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Solutions for Chapter 2 - Conversion and Reactor Sizing

P2-1. This problem will keep students thinking about writing down what they learned every chapter.

P2-2. This “forces” the students to determine their learning style so they can better use the resources in the text and on the CDROM and the web.

P2-3. ICMs have been found to motivate the students learning.

P2-4. Introduces one of the new concepts of the 4^{th} edition whereby the students “play” with the example problems before going on to other solutions.

P2-5. This is a reasonably challenging problem that reinforces Levenspiels plots.

P2-6. Straight forward problem alternative to problems 7, 8, and 11.

P2-7. To be used in those courses emphasizing bio reaction engineering.

P2-8. The answer gives ridiculously large reactor volume. The point is to encourage the student to question their numerical answers.

P2-9. Helps the students get a feel of real reactor sizes.

P2-10. Great motivating problem. Students remember this problem long after the course is over.

P2-11. Alternative problem to **P2-6** and **P2-8**.

P2-12. Novel application of Levenspiel plots from an article by Professor Alice Gast at Massachusetts Institute of Technology in CEE.

CDP2-A Similar to 2-8

CDP2-B Good problem to get groups started working together (e.g. cooperative learning).

CDP2-C Similar to problems 2-7, 2-8, 2-11.

CDP2-D Similar to problems 2-7, 2-8, 2-11.

Summary

		Assigned	Alternates	Difficulty	Time (min)
	P2-1	O			15
●	P2-2	A			30
●	P2-3	A			30

	P2-4	O			75
	P2-5	O		M	75
●	P2-6	AA	7,8,11	FSF	45
	P2-7	S		FSF	45
	P2-8	AA	6,8,11	SF	45
	P2-9	S		SF	15
●	P2-10	AA		SF	1
	P2-11	AA	6,7,8	SF	60
	P2-12	S		M	60
	CDP2-A	O	8,B,C,D	FSF	5
	CDP2-B	O	8,B,C,D	FSF	30
	CDP2-C	O	8,B,C,D	FSF	30
	CDP2-D	O	8,B,C,D	FSF	45

Assigned

● = Always assigned, AA = Always assign one from the group of alternates,
O = Often, I = Infrequently, S = Seldom, G = Graduate level

Alternates

In problems that have a dot in conjunction with AA means that one of the problems, either the problem with a dot or any one of the alternates are always assigned.

Time

Approximate time in minutes it would take a B/B^+ student to solve the problem.

Difficulty

SF = Straight forward reinforcement of principles (plug and chug)
FSF = Fairly straight forward (requires some manipulation of equations or an intermediate calculation).
IC = Intermediate calculation required
M = More difficult
OE = Some parts open-ended.

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*Note the letter problems are found on the CD-ROM. For example A ≡ CDP1-A.

Summary Table Ch-2

Straight forward	1,2,3,4,9
Fairly straight forward	6,8,11
More difficult	5,7, 12
Open-ended	12
Comprehensive Critical thinking	4,5,6,7,8,11,12 P2-8

P2-1 Individualized solution.

P2-2 (a) Example 2-1 through 2-3

If flow rate F_{AO} is cut in half.

$v_1 = v/2$, $F_1 = F_{AO}/2$ and C_{AO} will remain same.
Therefore, volume of CSTR in example 2-3,

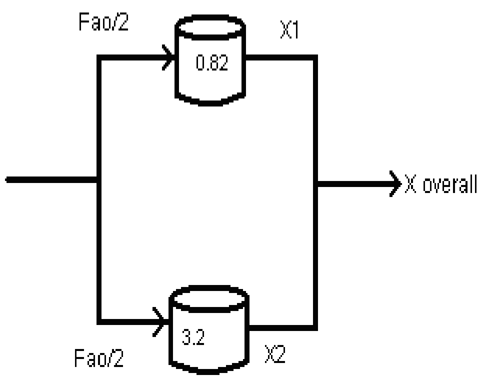
$$V_1 = \frac{F_1 X}{-r_A} = \frac{1}{2}\frac{F_{A0} X}{-r_A} = \frac{1}{2}6.4 = 3.2$$

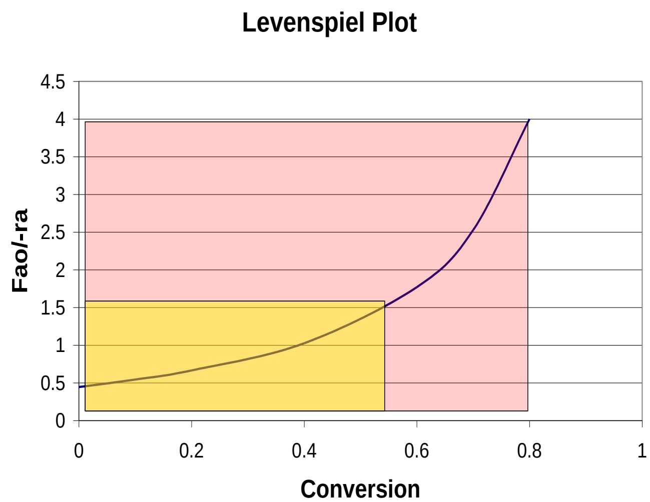
If the flow rate is doubled,

$F_2 = 2F_{AO}$ and C_{AO} will remain same,

Volume of CSTR in example 2-3,
$V_2 = F_2X/-r_A = 12.8\ m^3$

P2-2 (b) Example 2-4





Now, $F_{AO} = 0.4/2 = 0.2$ mol/s,

Table: Divide each term $\frac{F_{A0}}{-r_A}$ in Table 2-3 by 2.

X	0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{AO}/-r_{A]}(m^3)$	0.445	0.545	0.665	1.025	1.77	2.53	4

Reactor 1

$V_1 = 0.82m^3$

$V = (F_{AO}/-r_A)X$

$$0.82 = \left(\frac{F_{A0}}{-r_A}\right)_{X1}(X1)$$

Reactor 2

$V_2 = 3.2\ m^3$

$$3.2 = \left(\frac{F_{A0}}{-r_A}\right)_{X2}(X2)$$

By trial and error we get:

$X_1 = 0.546$ and $X_2 = 0.8$

Overall conversion $X_{Overall} = (1/2)X_1 + (1/2)X_2 = (0.546+0.8)/2 = 0.673$

P2-2 (c) Example 2-5

(1) For first CSTR,

at X=0 ;

$\frac{F_{A0}}{-r_A} = 1.28\text{m}^3$

at X=0.2 ; $\frac{F_{A0}}{-r_A} = .94\ \text{m}^3$

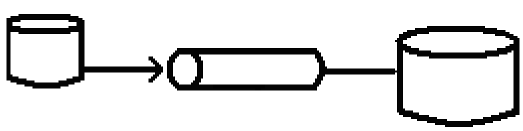
From previous example; V1 (volume of first CSTR) = .188 m^3

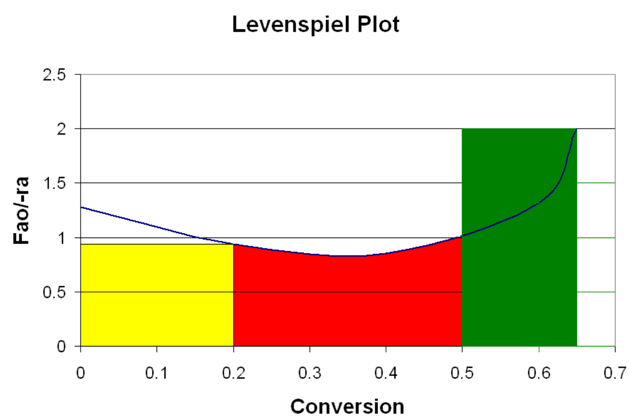
Also the next reactor is PFR, Its volume is calculated as follows

$$V_2 = \int_{0.2}^{0.5} \left(\frac{F_{AO}}{-r_A} \right) dX$$
$$= 0.247 m^3$$

For next CSTR,

$X_3 = 0.65$, $\frac{F_{AO}}{-rA} = 2m^3$, $V_3 = \frac{F_{AO}(X_3 - X_2)}{-rA} = .3m^3$





(2)
Now the sequence of the reactors remain unchanged.

But all reactors have same volume.
First CSTR remains unchanged

$V_{cstr} = .1 = (F_{A0}/-r_A)*X_1$
=> X1 = .088
Now
For PFR:

$$V = \int_{0.088}^{X_2} \left(\frac{F_{AO}}{-r_A} \right) dX$$

,

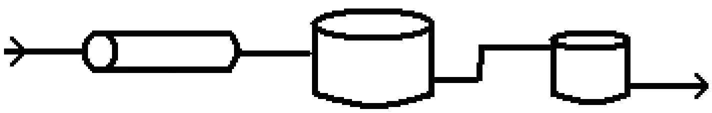
By estimation using the levenspiel plot
$X_2 = .183$

For CSTR,

$V_{CSTR2} = \frac{F_{AO} \quad X_3 - X_2}{-rA} = 0.1 m^3$

=> X_3 = .316

(3) The worst arrangement is to put the PFR first, followed by the larger CSTR and finally the smaller CSTR.



Conversion	Original Reactor Volumes	Worst Arrangement
X1 = 0.20	V1 = 0.188 (CSTR)	V1 = 0.23 (PFR)
X2 = 0.60	V2 = 0.38 (PFR)	V2 = 0.53 (CSTR)
X3 = 0.65	V3 = 0.10 (CSTR)	V3 = 0.10 (CSTR)

For PFR,

$X_1 = 0.2$

$$V_1 = \int_0^{X_1} \left(\frac{F_{AO}}{-r_A} \right) dX$$

Using trapezoidal rule,

$X_O = 0.1$, $X_1 = 0.1$

$$V_1 = \frac{(X_1 - X_O)}{-rA} \left[f(X_O) + f(X_1) \right]$$

$$= \frac{0.2}{2} [1.28 + 0.98] m^3$$

$$= 0.23 m^3$$

For CSTR,

For $X_2 = 0.6$, $\frac{F_{AO}}{-rA} = 1.32 m^3$, $V_2 = \frac{F_{AO}}{-r_A}(X_2 - X_1)$ = 1.32(0.6 – 0.2) = 0.53 m^3

For 2nd CSTR,

For $X_3 = 0.65$, $\frac{F_{AO}}{-rA} = 2 m^3$, $V_3 = 0.1\ m^3$

P2-3 Individualized solution.

P2-4 Solution is in the decoding algorithm given with the modules.

P2-5

X	0	0.1	0.2	0.4	0.6	0.7	0.8
$F_{AO}/-r_A$ (m^3)	0.89	1.08	1.33	2.05	3.54	5.06	8.0

$V = 1.6\ m^3$

P2-5 (a) Two CSTRs in series

For first CSTR,

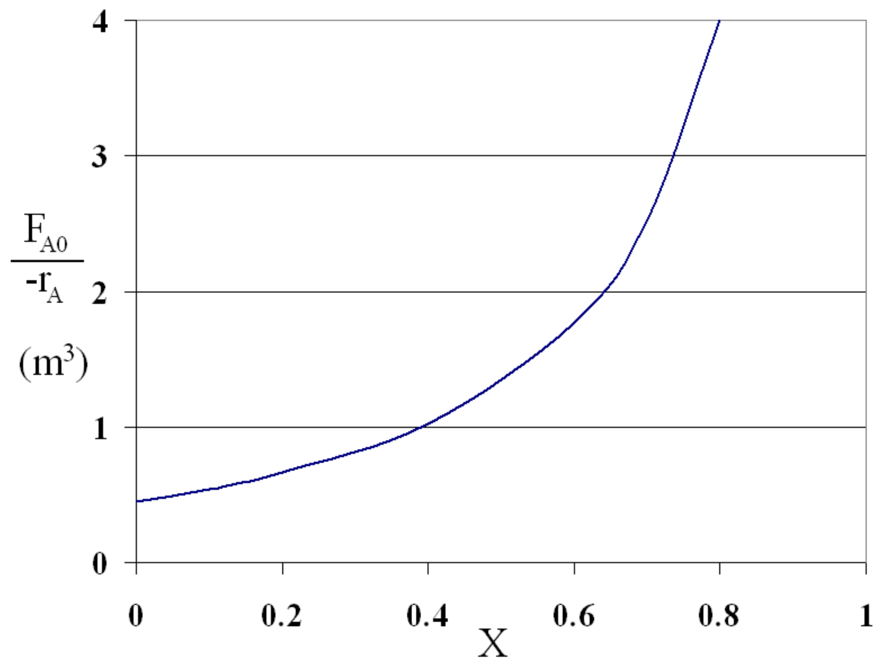
$V = (F_{Ao}/-r_{AX1})\ X$

=> X1 = 0.53

For second CSTR,

$V = (F_{Ao}/-r_{AX2})\ (X_2 - X_1)$

=> X2 = 0.76



P2-5 (b)

Two PFRs in series

$$V = \int_0^{X_1} \left(\frac{F_{Ao}}{-r_A}\right) dX + \int_{X_1}^{X_2} \left(\frac{F_{Ao}}{-r_A}\right) dX$$

By extrapolating and solving, we get

$X_1 = 0.62$ $X_2 = 0.84$

P2-5 (c)

Two CSTRs in parallel with the feed, F_{AO}, divided equally between two reactors. $F_{ANEW}/-r_{AX1} = 0.5F_{AO}/-r_{AX1}$

$V = (0.5F_{AO}/-r_{AX1})\ X_1$

Solving we get, $X_{out} = 0.68$

P2-5 (d)

Two PFRs in parallel with the feed equally divided between the two reactors.

$F_{ANEW}/-r_{AX1} = 0.5F_{AO}/-r_{AX1}$

By extrapolating and solving as part (b), we get

$X_{out} = 0.88$

P2-5 (e)

A CSTR and a PFR are in parallel with flow equally divided

Since the flow is divided equally between the two reactors, the overall conversion is the average of the CSTR conversion (part C) and the PFR conversion (part D)

$X_o = (0.60 + 0.74) / 2 = 0.67$

P2-5 (f)

A PFR followed by a CSTR,

$X_{PFR} = 0.50$ (using part(b))

$V = (F_{Ao}/-r_{A-XCSTR}) (X_{CSTR} - X_{PFR})$

Solving we get, $X_{CSTR} = 0.70$

P2-5 (g)

A CSTR followed by a PFR,

$X_{CSTR} = 0.44$ (using part(a))

$$V = \int_{X_{CSTR}}^{X_{PFR}} \frac{F_{AO}}{-r_A} dX$$

By extrapolating and solving, we get $X_{PFR} = 0.72$

P2-5 (h)

A 1 m^3 PFR followed by two 0.5 m^3 CSTRs,

For PFR,

$X_{PFR} = 0.50$ (using part(b))

$CSTR_1$: $V = (F_{Ao}/-r_{A-XCSTR}) (X_{CSTR} - X_{PFR}) = 0.5\ m^3$

$X_{CSTR} = 0.63$

$CSTR_2$: $V = (F_{Ao}/-r_{A-XCSTR2}) (X_{CSTR2} - X_{CSTR1}) = 0.5\ m^3$

$X_{CSTR2} = 0.72$

P2-6

Exothermic reaction: A → B + C

X	r(mol/dm³.min)	1/-r(dm³.min/mol)
0	1	1
0.20	1.67	0.6
0.40	5	0.2
0.45	5	0.2
0.50	5	0.2
0.60	5	0.2
0.80	1.25	0.8
0.90	0.91	1.1

P2-6 (a)

To solve this problem, first plot 1/-rA vs. X from the chart above. Second, use mole balance as given below.

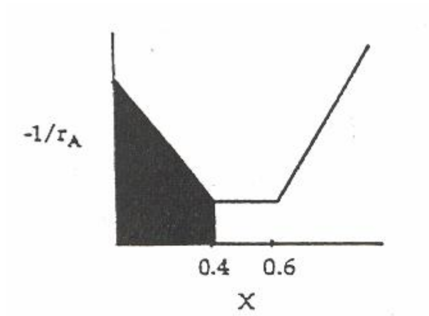
CSTR:

Mole balance: $V_{CSTR} = \frac{F_{A0}X}{-r_A} = \frac{(300 mol/\min)(0.4)}{(5 mol/dm^3.\min)}$ =>

=>V_{CSTR} = 24 dm^3

PFR:

Mole balance: $V_{PFR} = F_{A0}\int_0^X \frac{dX}{-r_A}$



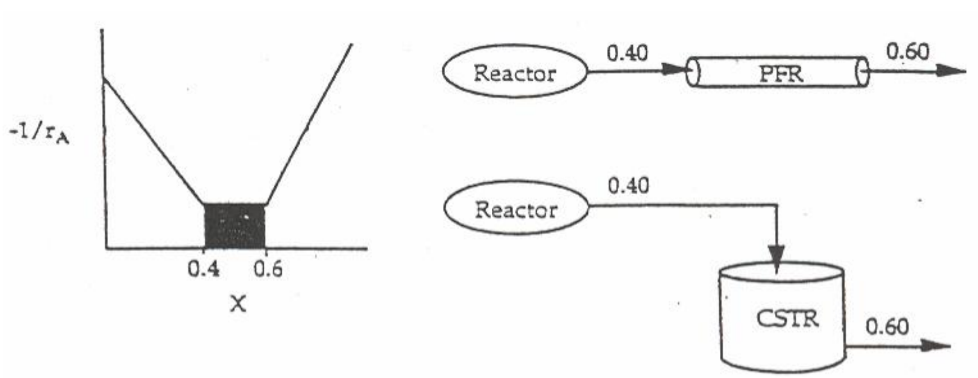
= 300(area under the curve)

V_{PFR} = 72 dm^3

P2-6 (b)

For a feed stream that enters the reaction with a previous conversion of 0.40 and leaves at any conversion up to 0.60, the volumes of the PFR and CSTR will be identical because of the rate is constant over this conversion range.

$$V_{PFR} = \int_{.4}^{.6} \frac{F_{A0}}{-r_A} dX = \frac{F_{A0}}{-r_A}\int_{.4}^{.6} dX = \frac{F_{A0}}{-r_A} X\Big|_{.4}^{.6}$$



P2-6 (c)

V_{CSTR} = 105 dm^3

Mole balance: $V_{CSTR} = \frac{F_{A0}X}{-r_A}$

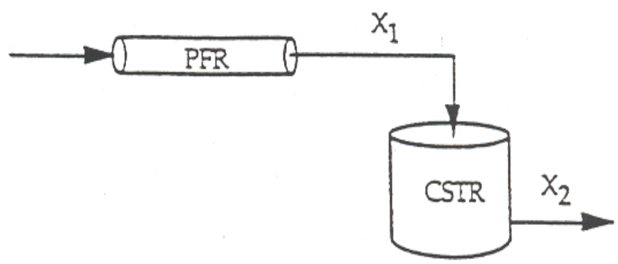
$$\frac{X}{-r_A} = \frac{105dm^3}{300mol/\min} = 0.35dm^3 \min/\ mol$$

Use trial and error to find maximum conversion.

At X = 0.70, 1/-rA = 0.5, and X/-rA = 0.35 dm3.min/mol

Maximum conversion = 0.70

P2-6 (d)



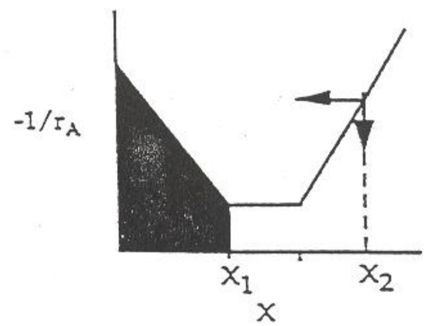
From part (a) we know that $X_1 = 0.40$.

Use trial and error to find X_2.

Mole balance: $V = \frac{F_{A0}(X_2 - X_1)}{-r_A|_{X_2}}$

Rearranging, we get

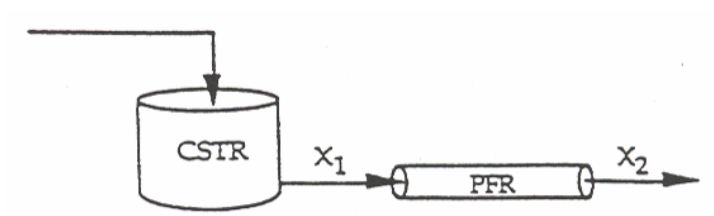
$$\frac{X_2 - 0.40}{-r_A|_{X_2}} = \frac{V}{F_{A0}} = 0.008$$



At $X_2 = 0.64$, $\frac{X_2 - 0.40}{-r_A|_{X_2}} = 0.008$

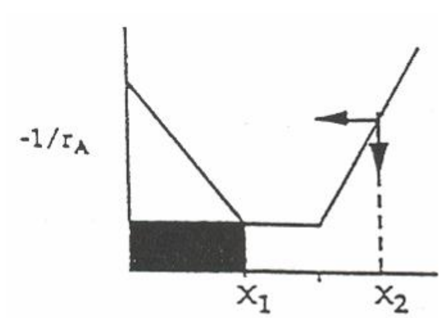
Conversion = 0.64

P2-6 (e)



From part (a), we know that $X_1 = 0.40$. Use trial and error to find X_2.

Mole balance: $V_{PFR} = 72 = F_{A0}\int_{0.40}^{X_2}\frac{dX}{-r_A} = 300\int_{0.40}^{X_2}\frac{dX}{-r_A}$



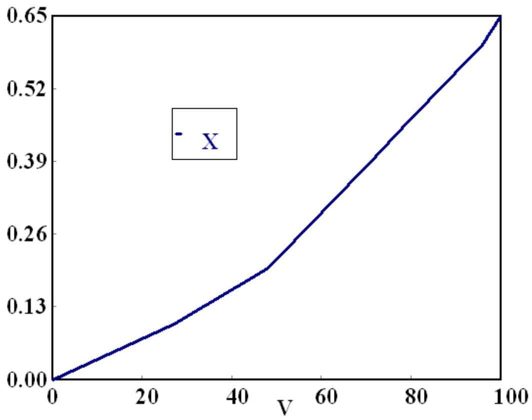
At $X_2 = 0.908$, V = 300 x (area under the curve)

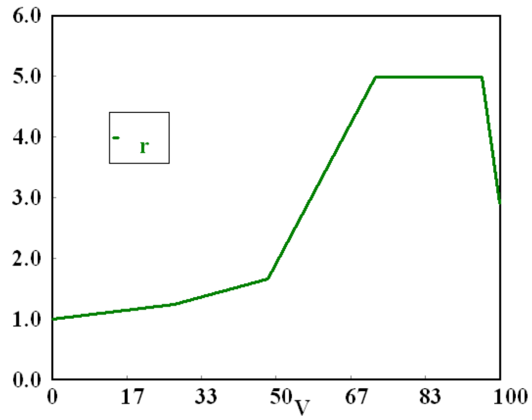
=> V = 300(0.24) = 72dm^3

Conversion = 0.908.

P2-6 (f)

See Polymath program P2-6-f.pol.





P2-7 (a)

$$V = \frac{F_{S0}X}{-r_S}$$

F_{S0} = 1000 g/hr

At a conversion of 40% $\frac{1}{-r_S} = 0.15\frac{dm^3 hr}{g}$

Therefore $V = (0.15)(1000)(0.40) = 60\, dm^3$

P2-7 (b)

At a conversion of 80%, $\frac{1}{-r_S} = 0.8\frac{dm^3 hr}{g}$

F_{S0} = 1000 g/hr

Therefore $V = (0.8)(1000)(0.80) = 640\, dm^3$

P2-7 (c)

$$V_{PFR} = F_{S0}\int_0^X \frac{dX}{-r_S}$$

From the plot of $1/-r_S$ Calculate the area under the curve such that the area is equal to V/F_{S0} = 80 / 1000 = 0.08

X = 12%

For the 80 dm^3 CSTR, $V = 80\, dm^3 = \frac{F_{S0}X}{-r_S}$

$X/-r_s$ = 0.08. From guess and check we get X = 55%

P2-7 (d)

To achieve 80% conversion with a CSTR followed by a CSTR, the optimum arrangement is to have a CSTR with a volume to achieve a conversion of about 45%, or the conversion that corresponds to the minimum value of $1/\text{-}r_s$. Next is a PFR with the necessary volume to achieve the 80% conversion following the CSTR. This arrangement has the smallest reactor volume to achieve 80% conversion.

For two CSTR's in series, the optimum arrangement would still include a CSTR with the volume to achieve a conversion of about 45%, or the conversion that corresponds to the minimum value of $1/\text{-}r_s$, first. A second CSTR with a volume sufficient to reach 80% would follow the first CSTR.

P2-7 (e)

$-r_s = \frac{kC_S C_C}{K_M + C_S}$ and $C_C = 0.1[C_{S0} - C_S] + 0.001$

$$-r_s = \frac{kC_S(0.1[C_{S0} - C_S] + 0.001)}{K_M + C_S}$$

$$-\frac{1}{r_s} = \frac{K_M + C_S}{kC_S(0.1[C_{S0} - C_S] + 0.001)}$$

Let us first consider when C_S is small.

C_{S0} is a constant and if we group together the constants and simplify then $-\frac{1}{r_s} = \frac{K_M + C_S}{k_1 C_S^2 + k_2 Cs}$

since $C_S < K_M$

$-\frac{1}{r_s} = \frac{K_M}{k_1 C_S^2 + k_2 Cs}$ which is consistent with the shape of the graph when X is large (if C_S is small X is large and as C_S grows X decreases).

Now consider when C_S is large (X is small)

As C_S gets larger C_C approaches 0:

$C_C = 0.1[C_{S0} - C_S] + 0.001$ and $C_S \approx C_{S0}$

If $-r_s = \frac{kC_S C_C}{K_M + C_S}$ then $-\frac{1}{r_s} = \frac{K_M + C_S}{kC_S C_C}$

As C_S grows larger, $C_S >> K_M$

And $-\frac{1}{r_s} = \frac{C_S}{kC_S C_C} = \frac{1}{kC_C}$

And since C_C is becoming very small and approaching 0 at X = 0, 1/-r_s should be increasing with C_S (or decreasing X). This is what is observed at small values of X. At intermediate levels of C_S and X, these driving forces are competing and why the curve of 1/-r_S has a minimum.

P2-8

Irreversible gas phase reaction

$$2A + B \rightarrow 2C$$

See Polymath program P2-8.pol.

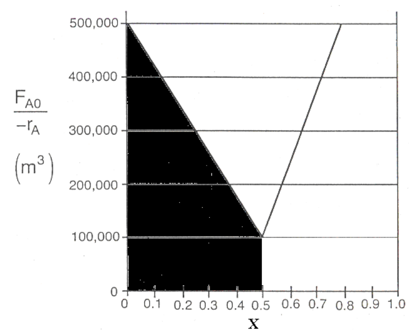
P2-8 (a)

PFR volume necessary to achieve 50% conversion

Mole Balance

$$V = F_{A0} \int_{X_1}^{X_2} \frac{dX}{(-r_A)}$$

Volume = Geometric area under the curve of (F_{A0}/-r_A) vs X)



$$V = \left(\frac{1}{2} \times 400000 \times 0.5\right) + (100000 \times 0.5)$$

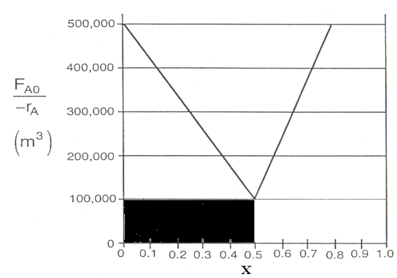
V = 150000 m^3

.

P2-8 (b)

CSTR Volume to achieve 50% conversion

Mole Balance



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

$$V = 0.5 \times 100000$$

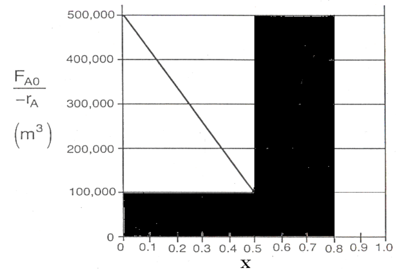
V = 50000m^3

P2-8 (c)
Volume of second CSTR added in series to achieve 80% conversion

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

$$V_2 = 500000 \times (0.8 - 0.5)$$

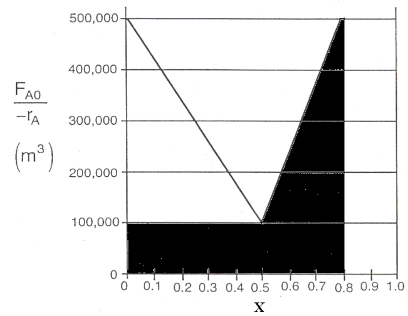
V_2 = 150000m^3



P2-8 (d)
Volume of PFR added in series to first CSTR to achieve 80% conversion

$$V_{PFR} = (\frac{1}{2} \times 400000 \times 0.3) + (100000 \times 0.3)$$

V_{PFR} = 90000m^3



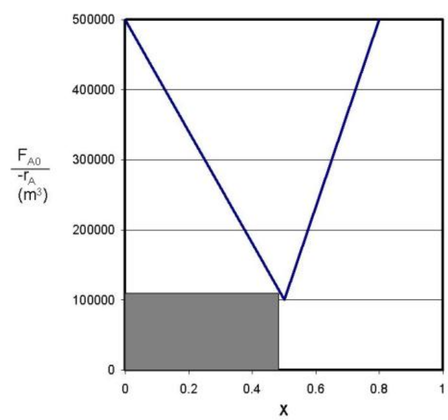
P2-8 (e)
For CSTR,
V = 60000 m^3 (CSTR)

Mole Balance

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

$$60000 = (-800000X + 500000)X$$

X = 0.463

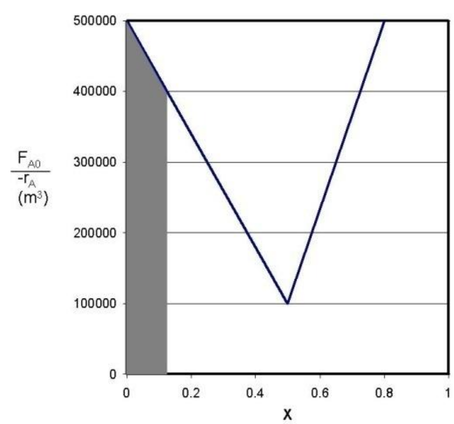


For PFR,
V = 60000 m^3 (PFR)
Mole balance

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

$$60000 = \int_0^X (-800000X + 100000)dX$$

X = 0.134



P2-8(f)
Real rates would not give that shape. The reactor volumes are absurdly large.

P2-9

Problem 2-9 involves estimating the volume of three reactors from a picture. The door on the side of the building was used as a reference. It was assumed to be 8 ft high.

The following estimates were made:

<u>CSTR</u>

h = 56ft   d = 9 ft

$V = \pi r^2 h = \pi(4.5\ ft)^2(56\ ft) = 3562\ ft^3 = 100{,}865\ L$

<u>PFR</u>

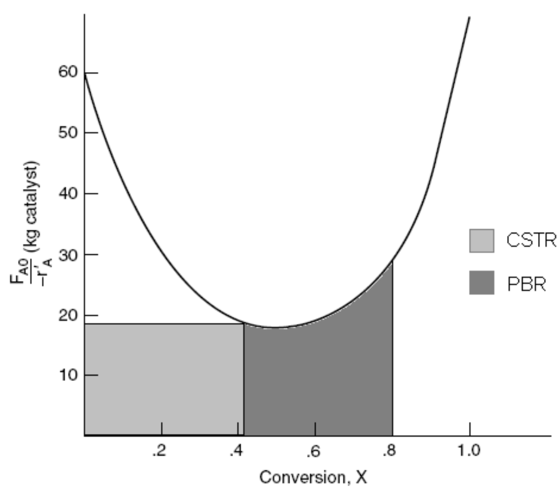
Length of one segment = 23 ft
Length of entire reactor = (23 ft)(12)(11) = 3036 ft
D = 1 ft
$V = \pi r^2 h = \pi(0.5\ ft)^2(3036\ ft) = 2384\ ft^3 = 67{,}507\ L$

Answers will vary slightly for each individual.

P2-10 No solution necessary.

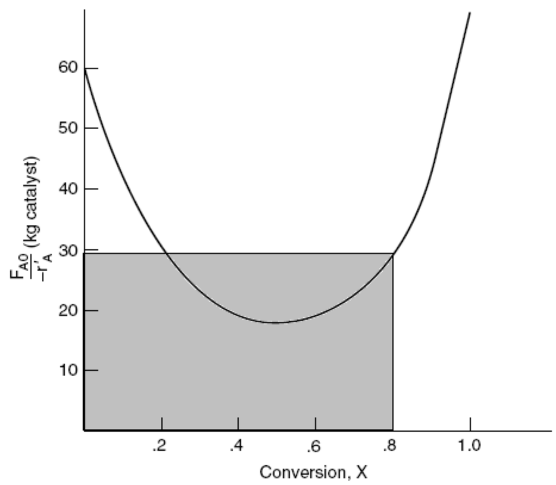
P2-11 (a)

The smallest amount of catalyst necessary to achieve 80 % conversion in a CSTR and PBR connected in series and containing equal amounts of catalyst can be calculated from the figure below.



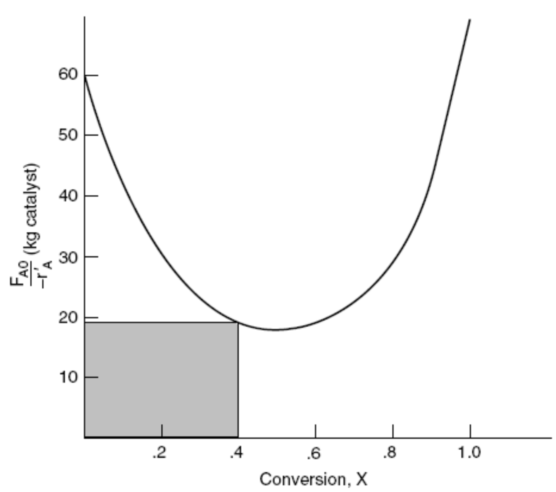
The lightly shaded area on the left denotes the CSTR while the darker shaded area denotes the PBR. This figure shows that the smallest amount of catalyst is used when the CSTR is upstream of the PBR.
See Polymath program P2-11.pol.

P2-11 (b)
Calculate the necessary amount of catalyst to reach 80 % conversion using a single CSTR by determining the area of the shaded region in the figure below.



The area of the rectangle is approximately 23.2 kg of catalyst.

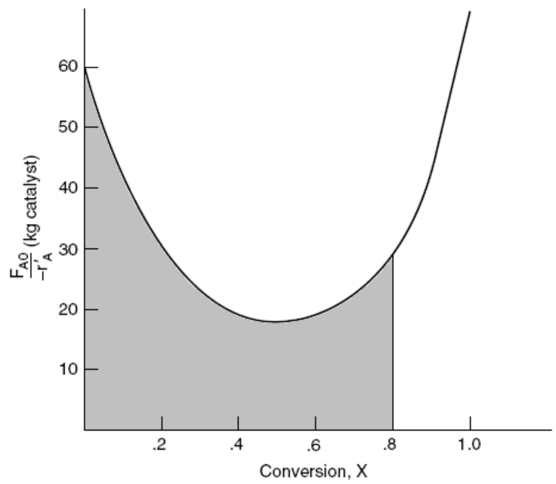
P2-11 (c)
The CSTR catalyst weight necessary to achieve 40 % conversion can be obtained by calculating the area of the shaded rectangle shown in the figure below.



The area of the rectangle is approximately 7.6 kg of catalyst.

P2-11 (d)

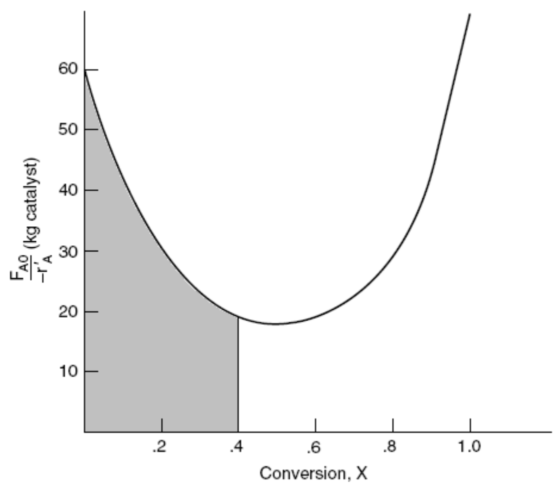
The catalyst weight necessary to achieve 80 % conversion in a PBR is found by calculating the area of the shaded region in the figure below.



The necessary catalyst weight is approximately 22 kg.

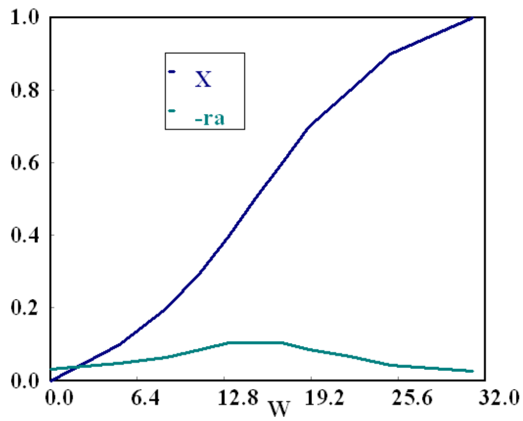
P2-11 (e)

The amount of catalyst necessary to achieve 40 % conversion in a single PBR can be found from calculating the area of the shaded region in the graph below.



The necessary catalyst weight is approximately 13 kg.

P2-11 (f)

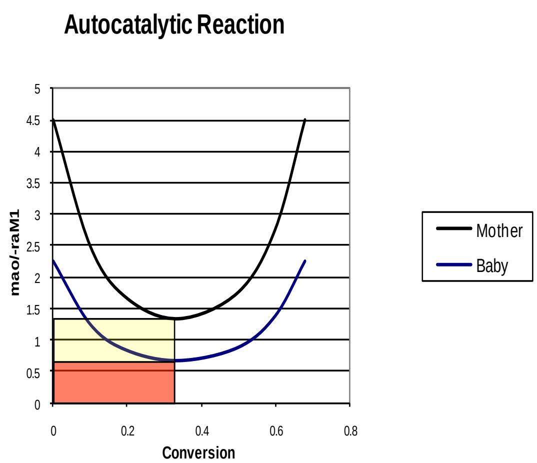


P2-11 (g)

For different ($-r_A$) vs. (X) curves, reactors should be arranged so that the smallest amount of catalyst is needed to give the maximum conversion. One useful heuristic is that for curves with a negative slope, it is generally better to use a CSTR. Similarly, when a curve has a positive slope, it is generally better to use a PBR.

P2-12 (a) Individualized Solution

P2-12 (b) 1) In order to find the age of the baby hippo, we need to know the volume of the stomach. The metabolic rate, $-r_A$, is the same for mother and baby, so if the baby hippo eats one half of what the mother eats then Fao (baby) = ½ Fao (mother). The Levenspiel Plot is shown:



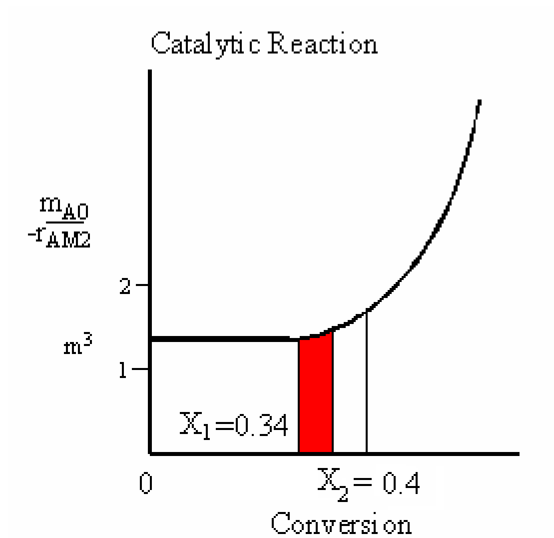
$$V_{baby} = \frac{FaoX}{-r_A} = \frac{1.36}{2} * 0.34 = 0.23m^3$$

Since the volume of the stomach is proportional to the age of the baby hippo, and the volume of the baby's stomach is half of an adult, then the baby hippo is half the age of a full grown hippo.

$$Age = \frac{4.5\,years}{2} = 2.25\,years$$

2) If Vmax and m_{ao} are both one half of the mother's then

$$\frac{m_{Ao}}{-r_{AM2}} = \frac{\left(\frac{1}{2} m_{A0_{mother}}\right)}{-r_{AM2}}$$



and since

$$-r_{AM2} = \frac{v_{max} C_A}{K_M + C_A} \text{ then}$$

$$-r_{AM2_{baby}} = \frac{\frac{1}{2} v_{max} C_A}{K_M + C_A} = -\frac{1}{2} r_{AM2_{mother}}$$

$$\left(\frac{m_{Ao}}{-r_{AM2}}\right)_{baby} = \left(\frac{\frac{1}{2} m_{Ao}}{-\frac{1}{2} r_{AM2}}\right)_{mother} = \left(\frac{m_{Ao}}{-r_{AM2}}\right)_{mother}$$

$\frac{m_{Ao}}{-r_{AM2}}$ will be identical for both the baby and mother.

Assuming that like the stomach the intestine volume is proportional to age then the volume of the intestine would be 0.75 m^3 and the final conversion would be 0.40

P2-12 (c)

$V_{stomach}$ = 0.2 m^3

From the web module we see that if a polynomial is fit to the autocatalytic reaction we get:

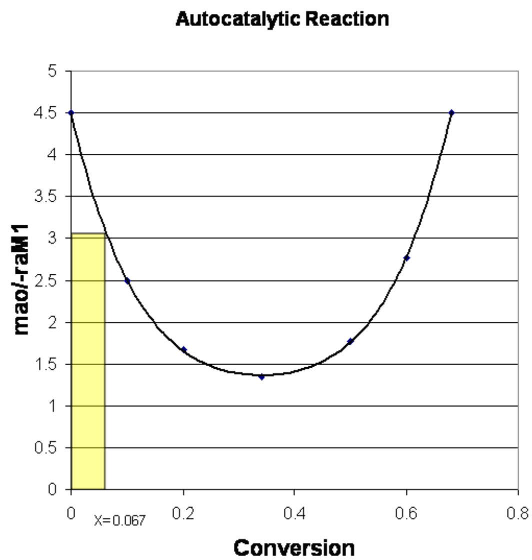
$\frac{m_{A0}}{-r_{AM1}}$ = $127X^4 - 172.36X^3 + 100.18X^2 - 28.354X + 4.499$

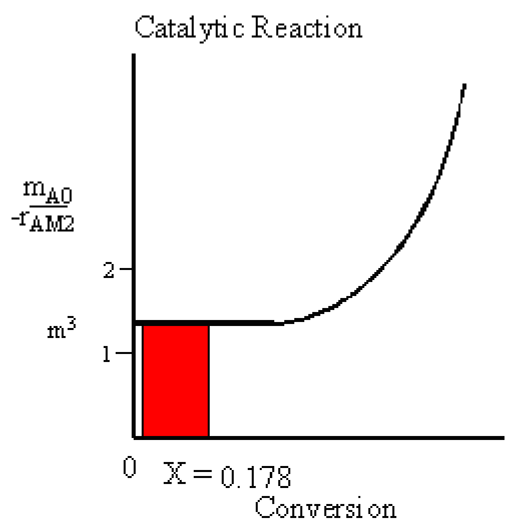
And since $V_{stomach} = \frac{m_{A0}}{-r_{AM1}} X$,

solve V= $127X^5 - 172.36X^4 + 100.18X^3 - 28.354X^2 + 4.499X = 0.2\ m^3$

$X_{stomach}$ = .067.

For the intestine, the Levenspiel plot for the intestine is shown below. The outlet conversion is 0.178. Since the hippo needs 30% conversion to survive but only achieves 17.8%, the hippo cannot survive.



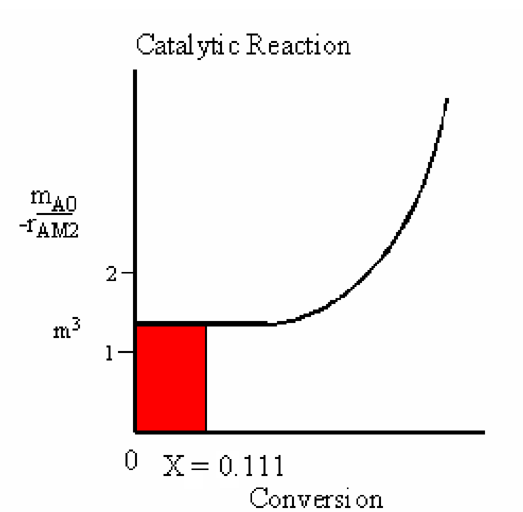


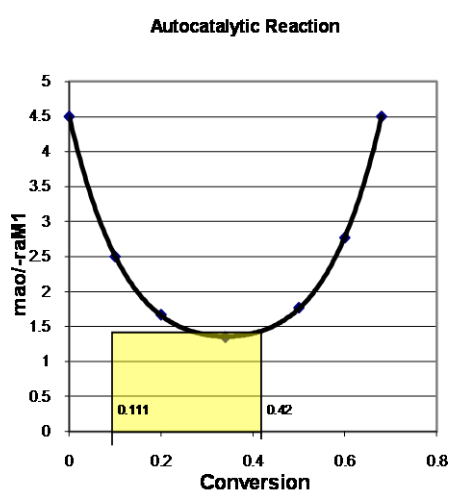
P2-12 (d)

PFR→ CSTR

PFR:

Outlet conversion of PFR = 0.111





CSTR:
We must solve

V = 0.46 = (X-0.111)(127X^4 - 172.36X^3 + 100.18X^2 - 28.354X + 4.499)

X=0.42

Since the hippo gets a conversion over 30% it will survive.

P2-13
For a CSTR we have :

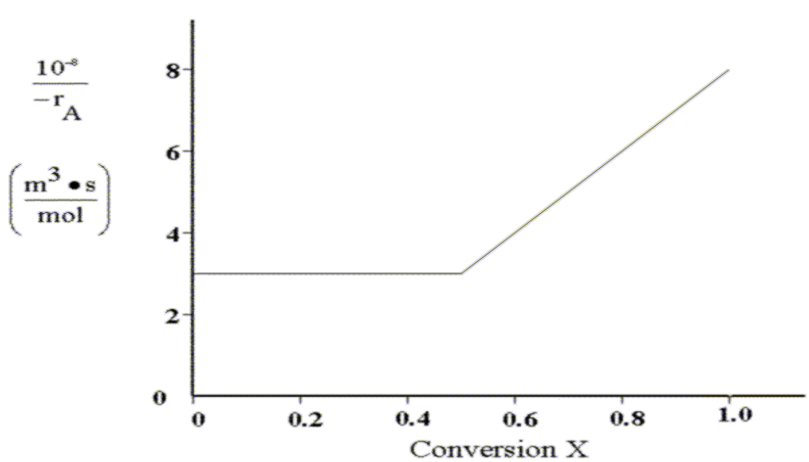
$$V = X \times \frac{F_{A0}}{-r_A|_{X=X_f}}$$

So the area under the $\frac{F_{A0}}{-r_A}$ versus X curve for a CSTR is a rectangle but the height of rectangle corresponds to the value of $\frac{F_{A0}}{-r_A}$ at X= X_f

But in this case the value of $\frac{F_{A0}}{-r_A}$ is taken at X= X_i and the area is calculated.

Hence the proposed solution is wrong.

CDP2-A (a)
Over what range of conversions are the plug-flow reactor and CSTR volumes identical?
We first plot the inverse of the reaction rate versus conversion.



Mole balance equations for a CSTR and a PFR:

CSTR: $V = \frac{F_{A0}X}{-r_A}$ PFR: $V = \int_0^X \frac{dX}{-r_A}$

Until the conversion (X) reaches 0.5, the reaction rate is independent of conversion and the reactor volumes will be identical.

i.e. $V_{PFR} = \int_0^{0.5} \frac{dX}{-r_A} = \frac{F_{A0}}{-r_A} \int_0^{0.5} dX = \frac{F_{A0}X}{-r_A} = V_{CSTR}$

CDP2-A (b)

What conversion will be achieved in a CSTR that has a volume of 90 L?

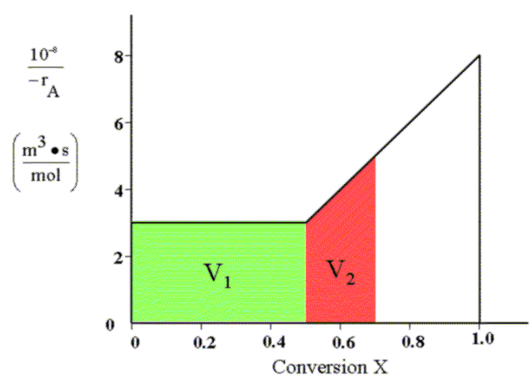
For now, we will assume that conversion (X) will be less that 0.5.

CSTR mole balance:

$$V = \frac{F_{A0}X}{-r_A} = \frac{v_0 C_{A0} X}{-r_A} \quad X = \frac{V}{\frac{v_0 C_{A0}}{-r_A}} = \frac{0.09m^3}{5\frac{m^3}{s} \times 200\frac{mol}{m^3} \times 3\times10^8 \frac{m^3.s}{mol}} = 3\times10^{-13}$$

CDP2-A (c)

This problem will be divided into two parts, as seen below:



- The PFR volume required in reaching X=0.5 (reaction rate is independent of conversion).

$$V_1 = \frac{F_{A0}X}{-r_A} = \frac{v_0 C_{A0} X}{-r_A} = 1.5\times10^{11} m^3$$

- The PFR volume required to go from X=0.5 to X=0.7 (reaction rate depends on conversion).

$$V_2 = F_{Ao}\int_{0.5}^{0.7}\frac{dX}{-r_A} = v_o C_{Ao} * \left(10^8 \frac{m^3 \bullet s}{mol}\right)\int_{0.5}^{0.7}(10X-2)dX$$

$$= 5\frac{m^3}{s} * 200\frac{mol}{m^3} * \left(10^8 \frac{m^3 \bullet s}{mol}\right) * (5X^2 - 2X)\Big|_{0.5}^{0.7}$$

$$= 10^{11} m^3 \left(\left[5(0.7)^2 - 2(0.7)\right] - \left[5(0.5)^2 - 2(0.5)\right]\right)$$

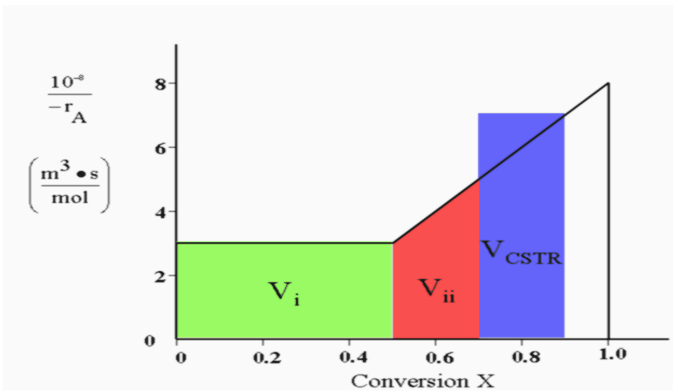
$$= 8 * 10^{10} m^3$$

Finally, we add V_2 to V_1 and get:

$$V_{tot} = V_1 + V_2 = 2.3 \times 10^{11} \ m^3$$

CDP2-A (d)

What CSTR reactor volume is required if effluent from the plug-flow reactor in part (c) is fed to a CSTR to raise the conversion to 90 %



We notice that the new inverse of the reaction rate (1/-rA) is 7*108. We insert this new value into our CSTR mole balance equation:

$$V_{CSTR} = \frac{F_{A0}\Delta X}{-r_A} = \frac{v_0 C_{A0}\Delta X}{-r_A} = 1.4 \times 10^{11} m^3$$

CDP2-A (e)

If the reaction is carried out in a constant-pressure batch reactor in which pure A is fed to the reactor, what length of time is necessary to achieve 40% conversion?

Since there is no flow into or out of the system, mole balance can be written as:

Mole Balance: $r_A V = \dfrac{dN_A}{dt}$

Stoichiometry: $N_A = N_{A0}(1 - X)$

Combine: $r_A V = N_{A0}\dfrac{dX}{dt}$

From the stoichiometry of the reaction we know that V = Vo(1+eX) and e is 1. We insert this into our mole balance equation and solve for time (t):

$$-r_A \frac{V_0}{N_{A0}}(1 + X) = \frac{dX}{dt}$$

$$\int_0^t dt = C_{A0}\int_0^X \frac{dX}{-r_A(1+X)}$$

After integration, we have:

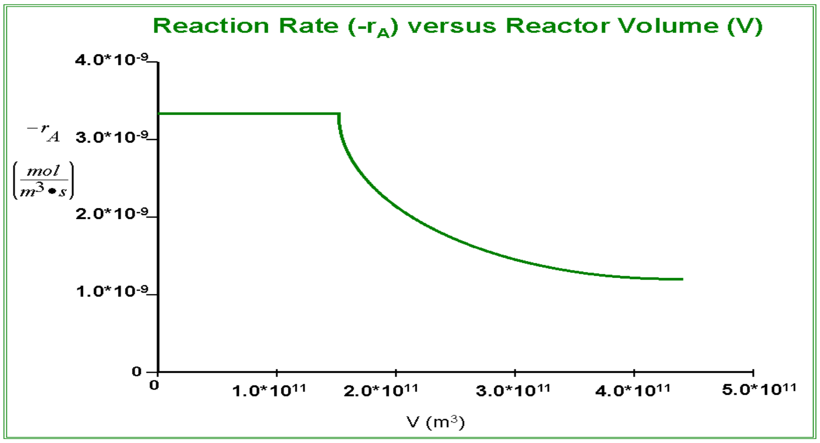
$$t = \frac{1}{-r_A} C_{A0} \ln(1 + X)$$

Inserting the values for our variables:
t = 2.02 x 10^{10} s
That is 640 years.

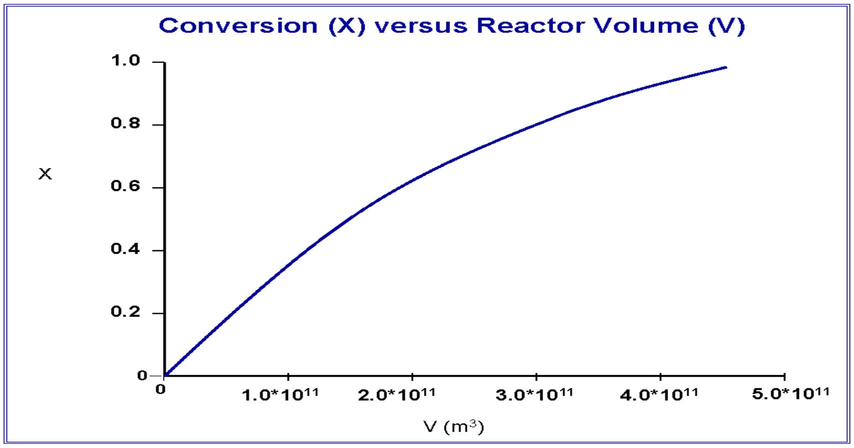
CDP2-A (f)

Plot the rate of reaction and conversion as a function of PFR volume.

The following graph plots the reaction rate ($-r_A$) versus the PFR volume:



Below is a plot of conversion versus the PFR volume. Notice how the relation is linear until the conversion exceeds 50%.



The volume required for 99% conversion exceeds 4*1011 m^3.

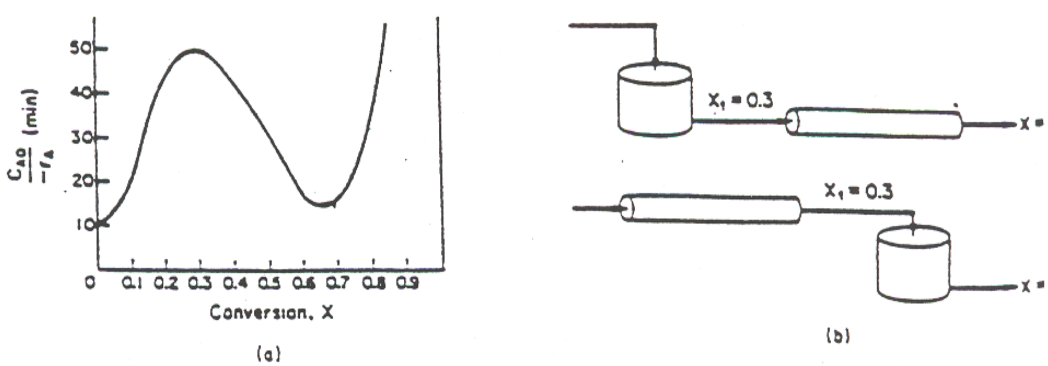
CDP2-A (g)

Critique the answers to this problem.

The rate of reaction for this problem is extremely small, and the flow rate is quite large. To obtain the desired conversion, it would require a reactor of geological proportions (a CSTR or PFR approximately the size of the Los Angeles Basin), or as we saw in the case of the batch reactor, a very long time.

CDP2-B Individualized solution

CDP2-C (a)



For an intermediate conversion of 0.3, Figure above shows that a PFR yields the smallest volume, since for the PFR we use the area under the curve. A minimum volume is also achieved by following the PFR with a CSTR. In this case the area considered would be the rectangle bounded by X =0.3 and X = 0.7 with a height equal to the $C_{A0}/-r_A$ value at X = 0.7, which is less than the area under the curve.

CDP2-C (b)

$v_o = 50\ l/min$

$V = v_o\ I$, where

I = area considered in part a.

$$I = \int_0^{0.3} \frac{C_{AO}}{-r_A} dX + (0.7-0.3) \left.\frac{C_{AO}}{-r_A}\right|_{X=0.7}$$

$$= (0.3 - 0)(10) + \frac{1}{2}(0.3-0)(50-10) + (0.7-0.3)(15)$$

$$= 15 \text{ min}$$

So $V = v_o\ I = (50\ l/min)\ (15\ min) = 750\ l = 750\ dm^3$.

CDP2-C (c)

The smallest area can be achieved by using only one CSTR with this system,

$$I = (0.7-0.0) \left.\frac{C_{AO}}{-r_A}\right|_{X=0.7} = (0.7-0)(15) = 10.5 \text{ min}$$

So $V = v_o\ I = (50)\ l/min\ (10.5)\ min = 525\ l$

We would further reduce the total volume by using a PFR at first up to the conversion that gives the same $C_{AO}/-r_A$ as X=0.7.

CDP2-C (d)

To obtain equal CSTR and PFR volumes the area under the curve must be equal to the area of the rectangle up to the specified conversion.

By trial and error we see that X=0.45 is a solution. For the CSTR,

$$I = (0.45-0) \left.\frac{C_{AO}}{-r_A}\right|_{X=0.7} = (0.45-0)(37) = 16.65 \text{ min}$$

So $V = v_o\ I = (50\ l/min)(16.65\ min) = 832.5\ l$

For the PFR,

$$I = \int_0^{0.45} \frac{C_{A0}}{-r_A} dX$$

Using Simpson's rule

$$I = \frac{0.05}{3}(10 + 4(15) + 2(20) + 4(35) + 2(43) + 4(48) + 2(50) + 4(48) + 2(43) + 37)$$

$$= \frac{0.05}{3}(10 + 4(15 + 35 + 48 + 48) + 2(20 + 43 + 50 + 43) + 37) = 15.72$$

So $V = v_o I$ = (50 l/min)(15.72 min) = 786 l   6% difference, pretty cl

There is also a solution at an X>0.7

Try X = 0.8

For the CSTR

$I = (0.8-0)(33) = 26.4$ min

For the PFR

$$I = \int_0^{0.8} \frac{C_{A0}}{-r_A} dX$$

$$= \frac{0.1}{3}(10 + 4(20) + 2(43) + 4(50) + 2(43) + 4(32) + 2(17) + 4(15) + 33)$$

$$= \frac{0.1}{3}(10 + 4(20 + 50 + 32 + 15) + 2(43 + 43 + 17) + 33) = 23.9 \text{ min}$$

Try X=0.79

For the CSTR

$I = (0.79)(30) = 23.7$ min

So $V = v_o I$ = (50 l/min)(23.7 min) = 1185 l (dm³)

For the PFR

$$I = 23.9 - \frac{1}{2}(0.8-0.79)(30+33) = 23.9 - 0.315 = 23.58 \text{ min}$$

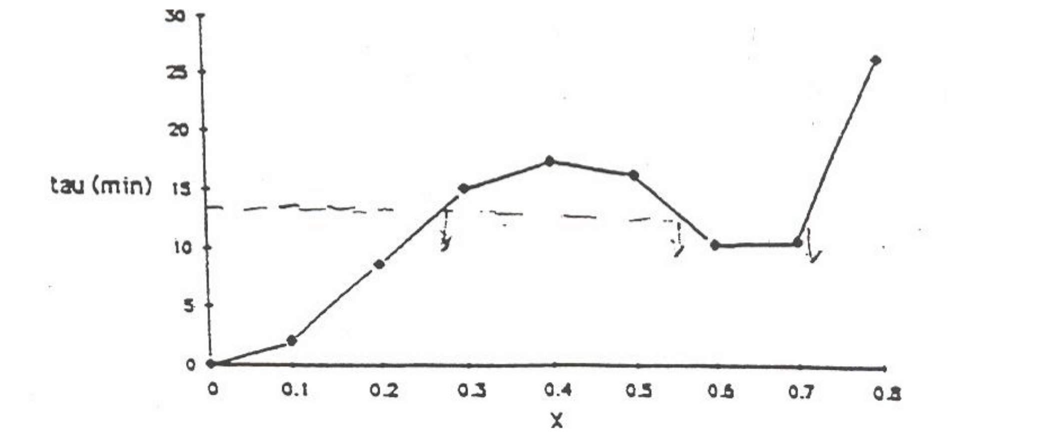
So $V = v_o I$ = (50 l/min)(23.58 min) = 1179 l

0.5% difference

CDP2-C (e)

$$\tau = \frac{V}{v_o} = \frac{v_o X\left[\frac{C_{Ao}}{(-r_A)_X}\right]}{v_o} = X\frac{C_{Ao}}{(-r_A)_X}$$

X	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$C_{A0}/-r_A$(min)	10	20	43	50	43	32	17	15	33
τ(min)	0.0	2.0	8.6	15.0	17.2	16.0	10.2	10.5	26.4



For our particular case

$$\tau = \frac{V}{v_o} = \frac{700\ l}{50\ l/min} = 14\ min$$

The graph yields three possible steady states

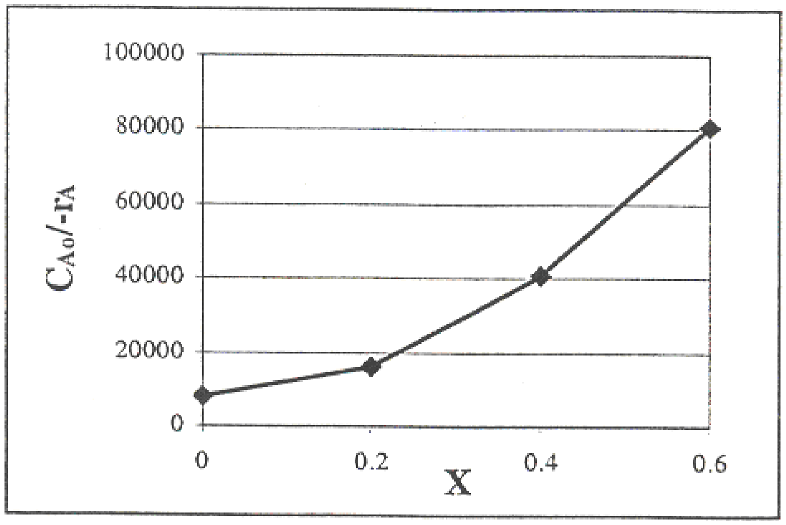
$X_1 = 0.285$, $X_2 = 0.535$, and X_3 0.730.

CDP2-D

Data taken at 1013 kPa (10 atm) and 227°C (500.2 K)

$$y_{Ao} = 0.333 \qquad C_{Ao} = \frac{y_{Ao}P}{RT} = \frac{(0.333)(10)}{(0.082)(500.2)} = 0.08113\ \text{gmol/dm}^3$$

$-r_A$	0.000010	0.000005	0.000002	0.000001
X	0	0.2	0.4	0.6
$C_{Ao}/-r_A$	8112.77	16225.54	40563.84	81127.68



CDP2-D (a)

30% conversion in PFR:

$$\tau_{PFR} = C_{Ao}\int_0^{0.3}\frac{dX}{-r_A} = 4{,}664.84\ \text{s} \quad \Rightarrow \quad V = v_o\tau = (4664.84\ \text{s})\left(\frac{1\ \text{min}}{60\ \text{s}}\right)(2\ \text{m}^3/\text{min}) = 155.5\ \text{m}^3$$

CDP2-D (b)

30 to 50% conversion in CSTR:

$$\tau_{CSTR} = \frac{C_{Ao}(X_2 - X_1)}{-r_{A2}} = 12{,}169.2\ \text{s} \quad \Rightarrow \quad V_{CSTR} = (12{,}169.2\ \text{s})\left(\frac{1\ \text{min}}{60\ \text{s}}\right)(2\ \text{m}^3/\text{min}) = 405.64\ \text{m}^3$$

CDP2-D (c)

Total Volume:

$$V_{Total} = 155.5 + 405.6 = 561.1\ \text{m}^3$$

CDP2-D (d)

60% conversion in PFR:

$$\tau_{PFR} = C_{Ao}\int_0^{0.6}\frac{dX}{-r_A} = 20{,}281.9\ \text{s} \quad \Rightarrow \quad V_{PFR} = (20{,}281.9\ \text{s})\left(\frac{1\ \text{min}}{60\ \text{s}}\right)(2\ \text{m}^3/\text{min}) = 676.06\ \text{m}^3$$

80% conversion in PFR:

r_A is not known for X>0.60 – can not do.

CDP2-D (e)

50 % in CSTR:

$$\tau = C_{Ao}\frac{X}{-r_A} = 30{,}422.9\ \text{s}$$

$$V = v_o\tau = (30{,}422.9\ \text{s})\left(\frac{1\ \text{min}}{60\ \text{s}}\right)(2\ \text{m}^3/\text{min}) = 1014.1\ \text{m}^3$$

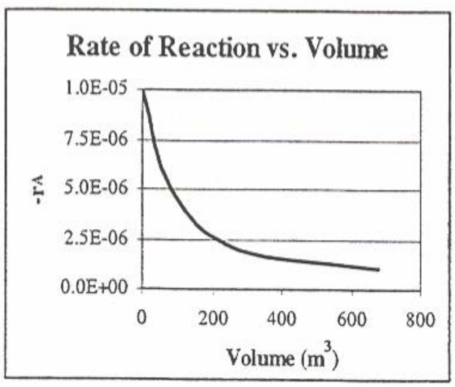
CDP2-D (f)

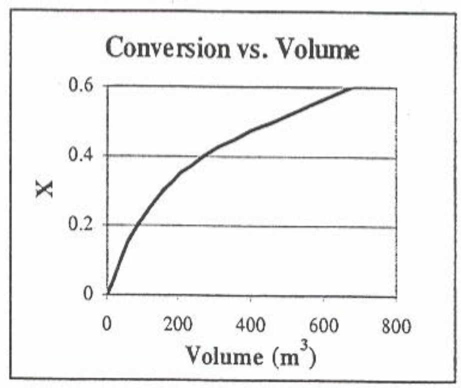
50 to 60% conversion in CSTR:

$$\tau = \frac{C_{Ao}(X_2 - X_1)}{-r_{A2}} = 8112.8$$

$$V = v_o\tau = (8112.8\ \text{s})\left(\frac{1\ \text{min}}{60\ \text{s}}\right)(2\ \text{m}^3/\text{min}) = 270.4\ \text{m}^3$$

CDP2-D (g)





CDP2-D (h)

Critique
Answers are Valid:

1. Constant Temperature and Pressure
   No heat effects
   No pressure drop
2. Single interpolation to $X_A = 0.15, 0.30, 0.45$, and 0.50 allowable
3. Huge volume (the size of the LA Basin)! Raise T? Raise P?

CDP2-E

For the CSTR:

$$V_1 = \frac{F_{Ao}X_1}{-r_A} = F_{Ao}(\text{Area})$$

$$\text{Area} = V_1 = 1200\ \text{dm}^3$$

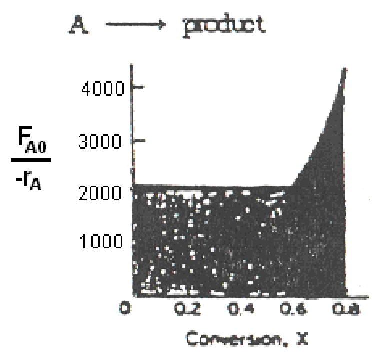
From the graph we can see that $X_1 = 0.60$

For the PFR:

$$V_2 = \frac{F_{Ao}(X_2 - X_1)}{-r_A} = F_{Ao}(\text{Area under curve})$$

$$\text{Area under curve} = V_2 = 600\ \text{dm}^3$$

From the graph we can see that $X_2 = 0.80$



CDP2-F (a)

Find the conversion for the CSTR and PFR connected in series.

X	$-r_A$	$1/(-r_A)$
0	0.2	5
0.1	0.0167	59.9
0.4	0.00488	204.9
0.7	0.00286	349.65
0.9	0.00204	490.19

400 L CSTR and 100 L PFR   Feed is 41% A, 41% B, and 18% I.

$P = 10\ \text{atm} \qquad T = 227°C = 500\ K$

$$C_{To} = \frac{P}{RT} = \frac{10\ \text{atm}}{(0.082\ \text{L}\cdot\text{atm/mol}\cdot\text{K})(500\ \text{K})} = 0.244\ \text{mol/L}$$

$$C_{Ao} = 0.41C_{To} = 0.41(0.244\ \text{mol/L}) = 0.1\ \text{mol/L}$$

$$F_{Ao} = \upsilon_o C_{Ao} = 1\ \text{L/s}(0.1\ \text{mol/L}) = 0.1\ \text{mol/s} = 6\ \text{mol/min}$$

There are two possible arrangements of the system:

1. CSTR followed by the PFR
2. PFR followed by the CSTR

Case 1: CSTR → PFR

CSTR: $V_1 = F_{Ao}(\text{Area})$

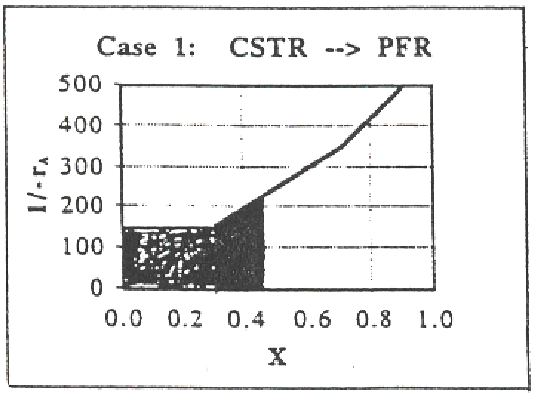
$$\text{Area} = \frac{V_1}{F_{Ao}} = \frac{400}{6} = 66.67$$

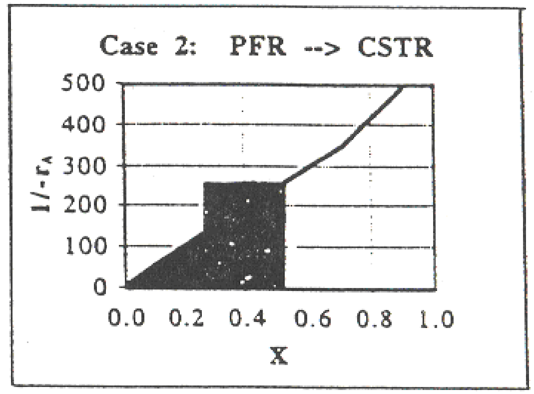
From the graph - $X_1 = 0.36$

PFR: $V_2 = F_{Ao}(\text{Area under curve})$

$$\text{Area under curve} = \frac{V_2}{F_{Ao}} = \frac{100}{6} = 16.667$$

From the graph - $X_2 = 0.445$





Case 2: PFR $\rightarrow$ CSTR

PFR: Area under curve = 16.67

From the graph - $X_1 = 0.259$

CSTR: Area = 66.67

From the graph - $X_2 = 0.515$

CDP2-F (b)

Two 400 L CSTR's in series.

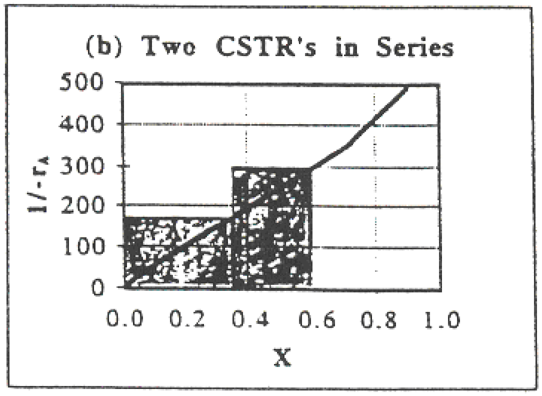
CSTR1: $V = F_{Ao}(\text{Area})$

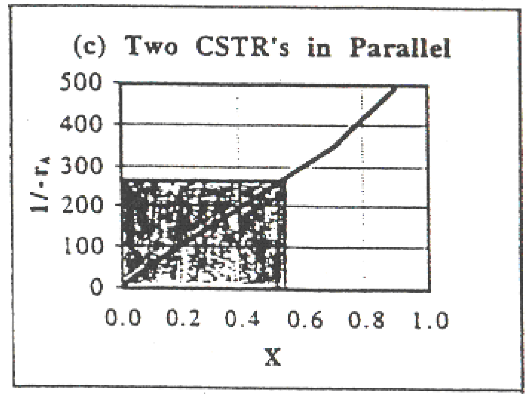
Area = 66.67

From the graph - $X_1 = 0.36$

CSTR2: Area = 66.67

From the graph - $X_2 = 0.595$





CDP2-F (c)

Two 400 L CSTR's in parallel.

To each CSTR goes half of the feed.

$F_{Ao} = 6/2 = 3$ mol/min

$V = F_{Ao}(\text{Area})$

$$\text{Area} = \frac{V}{F_{Ao}} = \frac{400}{3} = 133.3$$

From the graph : $X = 0.52$

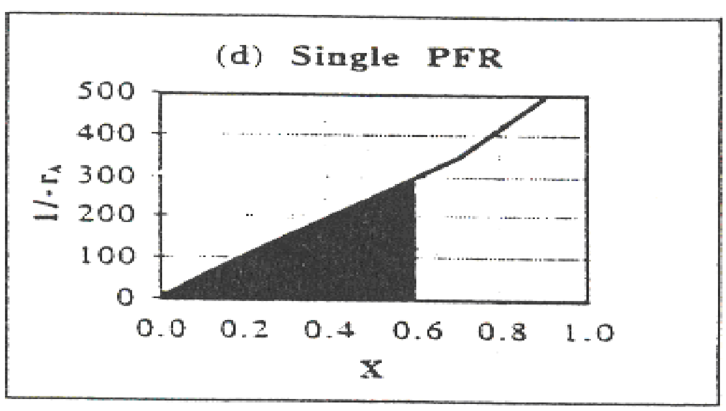
CDP2-F (d)

PFR : $V = F_{Ao}(\text{Area under curve})$

From the graph we can find the area under the curve for a conversion of 0.60:

$$\text{Area} = \frac{(0.60)(300)}{2} = 90$$

$V = (2 \text{ mol/min})(90) = 180$ L



CDP2-F (e)

Pressure reduced by a factor of 10.

A decrease in pressure would cause a decrease in the overall concentration which would in turn cause a decrease in C_{Ao} and F_{Ao}. By looking at the design equation:

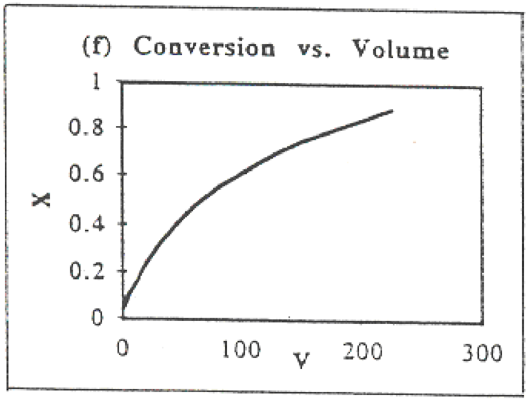
$$V = \frac{F_{Ao}X}{-r_A}$$

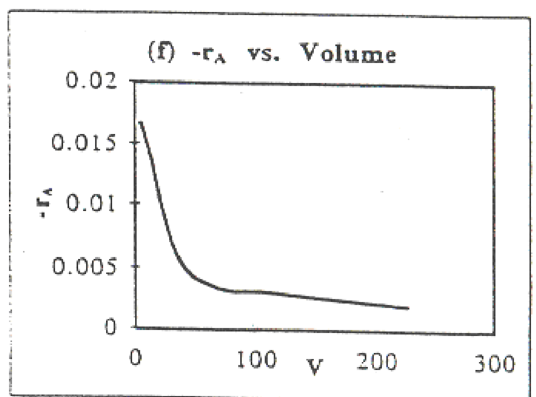
it is apparent that to compensate for the decrease in F_{Ao} there would be and increase in X.

CDP2-F (f)

Use the graph of $1/-r_A$ vs. X to find values for all volumes. (Assume a flow rate of 1 mol/min.) Generate the following table and graphs:

X	$-r_A$	V
0	0.2	0
0.1	0.0167	3.494
0.4	0.00488	42.984
0.7	0.00286	125.878
0.9	0.00204	225.088





CDP2-F (g) Individualized solution