SOLUTION:

PART = A

CASE1

Sol

(A) case I Dissociative adsorption of hydrogen.

Iso octane + H_2 $\longrightarrow$ Iso octane

A + B_2 $\longrightarrow$ C.

$$A + S \rightleftharpoons A\cdot S$$

$$B_2 + 2S \rightleftharpoons 2B\cdot S$$

$$A\cdot S + 2B\cdot S \rightleftharpoons C\cdot S + 2S$$

$$C\cdot S \rightleftharpoons C + S$$

$$r_{AA} = k_{AA}\left[P_A C_v - \frac{C_{AS}}{K_{AA}}\right] \quad -(1)$$

$$r_{AB_2} = k_{AB_2}\left[P_{B_2} C_v^2 - C_{BS}^2\right] \quad -(2)$$

$$r_S = k_S\left[C_{AS} C_{BS}^2 - \frac{C_{CS} C_v^2}{K_S}\right] -(3)$$

$$r_D = k_d\left[C_{CS} - \frac{P_C C_v}{K_D}\right] -(4)$$

Rate limited step $\rightarrow$ surface Rnx step

then eq(1) = eq(2) = eq(4) = 0

$$eq(1) = 0 \Rightarrow C_{AS} = K_{AA} P_A C_v$$

$$eq(2) = 0 \Rightarrow C_{BS} = (K_{AB_2} P_{B_2})^{1/2} C_v$$

$$eq(4) = 0 \Rightarrow C_{CS} = \frac{P_C C_v}{K_D}$$

$$C_T = C_v + C_{AS} + C_{BS} + C_{CS} = C_v + K_{AA} P_A C_v + (K_{AB_2} P_{B_2})^{1/2} C_v + \frac{P_C C_v}{K_D}$$

$$C_v = \frac{C_T}{1 + K_{AA} P_A + (K_{AB_2} P_{B_2})^{1/2} + \frac{P_C}{K_D}}$$

$$r_S = k_S\left[K_{AA} P_A C_v K_{AB_2} P_{B_2} C_v^2 - \frac{P_C}{K_D} C_v^3\right]$$

$$\boxed{r_S = -r_A' = \frac{k_S\left[K_{AA} K_{AB_2} P_A P_{B_2} - \frac{P_C}{K_D}\right] C_T^3}{\left[1 + K_{AA} P_A + \frac{P_C}{K_D} + K_{AB_2}^{1/2} P_{B_2}^{1/2}\right]^3}} \quad -(5)$$

$$-r_A'' = r_S = \frac{k_S\left[K_{AA}K_{AB_2}P_AP_{B_2} - \frac{P_C}{K_D}\right]C_T^3}{\left[1 + K_{AA}P_A + \frac{P_C}{K_D} + K_{AB_2}^{1/2}P_{B_2}^{1/2}\right]^3}$$

Assume : Irreversible rxn for easy calculation.

$$r_S = \frac{\left(k_S K_{AA}K_{AB_2}C_T^3\right)P_AP_{B_2}}{\left[1 + K_{AA}P_A + \frac{P_C}{K_D} + K_{AB_2}^{1/2}P_B^{1/2}\right]^3}$$

** $$\boxed{r_S = \frac{K_1P_AP_{B_2}}{\left[1+K_2P_A + K_3P_C + K_4P_{B_2}^{1/2}\right]^3}}$$ ** —— (6)

$$\left(\frac{P_AP_{B_2}}{r_S}\right)^{1/3} = \frac{1}{K_1^{1/3}}\left[1 + K_2P_A + K_3P_C + K_4P_{B_2}^{1/2}\right]$$

→ For linearization of equation.

$$\Rightarrow \left(\frac{P_AP_{B_2}}{r_S}\right)^{1/3} = \frac{1}{K_1^{1/3}} + \frac{K_2}{K_1^{1/3}}P_A + \frac{K_3}{K_1^{1/3}}P_C + \frac{K_4}{K_1^{1/3}}P_{B_2}^{1/2}$$

RUN	RATE	Pb2	Pa	Pc	(Pa*Pb2/RATE)^0.33
1	0.0362	1	1	0	3.022946607
2	0.0239	1	1	1	3.471634799
3	0.039	3	1	1	4.252903703
4	0.0351	1	3	1	4.40492021
5	0.0114	1	1	3	4.443225787
6	0.0534	10	1	0	5.721188377
7	0.028	1	10	0	7.09491706
8	0.0033	1	1	10	6.716793862
9	0.038	2	2	2	4.721631957
10	0.009	1	1	4	4.807498568
11	0.0127	0.6	0.6	0.6	3.049062031
12	0.0566	5	5	5	7.615665478

WHEN Pa=Pb2=1

RUN	RATE	Pb2	Pa	Pc	(Pa*Pb2/RATE)^0.33
1	0.0362	1	1	0	3.022946607
2	0.0239	1	1	1	3.471634799
5	0.0114	1	1	3	4.443225787
8	0.0033	1	1	10	6.716793862
10	0.009	1	1	4	4.807498568

MALTAB CODE FOR MAKING GRAPH AND PLOT

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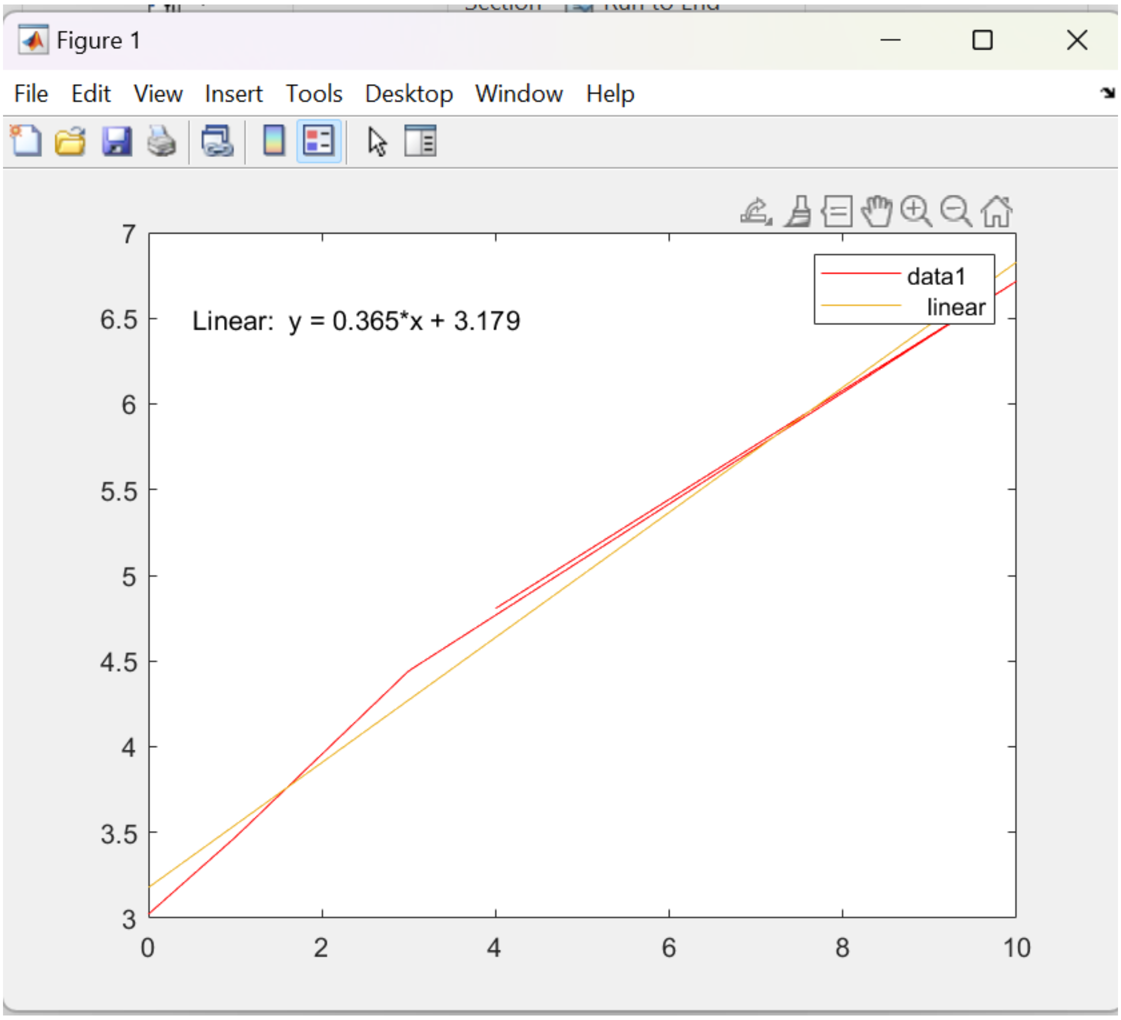
```
x = [0 1 3 10 4]
y = [3.022946607 3.471634799 4.443225787 6.716793862 4.807498568]
figure
plot(x,y,'r-')
```



→ for $P_A = P_B = 1$

$$\left(\frac{P_A P_{B_2}}{r_s}\right)^{1/3} = \left[\frac{1}{K_1^{1/3}} + \frac{K_2}{K_1^{1/3}} + \frac{K_4}{K_1^{1/3}}\right] + \frac{K_3}{K_1^{1/3}} P_C$$

$$y = 3.179 + 0.365\,x$$

$$\frac{1}{K_1^{1/3}}\left[1+K_2+K_4\right] = 3.179 \qquad \frac{K_3}{K_1^{1/3}} = 0.365$$

WHEN Pc = 0

RUN	RATE	Pb2	Pa	Pc	(Pa*Pb2/RATE)^0.33
1	0.0362	1	1	0	3.022946607
6	0.0534	10	1	0	5.721188377
7	0.028	1	10	0	7.09491706

$\rightarrow P_C = 0$

$$\left(\frac{P_A P_{B_2}}{r_S}\right)^{1/3} = \frac{1}{K_1^{1/3}}\left[1 + K_2 P_A + K_4 P_B^{1/2}\right]$$

Put $K_1^{1/3} = K_5$

$$K_5\left(\frac{P_A P_{B_2}}{r_S}\right)^{1/3} - K_2 P_A - K_4 P_B^{1/2} = 1$$

we have three conditions:-

$K_5(3.023) - K_2(1) - K_4(1) = 1$

$K_5(5.721) - K_2(1) - K_4(10)^{1/2} = 1$

$K_5(7.095) - K_2(10) - K_4(1) = 1$

$K_5 = 0.756$

$K_2 = 0.342$

$K_4 = 0.944$

$K_3 = K_1^{1/3}(0.365) = K_5(0.365) = 0.2761$

$K_1 = (K_5)^3 = 0.432$

$$-r_A' = \boxed{r_S = \frac{0.432 P_A P_B}{[1 + 0.342 P_A + 0.276 P_C + 0.944 P_{B_2}^{1/2}]^3}} \quad \text{— (7)}$$

when
$$\left\{\begin{array}{l} K_{AA} = K_2 = 0.342 \\ K_{AB_2} = K_4^2 = 0.891136 \\ K_D = \frac{1}{K_3} = 3.6218 \\ k_S K_{AA} K_{AB_2} C_T^3 = K_1 \\ k_S C_T^3 = 1.417 \end{array}\right\}$$

CASE2

* case II

Associative adsorption of hydrogen.

Iso-octane + hydrogen $\longrightarrow$ Iso-octane

$A + B \longrightarrow C$

$A + S \rightleftharpoons A\text{-}S$

$B + S \rightleftharpoons B\text{-}S$

$A\text{-}S + B\text{-}S \rightleftharpoons C\text{-}S + S$

$C\text{-}S \rightleftharpoons C + S$

$$r_{AA} = k_{AA}\left[P_A C_v - \frac{C_{AS}}{K_{AA}}\right] \quad \text{--- (8)}$$

$$r_{AB} = k_{AB}\left[P_B C_v - \frac{C_{BS}}{K_{AB}}\right] \quad \text{--- (9)}$$

$$r_S = k_S\left[C_{AS} C_{BS} - \frac{C_{CS} C_v}{K_S}\right] \quad \text{--- (10)}$$

$$r_D = k_D\left[C_{CS} - \frac{P_C C_v}{K_D}\right] \quad \text{--- (11)}$$

Rate limited step $\rightarrow$ surface Rxn step

eq (8) = eq (9) = eq (11) = 0

eq (8) = 0 $\Rightarrow C_{AS} = K_{AA} P_A C_v$

eq (9) = 0 $\Rightarrow C_{BS} = K_{AB} P_B C_v$

eq (11) = 0 $\Rightarrow C_{CS} = \frac{P_C C_v}{K_D}$

$$C_T = C_v + C_{AS} + C_{BS} + C_{CS} = C_v + K_{AA} P_A C_v + K_{AB} P_B C_v + \frac{P_C C_v}{K_D}$$

$$C_v = \frac{C_T}{1 + K_{AA} P_A + K_{AB} P_B + \frac{P_C}{K_D}}$$

$$r_S = k_S\left[K_{AA} P_A C_v K_{AB} P_C C_v - \frac{P_C C_v C_v}{K_D K_S}\right]$$

$$\boxed{-r_A' = r_S = \frac{k_S\left[K_{AA} K_{AB} P_A P_B - \frac{P_C}{K_D K_S}\right] C_T^2}{\left[1 + K_{AA} P_A + K_{AB} P_B + \frac{P_C}{K_D}\right]^2}} \quad \text{--- (12)}$$

Assume Irreversible rxn for easy calculation.

$$-r_A' = r_S = \frac{k_S [K_{AA} K_{AB} P_A P_B] C_T^2}{[1 + K_{AA} P_A + K_{AB} P_B + \frac{P_C}{K_D}]^2}$$

$$= \frac{[k_S K_{AA} K_{AB} C_T^2] P_A P_B}{[1 + K_{AA} P_A + K_{AB} P_B + \frac{P_C}{K_D}]^2}$$

★★

$$\boxed{-r_A' = r_S = \frac{k_6 P_A P_B}{[1 + k_7 P_A + k_8 P_B + k_9 P_C]^2}}$$

★★

where

$$\left\{ \begin{array}{l} k_6 = k_S K_{AA} K_{AB} C_T^2 \\ k_7 = K_{AA} \\ k_8 = K_{AB} \\ k_9 = \frac{1}{K_D} \end{array} \right\}$$

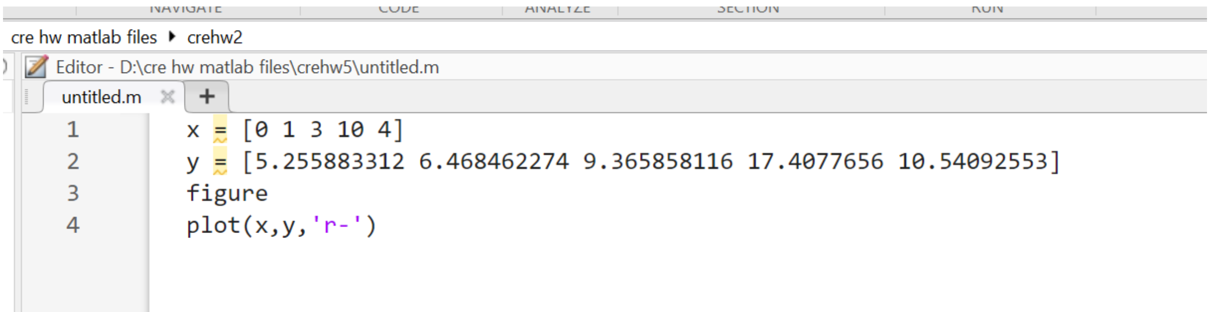
→ for linearization this equation.

$$\rightarrow \left(\frac{P_A P_B}{r_S}\right)^{1/2} = \frac{1}{k_6^{0.5}} + \frac{k_7}{k_6^{0.5}} P_A + \frac{k_8}{k_6^{0.5}} P_B + \frac{k_9}{k_6^{0.5}} P_C$$

RUN	RATE	Pb	Pa	Pc	(Pa*Pb/RATE)^0.5
1	0.0362	1	1	0	5.255883312
2	0.0239	1	1	1	6.468462274
3	0.039	3	1	1	8.770580193
4	0.0351	1	3	1	9.24500327
5	0.0114	1	1	3	9.365858116
6	0.0534	10	1	0	13.68451379
7	0.028	1	10	0	18.89822365
8	0.0033	1	1	10	17.4077656
9	0.038	2	2	2	10.25978352
10	0.009	1	1	4	10.54092553
11	0.0127	0.6	0.6	0.6	5.324139056
12	0.0566	5	5	5	21.01656759

WHEN Pa = Pb = 1

RUN	RATE	Pb	Pa	Pc	(Pa*Pb/RATE)^0.5
1	0.0362	1	1	0	5.255883312
2	0.0239	1	1	1	6.468462274
5	0.0114	1	1	3	9.365858116
8	0.0033	1	1	10	17.4077656
10	0.009	1	1	4	10.54092553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untitled.m
x = [0 1 3 10 4]
y = [5.255883312 6.468462274 9.365858116 17.4077656 10.54092553]
figure
plot(x,y,'r-')

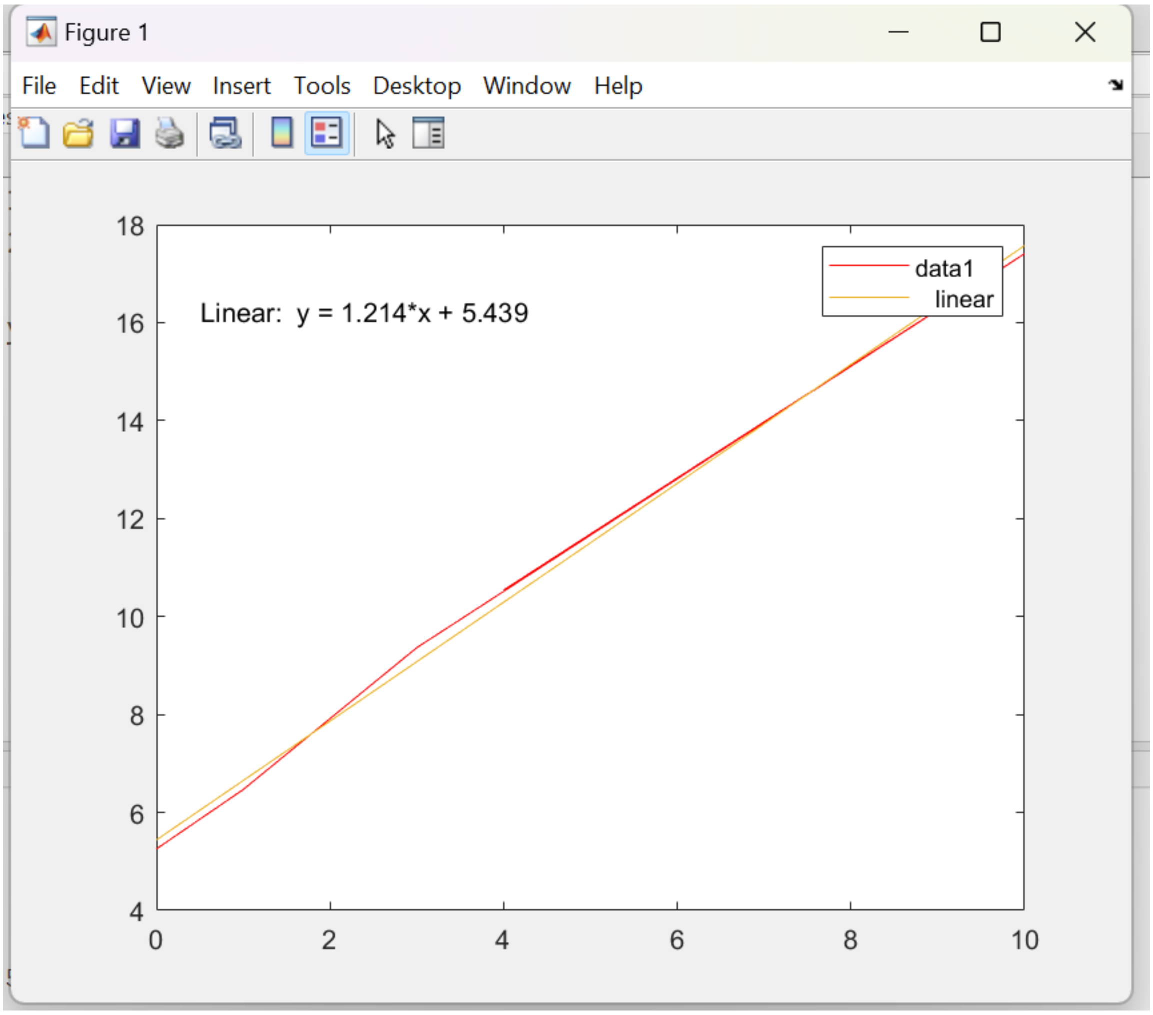
Figure 1
File Edit View Insert Tools Desktop Window Help
Linear: y = 1.214*x + 5.439
data1
linear
18
16
14
12
10
8
6
4
0
2
4
6
8
10

$\rightarrow$ for $P_A = P_B \neq 1$

$$\left(\frac{P_A P_B}{r_S}\right)^{1/2} = \left(\frac{k_9}{k_6^{0.5}}\right) P_C + \left(\frac{1}{k_6^{0.5}} + \frac{k_7}{k_6^{0.5}} + \frac{k_8}{k_6^{0.5}}\right)$$

$$y = 1.214 P_C + 5.439$$

$$\frac{k_9}{k_6^{0.5}} = 1.214 \qquad \frac{1}{k_6^{0.5}}\left(1 + k_7 + k_8\right) = 5.439$$

WHEN Pa = Pb = Pc

	A	B	C	D	E	F
1	RUN	RATE	Pb	Pa	Pc	(Pa*Pb/RATE)^0.5
2	2	0.0239	1	1	1	6.468462274
3	9	0.038	2	2	2	10.25978352
4	11	0.0127	0.6	0.6	0.6	5.324139056
5	12	0.0566	5	5	5	21.01656759
6						

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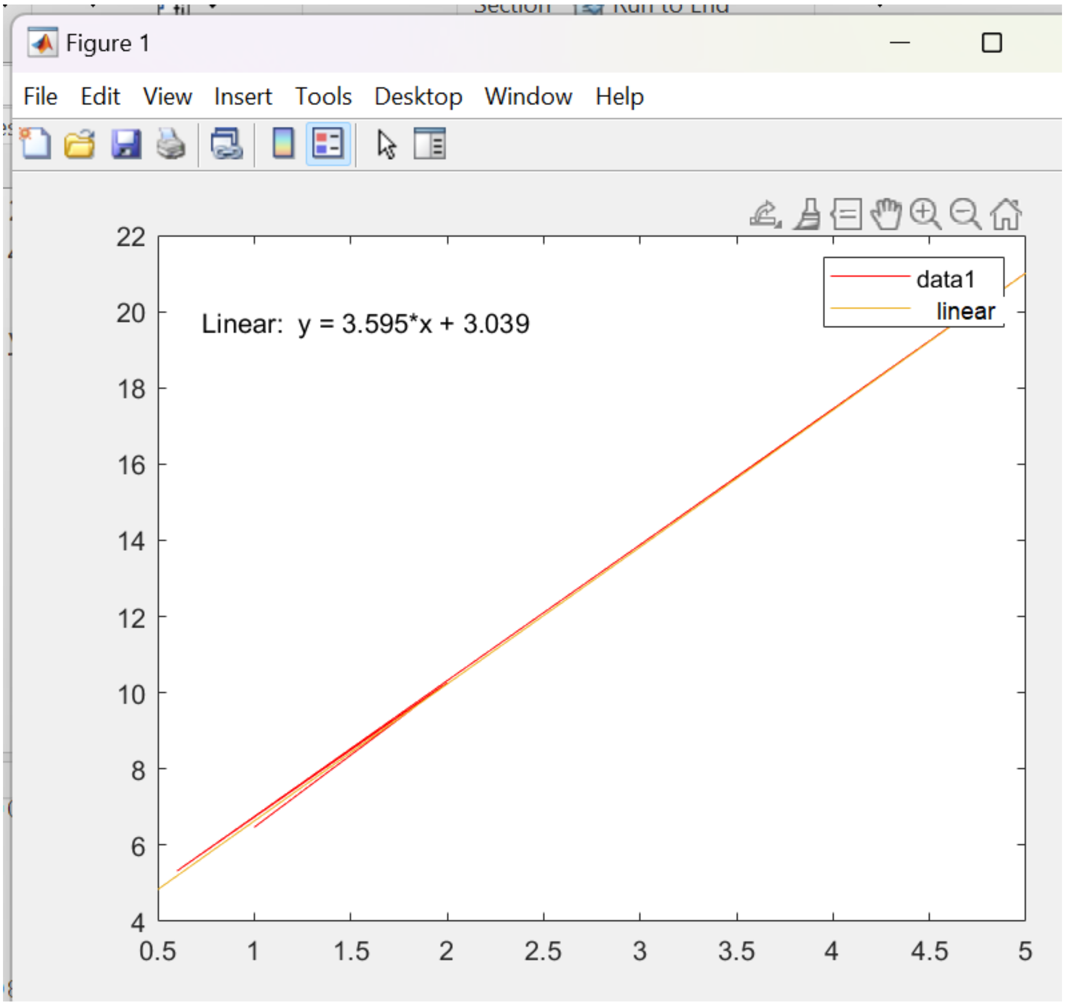
untitled2.m

```
x = [1 2 0.6 5]
y = [6.468462274 10.25978352 5.324139056 21.01656759]
figure
plot(x,y,'r-')
```



$\rightarrow \cdot P_A = P_B = P_C$.

$$\left(\frac{P_A P_B}{r_S}\right)^{1/2} = \frac{1}{K_6^{0.5}} + \frac{1}{K_6^{0.5}}\left(K_7+K_8+K_9\right) P_C$$

$$y = 3.039 + 3.595\, P_C$$

$$\frac{1}{K_6^{0.5}} = 3.039 \qquad \frac{1}{K_6^{0.5}}\left(K_7+K_8+K_9\right) = 3.595$$

$$K_9 = \frac{1.214}{3.039} = 0.3995$$

$$K_6 = \frac{1}{(3.039)^2} = 0.1083$$

WHEN Pc = 0

	A	B	C	D	E	F
1	RUN	RATE	Pb	Pa	Pc	(Pa*Pb/RATE)^0.5
2	1	0.0362	1	1	0	5.255883312
3	6	0.0534	10	1	0	13.68451379
4	7	0.028	1	10	0	18.89822365

$\rightarrow P_C = 0$

$$13.68451 = 3.039 [1 + K_7(1) + K_8(10)]$$
$$18.8982 = 3.039 [1 + K_7(10) + K_8(1)]$$

$$K_7 + 10K_8 = 3.50296$$
$$10K_7 + K_8 = 5.218567$$
$$K_7 = 0.491744$$
$$K_8 = 0.301122$$

$\rightarrow$ final result.

$$-r_A' = r_S = \frac{0.1083\, P_A P_B}{[1 + (0.491744) P_A + (0.301122) P_B + (0.3995) P_C]^2}$$

$$K_{AA} = K_7 = 0.491744$$
$$K_{AB} = K_8 = 0.301122$$
$$K_D = 1/K_9 = 2.50312$$
$$k_S C_T^2 = \frac{K_6}{K_7 K_8} = 0.731386$$

PART = B

Calculated rate means rate calculated by putting the valves of partial pressure of each species in rate equation defined in part 1 for both cases.

ERROR IN EXCEL SHEET MEANS

PERCENTAGE ERROR = (EXP RATE-CALCULATED RATE)/EXP RATE *100

RATE MEANS IN EXCEL SHEET = EXP RATE

Case 1

	A	B	C	D	E	F	G
1	RUN	RATE	Pb2	Pa	Pc	CALCULATED RATE	ERROR
2	1	0.0362	1	1	0	0.036162219	-0.104368169
3	2	0.0239	1	1	1	0.025688951	7.485150686
4	3	0.039	3	1	1	0.037647002	-3.469225443
5	4	0.0351	1	3	1	0.037893041	7.957380598
6	5	0.0114	1	1	3	0.01430632	25.49403137
7	6	0.0534	10	1	0	0.053317014	-0.155404487
8	7	0.028	1	10	0	0.027990937	-0.03236728
9	8	0.0033	1	1	10	0.003362343	1.88918031
10	9	0.038	2	2	2	0.037946154	-0.141699946
11	10	0.009	1	1	4	0.011088803	23.20891774
12	11	0.0127	0.6	0.6	0.6	0.016744654	31.84766906
13	12	0.0566	5	5	5	0.045297107	-19.96977622
14							

Case 2

	A	B	C	D	E	F	G
1	RUN	RATE	Pb	Pa	Pc	CALCULATED RATE	ERROR
2	1	0.0362	1	1	0	0.033692466	-6.92689
3	2	0.0239	1	1	1	0.022532135	-5.72329
4	3	0.039	3	1	1	0.041601338	6.670096
5	4	0.0351	1	3	1	0.032212813	-8.2256
6	5	0.0114	1	1	3	0.012102897	6.165766
7	6	0.0534	10	1	0	0.053411098	0.020783
8	7	0.028	1	10	0	0.028005835	0.020838
9	8	0.0033	1	1	10	0.003232894	-2.0335
10	9	0.038	2	2	2	0.03781289	-0.49239
11	10	0.009	1	1	4	0.009419052	4.656135
12	11	0.0127	0.6	0.6	0.6	0.013249217	4.324545
13	12	0.0566	5	5	5	0.055862663	-1.30272

By seeing the error in both cases we can say case **2 modal is more accurate**. AS 2ND MODEL SHOW LESS ERROR

PART = C

(c) $A + B \longrightarrow C$

Gas Associative adsorption show less error. therefore we solve using 2^{nd} case mechanism.

$\Rightarrow F_{A0} = F_{B0} = 2.5 \text{ mol/min} = 2.5 \frac{\text{mol}}{\text{min}} \times \frac{60 \text{ min}}{\text{hr}} = 150 \frac{\text{mole}}{\text{hr}}$

$\Rightarrow P_T = 4 \text{ atm}$ $\quad T = 300°C$.

$\Rightarrow P_{A_0} = y_{A_0} P_{T_0} = 2$ $\quad [y_{A0} = 0.5]$

$\Rightarrow P_{A_0} = C_{A_0} RT = 2$

$\Rightarrow X_A = 0.8$

$$\Rightarrow -r_A' = \frac{(0.1083) P_A P_B}{[1 + (0.491744) P_A + (0.301122) P_B + (0.3995) P_C]^2}$$

$$\rightarrow P_A = C_A RT = C_{A0} RT \left[\frac{1 - X_A}{1 + \epsilon X_A}\right]$$

$$= C_{A0} RT \left[\frac{1 - X_A}{1 - 0.5 X_A}\right]$$

$$\left\{ \begin{array}{l} \delta = \frac{1 - 1 - 1}{1} = -1 \\ y_{A0} = 0.5 \\ \epsilon = \delta y_{A0} = -0.5 \end{array} \right.$$

$$\rightarrow P_B = C_B RT = C_{A0} RT \left[\frac{\theta_{BA} - X_A}{1 + \epsilon X_A}\right] \qquad \{\theta_{BA} = 1\}$$

$$= C_{A0} RT \left[\frac{1 - X_A}{1 - 0.5 X_A}\right]$$

$$\rightarrow P_C = C_C RT = C_{A0} RT \left[\frac{\theta_{CA} + X_A}{1 - 0.5 X_A}\right] \qquad \{\theta_{CA} = 0\}$$

$$= C_{A_0} RT \left[\frac{X_A}{1 - 0.5 X_A}\right]$$

$$\rightarrow -r_A' = \frac{(0.1083)(C_{A0}RT)^2 \left[\frac{1-X_A}{1-0.5X_A}\right]^2}{\left[1+\frac{C_{A0}RT}{(1-0.5X_A)}\left\{(1-X_A)(0.491744+0.301122)+0.3995X_A\right\}\right]^2}$$

{ Put value of $C_{A0}RT = 2$ }

$$-r_A' = \frac{0.4332\left[\frac{1-X_A}{1-0.5X_A}\right]^2}{\left[1+\frac{2}{(1-0.5X_A)}\left\{0.792866(1-X_A)+0.3995X_A\right\}\right]^2}$$

$$-r_A' = \frac{0.4332\left[\frac{1-X_A}{1-0.5X_A}\right]^2}{\left[1+\frac{2}{(1-0.5X_A)}\left[0.792866-0.393366X_A\right]\right]^2}$$

→ For CSTR

$$\boxed{W = \frac{F_{A0}X_A}{-r_A'}}$$

$$= \frac{150 \times 0.8}{\frac{0.4332\left[\frac{1-(0.8)}{1-(0.8)0.5}\right]^2}{\left[1+\frac{2}{0.6}\left[0.792866-0.393366X_A\right]\right]^2}}$$

$= 16774.335 g$

$= \underline{16.774 \text{ kg}}$

→ For PFR

$$w = 150\int_0^{X_{Af}} \frac{dX_A}{-r'_A}$$

$$= 150\int_0^{X_{Af}} \frac{dX_A}{\dfrac{0.4332\left[\dfrac{1-X_A}{1-0.5X_A}\right]^2}{\left[1+\dfrac{2}{(1-0.5X_A)}[0.792866-0.393366X_A]\right]^2}}$$

$$= \frac{150}{0.4332}\int_0^{X_{Af}} \frac{\left[1+\dfrac{2}{(1-0.5X_A)}[0.792866-0.393366X_A]\right]^2}{\left[\dfrac{(1-X_A)}{(1-0.5X_A)}\right]^2}dX_A$$

$$\cancel{= \frac{150}{0.4332}\int_0^{X_A}\left[(1-0.5X_A)^2 + \right.}$$

$$= \frac{150}{0.4332}\int_0^{X_{Af}} \frac{\left[(1-0.5X_A)+2[0.792866-0.393366X_A]\right]^2}{(1-X_A)^2}dX_A$$

$$= 346.26038\int_0^{X_{Af}} \frac{\left[2.585732-1.286732X_A\right]^2}{(1-X_A)^2}dX_A$$

$$= 346.26038\int_0^{X_{Af}} \left[\frac{2.585732-1.286732X_A}{1-X_A}\right]^2 dX_A$$

$$W = C\int_0^{0.8}\left(\frac{a-bX_A}{1-X_A}\right)^2 dX_A$$

where $a = 2.585732$

$b = 1.286732$

$c = 346.26038$

$$w = C b^2 \int_0^{0.8} \frac{(a/b - x_A)^2}{(1-x_A)^2} \, dx_A$$

$$= C b^2 \int_0^{0.8} \frac{(a/b - 1 + 1 - x_A)^2}{(1-x_A)^2} \, dx_A$$

Put $1 - x_A = t$ and $\frac{a}{b} - 1 = K = 1.0092$

$dx_A = -dt$

limit

$x_A = 0 \quad t = 1$

$x_A = 0.8 \quad t = 0.2$

$$= -C b^2 \int_1^{0.2} \frac{(K+t)^2}{t^2} \, dx_A$$

$$= -C b^2 \int_1^{0.2} \left(\frac{K^2}{t^2} + 2\frac{K}{t} + 1 \right) dt$$

$$= -C b^2 \left[-K^2 \frac{1}{t} + 2K \ln t + t \right]_1^{0.2}$$

$$= -C b^2 \left[-K^2 \left[\frac{1}{0.2} - 1 \right] + 2K \ln \left[\frac{0.2}{1} \right] + [0.2 - 1] \right]$$

Put the value of a, b, C, K then

$$w = 4656.621 \, g.$$

$$\boxed{w = 4.656 \text{ kg}}$$

PART = D

✱ PART → 4)

$F_{A0} = F_{B0} = 2.5 \ mol/min \quad = 150 \ \frac{mol}{hr}$

$P_{T0} = 4 atm \quad T = 300°C$

$P_{A0} = y_{A0} P_{T0} = 0.5(4) = 2 = C_{A0}(RT)$

$X_{Af} = 0.8$

1/8 inch catalyst Pallet 1 ½ inch SC 80 pipes 35 feet long

void fraction = 40%. density of the catalyst = 2.6 g/cm³

$F_A = F_{A0}(1-X_A) = \frac{F_0}{2}(1-X_A)$

$F_B = F_{B0}(1-X_A) = \frac{1}{2} F_0 (1-X_A)$

$F_C = F_{A0} X_A = \frac{1}{2} F_0 X_A$

$F_T = F_A + F_B + F_C = \frac{F_0}{2}(1-X_A + 1-X_A + X_A)$

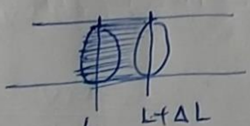
$F_T = \frac{F_0}{2}(2-X_A) \Rightarrow \frac{F_0}{F_T} = \frac{2}{2-X_A}$

$\frac{P_A}{P_T} = \frac{F_A}{F_T} = \frac{(1-X_A)}{2-X_A} \Rightarrow P_A = \left(\frac{1-X_A}{2-X_A}\right) P_T$

$\frac{P_B}{P_T} = \frac{F_B}{F_T} = \left(\frac{1-X_A}{2-X_A}\right) \Rightarrow P_B = \left(\frac{1-X_A}{2-X_A}\right) P_T$

$\frac{P_C}{P_T} = \frac{F_C}{F_T} = \frac{X_A}{2-X_A} \Rightarrow P_C = \left(\frac{X_A}{2-X_A}\right) P_T$

→



Mass balance.

In − Out + Generation = acc ↗ 0

$F_i|_L - F_i|_{L+\Delta L} + (r_i') A_t \rho_c (1-\phi)\, dL = 0$

$\frac{F_i|_{L+\Delta L} - F_i|_L}{dL} = (r_i') A_t \rho_c (1-\phi)$

$\frac{dF_A}{dL} = -(-r_A') A_t \rho_c (1-\phi) \qquad \{F_A = F_{A0}(1-X_A)\}$

$\frac{dX_A}{dL} = \frac{+(-r_A') A_t \rho_c (1-\phi)}{F_{A0}}$

$$A_t = T\left(\frac{\pi}{4} D^2\right) = T\left(\frac{\pi}{4} \left(\frac{1.682}{12}\right)^2 ft^2\right)$$

$$= T(0.01543) \quad ft^2$$

T → no of tubes

total crosssection Area = no of tubes × crosssection area of 1 tube.

$$= T\left(\frac{\pi}{4} d^2\right)$$

$\phi = 0.4$ · $\rho_c = 2.6 \, g/m^3 = 73623.8 \, g/ft^3$

$F_{i0} = 2.5 \frac{mol}{min} = 150 \, mol/hr$.

$$(-r_A') = \frac{0.4332 \, (1-x_A)^2}{(2.5857 - 1.286\, x_A)^2} \rightarrow \left(\text{from } 2^{nd} \text{ modal Part 3.}\right)$$

$$\frac{dx_A}{dL} = \frac{+(0.4332)\left(\frac{1-x_A}{2.5857-1.286x_A}\right)^2 T(0.01543)(0.6)(73623.8)}{150}$$

$$\boxed{\frac{dx_A}{dL} = (+1.9685)\, T \left(\frac{1-x_A}{2.5857-1.286x_A}\right)^2} \quad — (15)$$

→ Ergun equation.

$$\frac{dP}{dL} = \frac{G}{\rho g_0 D_p}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]$$

$$\boxed{\rho = \rho_0 \left(\frac{P}{P_0}\right)\left(\frac{2}{2-x}\right)} \qquad \left\{\frac{\rho}{\rho_0} = \left(\frac{P}{P_0}\right)\left(\frac{F_0}{F_t}\right)\right\}$$

$$\boxed{\frac{dP}{dL} = \frac{2-\cancel{x_A}\beta_0}{2P}} \quad — (16)$$

$$\beta_0 = \frac{P_0 G}{\rho_0 g_c D_p} \frac{(1-\phi)}{\phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]$$

$\phi = 0.4$

$$D_p = \left(\frac{1}{8} \text{inch}\right)\left(\frac{1}{12} ft/in\right) = \frac{1}{8 \times 12} ft.$$

$$= 4.17 \times 10^8 \frac{Lb\,m}{Lbf}\left(ft/hr^2\right)$$

$$G = \frac{F_{A_0} m_A + F_{B_0} m_B}{T(0.01543)} = \frac{(150)\frac{mol}{hr}(2+112)\ g/mol\left(\frac{Lb}{453.6 g}\right)}{T(0.01543)\ ft^2}$$

$$= \frac{2443.189}{T}\left(\frac{Lb\,m}{ft^2\,hr}\right)$$

$$P_0 = 4\,atm = 4\,atm \times \frac{2116.2166}{1\,atm}\left(\frac{Lb\,f}{ft^2}\right)$$

$$\rho_0 = \frac{mass}{vol} = C_T\left(\frac{mass}{mol}\right) = \frac{P}{RT}\ (\text{molecular weight})$$

$$\text{Avg M.W} = y_A M_A + y_B M_B = 57\,\frac{Lb}{Lb\,mol}$$

$$= \frac{57\left(\frac{Lb}{Lb\,mol}\right)\times(4\,atm)}{\left(0.7301\,\frac{ft^3 atm}{Lb\,mol\,R}\right)(200+273.15)(1.8)(R)}$$

$$= \frac{57\times4}{(0.7301)(473.15)(1.8)}\left(\frac{Lb}{ft^3}\right)$$

$$= 0.33667\left(\frac{Lb}{ft^3}\right)$$

Assume: [From Book]

$\mu = 0.02188\ \frac{Lbm}{ft\,hr}$ and $\boxed{T = 2}$

no of tubes.

$$\beta_0 = \frac{(4 \times 2116.21)\left(\frac{2443.189}{2}\right)(0.6)}{(0.3367)(4.17\times10^{8})\left(\frac{1}{8\times12}\right)(0.4)^3}\left[\frac{(150)(0.6)(0.02188)}{\left(\frac{1}{8\times12}\right)} + (1.75)\left(\frac{2443.189}{2}\right)\right]$$

$= 154246.2215$

put the value in eq (16)

$$\boxed{\frac{dP}{dL} = 77123.11075\left(\frac{2-x_A}{P}\right)}$$

then two ODE

$$\frac{dx_A}{dL} = 3.3969\left(\frac{1-x_A}{2.5857-1.286x_A}\right)^2$$

$x_{A0} = 0$

$$\frac{dP}{dL} = 77123.11075\left(\frac{2-x_A}{P}\right)$$

$P_0 = 8464.8664$

L ranges (0 - 35) ft.

as $L_{max} = 35$ ft (length of pipe)

for matlab code.

$$\boxed{\frac{dy_1}{dL} = 3.3969\left(\frac{1-y_1}{2.5857-1.286y_1}\right)^2} \quad \boxed{y_{10} = 0}$$

$$\boxed{\frac{dy_2}{dL} = 77123.110\left(\frac{2-y_1}{y_2}\right)} \quad \boxed{y_{20} = 8464.8664}$$

$L \to (0 - 35)$

After solving.

At $\boxed{x = 0.8}$ $\boxed{L = 3.3182 \text{ ft}}$ $\boxed{P = 8.5021\times10^3}$ lbf/ft²

$\boxed{P = 0.401 \text{ atm}}$

MATLAB CODE TO SOLVE ODES

Editor - D:\cre hw matlab files\crehw9\ques31.m

ques31.m

```
f =@(l,y) [(3.9369*((1-y(1))/(2.5857-1.286*y(1)))^2); (77123.11075*((2-y(1))/(y(2))))];
[l,y] = ode45(f,[0 35],[0; 8464.8664])
```

We know Xa = 0.8

Then find VALUES FOR L & P ACCORDING TO IT

THIS TABLE SHOW VALUE OF L

Variables - I

I

73x1 double

	1	2
1	0	
2	8.5316e-05	
3	1.7063e-04	
4	2.5595e-04	
5	3.4127e-04	
6	7.6785e-04	
7	0.0012	
8	0.0016	
9	0.0020	
10	0.0042	
11	0.0063	
12	0.0084	
13	0.0106	
14	0.0212	
15	0.0319	
16	0.0426	
17	0.0532	
18	0.1066	
19	0.1599	
20	0.2132	

21	0.2665	
22	0.4920	
23	0.7176	
24	0.9431	
25	1.1686	
26	1.4469	
27	1.7253	
28	2.0036	
29	2.2820	
30	2.6274	
31	2.9728	
32	3.3182	
33	3.6636	
34	4.1395	
35	4.6154	
36	5.0914	
37	5.5673	
38	6.2733	
39	6.9792	
40	7.6852	

41	8.3912	
42	9.2662	
43	10.1412	
44	11.0162	
45	11.8912	
46	12.7662	
47	13.6412	
48	14.5162	
49	15.3912	
50	16.2662	
51	17.1412	
52	18.0162	
53	18.8912	
54	19.7662	
55	20.6412	
56	21.5162	
57	22.3912	
58	23.2662	
59	24.1412	
60	25.0162	

THIS TABLE SHOW VALUE OF Xa AND P AS Y1 AND Y2 respectively

Variables - y

y

73x2 double

	1	2
1	0	8.4649e+03
2	5.0236e-05	8.4649e+03
3	1.0047e-04	8.4649e+03
4	1.5070e-04	8.4649e+03
5	2.0093e-04	8.4649e+03
6	4.5204e-04	8.4649e+03
7	7.0308e-04	8.4649e+03
8	9.5406e-04	8.4649e+03
9	0.0012	8.4649e+03
10	0.0025	8.4649e+03
11	0.0037	8.4650e+03
12	0.0050	8.4650e+03
13	0.0062	8.4651e+03
14	0.0124	8.4653e+03
15	0.0186	8.4654e+03
16	0.0248	8.4656e+03
17	0.0309	8.4658e+03
18	0.0608	8.4668e+03
19	0.0898	8.4677e+03
20	0.1178	8.4686e+03

21	0.1449	8.4695e+03
22	0.2499	8.4732e+03
23	0.3404	8.4767e+03
24	0.4179	8.4801e+03
25	0.4843	8.4832e+03
26	0.5531	8.4870e+03
27	0.6098	8.4906e+03
28	0.6565	8.4940e+03
29	0.6954	8.4974e+03
30	0.7351	8.5014e+03
31	0.7671	8.5053e+03
32	0.7931	8.5091e+03
33	0.8146	8.5129e+03
34	0.8389	8.5179e+03
35	0.8581	8.5229e+03
36	0.8734	8.5278e+03
37	0.8861	8.5326e+03
38	0.9013	8.5396e+03
39	0.9131	8.5466e+03
40	0.9224	8.5535e+03

41	0.9300	8.5603e+03	
42	0.9378	8.5687e+03	
43	0.9442	8.5770e+03	
44	0.9493	8.5853e+03	
45	0.9537	8.5936e+03	
46	0.9574	8.6018e+03	
47	0.9605	8.6099e+03	
48	0.9633	8.6181e+03	
49	0.9657	8.6262e+03	
50	0.9678	8.6342e+03	
51	0.9697	8.6423e+03	
52	0.9713	8.6503e+03	
53	0.9728	8.6583e+03	
54	0.9742	8.6663e+03	
55	0.9754	8.6743e+03	
56	0.9765	8.6823e+03	
57	0.9776	8.6902e+03	
58	0.9785	8.6982e+03	
59	0.9794	8.7061e+03	
60	0.9802	8.7140e+03	

weight of catlyst $= (1-\phi) A_t\, z\, \rho_c$

ρ_c → density of catalyst

z → length of catalyst

$= (1-0.4)(2\times 0.01543)(3.3182)(73623.8)$

$= 4523.43$ gram

$= \underline{\underline{4.52\ Kg}}$