume = $120 + 119 + 180 = 419 \text{ dm}^3$

Reactor Sequencing

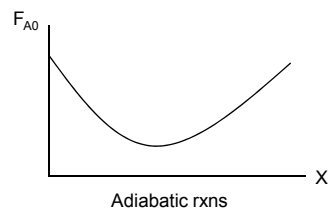
Is there any differences between having a CSTR – PFR system & PFR – CSTR system? Which arrangement is best?



The volumes are different!

$$V_1 + V_2 \neq V_3 + V_4$$

For isothermal rxns



The choice of reactors depend on ;
the Levenspiel plots
relative reactor sizes.

Space Time

The space time, tau, is obtained by dividing the reactor volume by the volumetric flow rate entering the reactor:

$$\tau = \frac{V}{v_0}$$

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. It is also called holding time or mean residence time.

Example: $v_0 = 0.01 \text{ m}^3/\text{s}$ and $V = 0.2 \text{ m}^3 \rightarrow \tau = 0.2 \text{ m}^3 / 0.01 \text{ m}^3/\text{s} = 20 \text{ s}$

It would take 20 s for the fluid at the entrance to move to the exit.

Typical space time for different reactors:

Batch : 15 min – 20 h (few kg/day – 100,000 tons/year \approx 280 tons/day)

CSTR : 10 min – 4 h (10 to 3×10^6 tons/yr)

Tubular: 0.5s – 1h (50 to 5×10^6 tons/yr)

Space Velocity (SV) is defined as:

$$SV = \frac{v_0}{V} = \frac{1}{\tau}$$

instead of using volumetric flow rate at the entrance, you use liquid – hourly & gas – hourly space velocities (LHSV, GHSV).

v_0 (for LHSV) is that of a liquid feed rate at 60°F or 75°F.

v_0 (for GHSV) is that of the one that measured at STP.

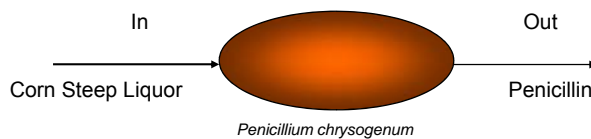
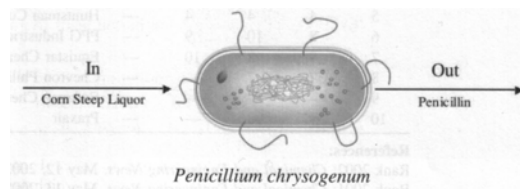
$$LHSV = \frac{v_0|_{liq}}{V} \quad GHSV = \frac{v_0|_{STP}}{V}$$

Sample Industrial Space Times

	Reaction	Reactor	Temperature	Pressure atm	Space Time
(1)	$C_2H_6 \rightarrow C_2H_4 + H_2$	PFR	860°C	2	1 s
(2)	$CH_3CH_2OH + HCH_3COOH \rightarrow CH_3CH_2COOCH_3 + H_2O$	CSTR	100°C	1	2 h
(3)	Catalytic cracking	PBR	490°C	20	$1 \text{ s} < \tau < 400 \text{ s}$
(4)	$C_6H_5CH_2CH_3 \rightarrow C_6H_5CH = CH_2 + H_2$	PBR	600°C	1	0.2 s
(5)	$CO + H_2O \rightarrow CO_2 + H_2$	PBR	300°C	26	4.5 s
(6)	$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$	CSTR	50°C	1	20 min

- HW (due date: Feb 25):
- Solve the prpbem in your own way.
- http://www.engin.umich.edu/~cre/web_mod/hippo/index.htm
- Suggested problems from the web:
- <http://www.engin.umich.edu/~cre/>
- [Additional Homework Problems](#) at each chapter

Example: Consider cell as a reactor. The nutrient corn steep liquor enters the cell of the microorganism *Penicillium chrysogenum* and is decomposed to form such products as amino acids, RNA and DNA. Write an unsteady mass balance on (a) the corn steep liquor, (b) RNA, and (c) pencillin. Assume the cell is well mixed and that RNA remains inside the cell.



Assumption:

Penicillin is produced in the stationary state.

→ no cell growth & nutrients are used in making the product.

Mass balance for penicillin: $In - Out + Generation = Accumulation$

$$F_{in} + F_{out} + G_p = \frac{dN_p}{dt}$$

$$F_{in} = 0 \text{ (no penicillin in flow)}$$

$$G_p = \int_V r_p \cdot dV \Rightarrow \int_V r_p \cdot dV - F_{out} = \frac{dN_p}{dt}$$

Assuming steady state for the rate of production of penicillin in the cells stationary state,

$$\frac{dN_p}{dt} = 0$$

$$V = \frac{F_{in} - F_{out}}{-r_p} \Rightarrow V = \frac{F_{out}}{r_p}$$

Similarity, for Corn Steep Liquor with $F_C = 0$

$$V = \frac{F_{C0} - F_C}{-r_C} = \frac{F_{C0}}{-r_C}$$

No RNA is generated or destroyed.

Summary

<u>Batch</u>	<u>Flow</u>
$X = \frac{(N_{A0} - N_A)}{N_{A0}}$	$X = \frac{(F_{A0} - F_A)}{F_{A0}}$

$$X = \frac{\text{Moles of A reacted}}{\text{Moles of A fed}}$$

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. $X = X_e$.

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

*Batch reactor design eq'n
(in differential form)*

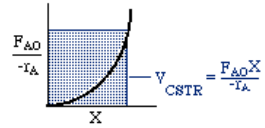
$$V = \frac{F_{A0} \cdot X}{(-r_A)_{exit}}$$

CSTR

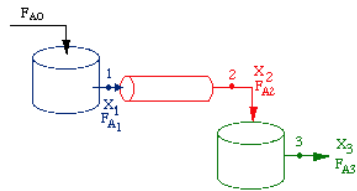
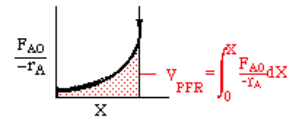
$$V = F_{A0} \cdot \int_0^X \frac{dX}{-r_A}$$

PFR

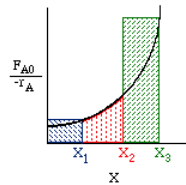
CSTR



PFR



Reactors in series



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

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

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

Space time

$$\tau = \frac{V}{v_0}$$