Advanced chemical reaction engineering

Prof. H.S. Shankar
Department of Chemical Engineering
Indian Institute of Technology, Bombay

Lecture - 13

Illustrative example
1. Determination of deactivation parameters
2. Design for deactivation catalyst

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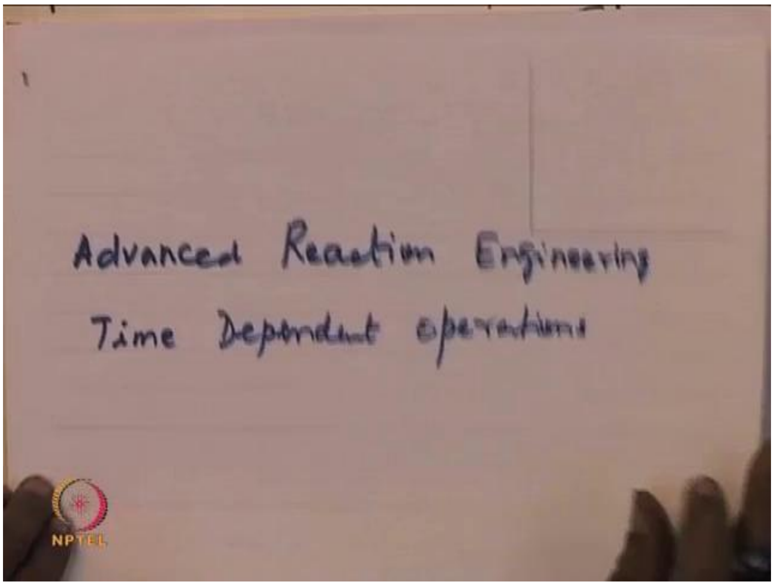

Advanced Reaction Engineering
Time Dependent operations

This look at here advanced reaction engineering; today, will continue and look at time dependent operations.

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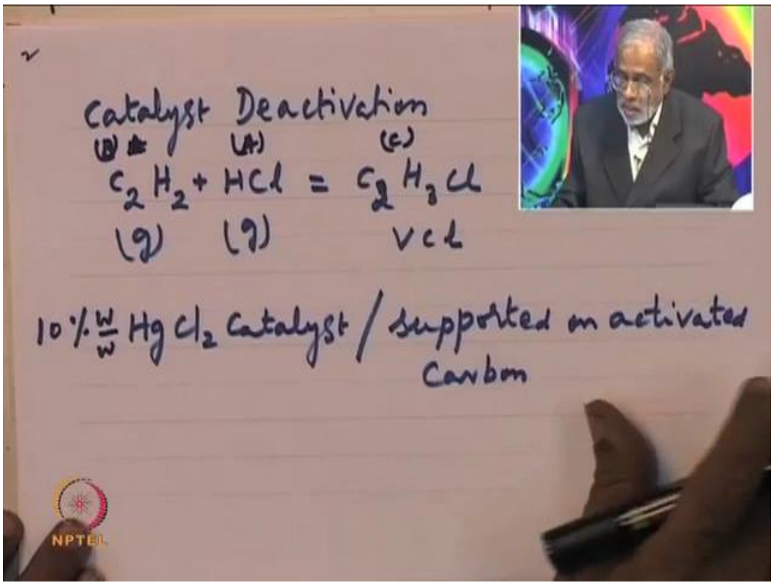

Catalyst Deactivation

(B) (A) (C)

$C_2H_2 + HCl = C_2H_3Cl$

(g) (g) VCl

10% $\frac{w}{w}$ $HgCl_2$ catalyst / supported on activated Carbon

Now, we said at an earlier class that there are several situations where we have deal the time dependence. And, the time dependence we are going to be looking at today is catalyst deactivation. So, the context is catalyst deactivation; of course, there are lot of literature on this subject. And, the example I take here is just to illustrate how we can determine the catalyst activity variation dependence or what is called as rate function for catalytic Activation; as an example. This is an example situation we are looking at; we looking at 1 ((Refer Time: 01:34)) production from a acetylene and H C l this gas, this also a gas it gives you sorry; C 2 H 3 C l this called vinyl chloride ok.

This reaction takes place over mercuric chloride catalyst which is supported on activated carbon. Let me tell you how these catalysts are prepared by making the solution of mercury chloride; because mercuric chloride very poisonous you have to handle with great care and so on. And, you dissolve it in water; and then you put so many grams of Activated carbon and then allow it in to the undergo the absorption. And, it absorbs very rapidly; actually, you do not have to wait very long. And, then you filter of the solution and you can determine the unabsorbed mercury chloride in the solution; you can do it in various ways by if you can start with analog grade mercury chloride you can just do chloride analysis.

But better think to do would to be do mercury analysis; there is atomic Absorption techniques that we can use by which you can kill determine how much mercury chloride has been absorbed. And, therefore you can determine; what is the loading of mercury chloride on the activated carbon.

Now, typically this is 10 percent weight by weight this is what is typical? Of course, this is a well studied reaction. And, it also known this catalyst undergoes deactivation and as a result of deactivation the catalyst loses the activity and so on. And, it seems to good example to illustrate how we can determine deactivation kinematics.

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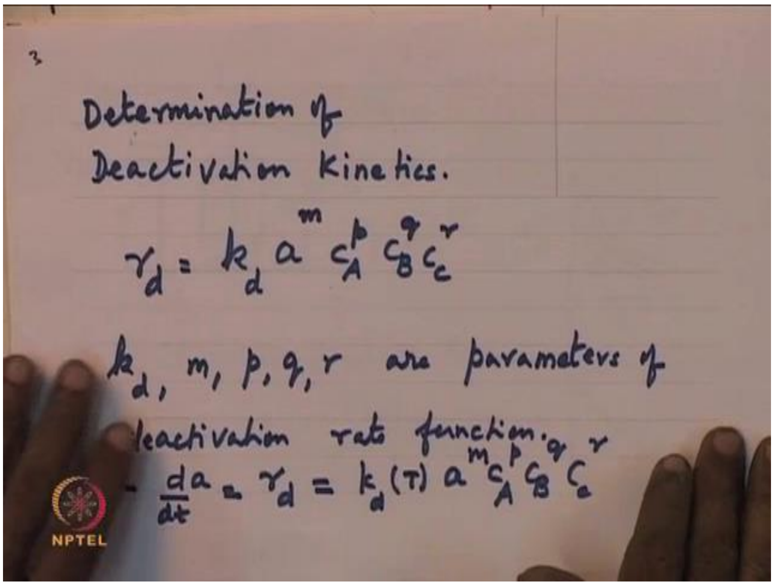

Determination of
Deactivation Kinetics.

$$r_d = k_d a^m C_A^p C_B^q C_c^r$$

k_d, m, p, q, r are parameters of deactivation rate function.

$$-\frac{da}{dt} = r_d = k_d(T) a^m C_A^p C_B^q C_c^r$$

So, what we are trying to do is to determine deactivation kinematics first. And, then use the kind of result to understand how we can design, operate, processes in which there is catalyst deactivation. Now, determination of deactivation kinematic; so, what we are looking for is a rate function which we think will depend upon activity; sum to the power of I just put to power of m it may also depend upon we have 3 comp1nts here. If you recall in our vinyl chloride monument reactions; please recall if there call this as A, I will call this as B, call this as A, call this as C.

So, it depends upon A, B and C it could; we do not know what is the dependence. But you saying is that our intension in this is to determine what is the function that determines catalyst deactivation? So, we expect that the r d the catalyst deactivation function would depend upon activity itself; it could also depend upon the composition of A, B and C which some exp1nts say p, q, r. So, what in another words what we are saying is that k, d, m, p, q, r are parameters of deactivation rate function. And, the object of what are trying to do today is to find the way by which we determine; what are m, p, q, r and k, d.

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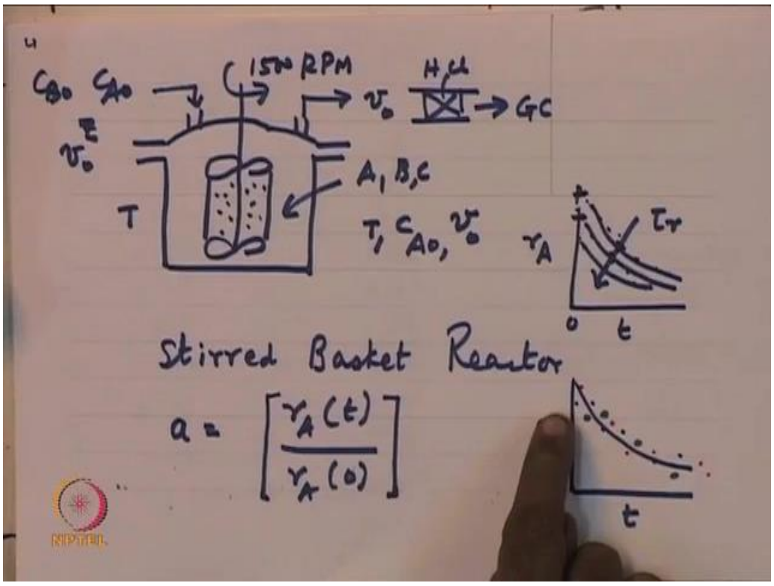

And, more importantly how k, d for example, depends upon temperature; therefore, we are interested in the whole range of things that will help us to understand the deactivation rate function. How is it d1? We do this case by recognizing that we have; let us say stirred tank, it also called stirred basket reactor. Why is it called stirred basket reactor? We have this stirred; then, you a have this impellers and your basket is mounted like this and your catalyst is sitting like this and you are rotating this.

And, of course, this is a tank and then it is called a closure; and there is a value here through which gas is coming and there is a valve here through which gas is going out. And, this is pinning under rapid rate; so that we are able to keep the compositions around the catalyst uniform, we are able to keep the temperature uniform, compositions uniform and so on. So that whatever the data we get the composition in temperatures are well known in the environment of the catalyst.

Now, when we talk about this little earlier; we said our activity a is actually defined as at time T divided by time 0. We recall, we said this we recall this, we just put in the context; we said that when we make a plot, I just brought it here; plot of r A verses time.

And, we can do this for different residence times we have d1 all these; it is not new to you. Therefore, and if you just extrapolate this; so this gives you this is 0 times so you get reaction rate at 0 time and reaction rate at any time. So, at 1 residence time you get this kind of curves; otherwise you get this kind of curves, otherwise you get this kind of curves.

On the other words what we are trying to say is that we can operate this equipment at different; you can do this at different C A 0s, you can do this at different flow rates therefore, different residence times and so on. Therefore, we are able to determine; since, we are able to measure reaction rate at any time divided by reaction. therefore, you able to measure the activity of the catalyst in this way; so you are able to find activity so that say the some temperature T, you can do it at some temperature T; you can do it at different composition at C A naught. So, this and then we may also do at different v naught; so, these are the 3 variables at which we can do these experiments.

On other words if you are looking at this rate function after all our intension is what is this function? So, this function if you want to determine this function r d what is, which you would say that d by d t of A; we, expect that a to decrease with time equal to r d. Therefore, this is equal to k d which is a function of temperature a to the power m C A to the power of p c B to the power q c c to the power r. On, other words now this d by d t of A is given by the right hand side; now, what is the we have determine the right hand side is r d.

So, we have determine this activity a as a function of time; therefore, in a sense we have data to determine what is k, d? What is m, p, q, r? We, have data to determine m, p, q and r. Now, we also said 1 more thing; for example, let us say we make a plot of A verses time can we do this? Answer is yes; because we have determine a which is at r A at any time t divided by r A at 0 time. So, you can find out what is 0 time r A? What is r A at any other time? This divided by this is the activity corresponding to this kind of operation.

We, can get activity for different conditions; for the every condition that we for which for we get data the compositions A, B, C. These compositions have A, B and C could be quite different; let us say our data looks like this for 1 set of 1 residence time. Now, we do it for another residence time; let us say means at this point we got data and again we get another curve. Let we draw it by another color; let us say previous data and this putting the previous data. Now, when we do this data that is mean the different residence time; let us say our greens are here. And, let us say 1 more set of experiments in which we again do the experiments for another residence time; let us say our data looks like this.

What we are try to say here is that if it so happens that a verses time data actually collapses into single curve, collapses into a single curve; irrespective of the choice of residence time. On other words every residence time; the composition of A, B and C would be different in square obvious. Because depending on residence time the extend of reaction would change; and therefore, the composition would change. Therefore, every choice of residence time we get different compositions. And, then we find that the activity has determine by this function r A T at r A at 0; we get, let us say the black dots and then for the another residence time we get this green dots and for the another residence time we get this red dots; all of them seem to be collapsing into 1 curve suggesting that this form of deactivation is concentration independent.

What are we saying is that if you look at this deactivation rate function; what you find is that when we change composition A, B, C by appropriate choice of the residence time composition of A, B, C change. But in spite of that we find that our activity time relationship collapses onto a single curve; showing that the concentration dependence is not there in this data. We talking about this particular data we do not know; no, different data may be different accordingly this function could be different this exp1nts could be different.

What is being said here is that if you find this concentration dependence is not there; it means that p, q and r of this rate function are 0; that is all it means. And, in a particular case; if you find this dependence is there and we will be able to determine what the value is from your data.

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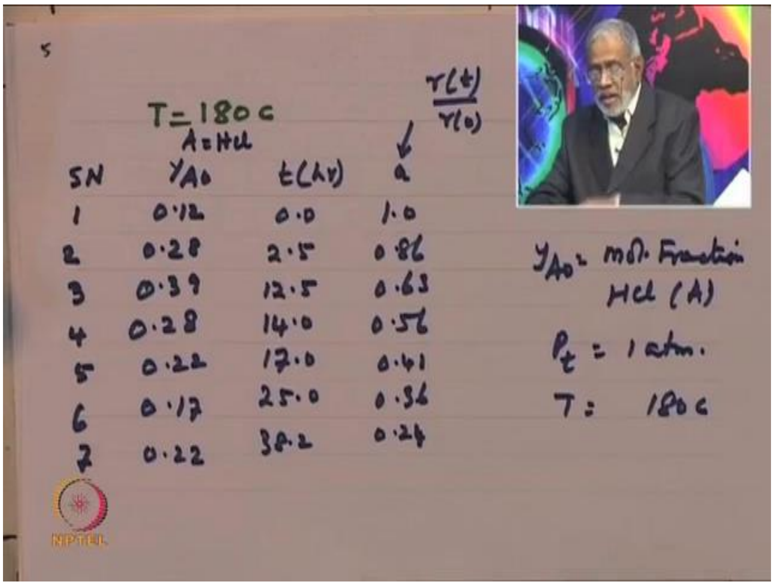

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$T = 180\,C$

$A = HCl$

SN	y_{A0}	$t\,(hr)$	a ↙ $\frac{r(t)}{r(0)}$
1	0.12	0.0	1.0
2	0.28	2.5	0.86
3	0.39	12.5	0.63
4	0.28	14.0	0.56
5	0.22	17.0	0.41
6	0.17	25.0	0.36
7	0.22	38.2	0.24

y_{A0} = mol. Fraction HCl (A)

P_t = 1 atm.

T : 180 C

So, in this particular case the example have taken is that p, q and r are seem to be 0; let us say all right having said this. Let us just take the data that we have I got some data here this is bare with the data write down the data. This is temperature is 180 C And data is serial number 1 serial number it is 1,2,3,4,5,6,7; I have got 7 sets of data Y A 0 this is a comes at 0.12, 0.28, 0.39, 0.28, 0.22, 0.17 and 0.22 data is available like this. And, time in hours; we are taking about 0.0 times in hours 2.5, 12.5, 14.0, 17.0, 25.0, 38.2. Activity is defined as r t at r 0; and I am just putting as 1.0, 0.86, 0.63, 0.56, 0.41, 0.36, 0.24 this is a data at 180 c.

Now, what is Y A O is mole fraction H C l in this case comp1nt (A). And, then pressure is 1 h, temperature in this data is 180 c; what have we d1? Now, let us recall how this experiment was d1 is quite interesting to know how these experiments are d1. Now, how do you do this experiment? You set the temperature as 180; how do you set this temperature as 180? You will have this particular reactor nicely covered; it is let say heating tapes or jackets. In this particular case it is heating tape and well insulated; so that the heating loses are small. Therefore, by adjusting the heating rate you can get the temperature that you desire all right.

So, and then composition how do you get; let us say Y A 0 as 0.10, 0.12; whatever you have a rot meter let us say which is all calibrated. So, adjust the flow of rot meter of hydrochloride gas as well as settling gas. And, adjust it appropriately as per a calibration;

so that you get the mole fraction of hydrogen chloride gas is 0.1 whatever. So, this composition of you have both A and B. Similarly, C B 0 in this case C A 0 is H c l, C B 0 is settling. And, the gas goes in undergoes reaction and this kept spinning; typically, at about 1500 R P M.

Let us say the mixing is satisfactory; and then product gas is come out and what happen to this the product gas? Generally, goes through what is called as a absorber of H c l, absorber before you have to remove the H c l. Before it can go for chromatography goes to a G C gas chromatograph; where the compositions are continuously monitored is that understand is this clear what we are saying. So, the gas goes into the H c l absorber to remove the H c l. And, generally absorber H c l absorber is the sodium hydrochloride in a lab; typically, it will be sodium hydroxide whatever or potassium hydroxide.

And, then the H c l free gas goes to gas chromatographer analysis; 1s again the gas chromatograph are calibrated. There are elaborate procedures for calibration with the internal standards and so on. So, you know as you put a gas to the chromatograph we get a response and you can compare the response with the standard; so that you can get your compositions. So, what we are trying to say here is that you can do a measurement of the activity at a given temperature; you can do this activity measurement by and to determine whether this concentration dependence is there or not by doing this experiments is varies composition that is what we have d1.

And, the data that is in front of you; this data in front of you tells you that H c l, A is H c l. So, data tells you that we have change the composition 0.12 to vary composition in that range to find out what happens to the activity is that clear. So, we find out the activity to be this.

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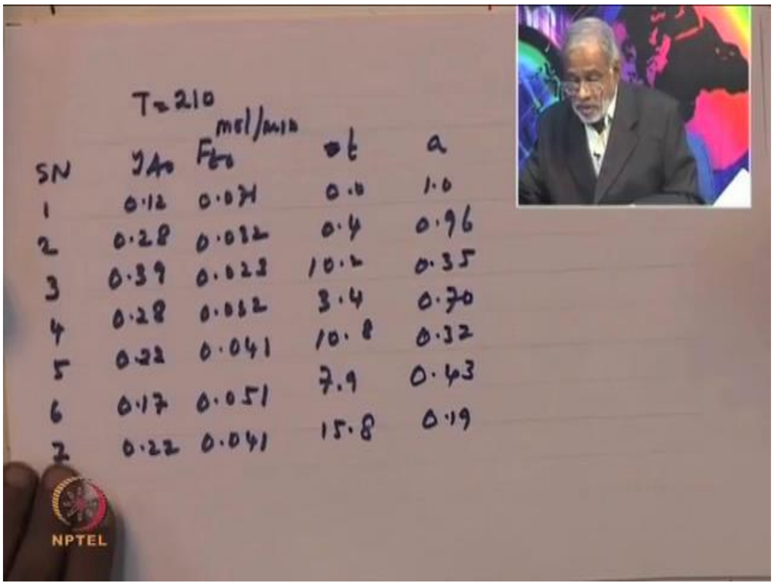

T = 210

SN	y_{A0}	F_{t0} mol/min	t	a
1	0.12	0.071	0.0	1.0
2	0.28	0.032	0.4	0.96
3	0.39	0.023	10.2	0.35
4	0.28	0.032	3.4	0.70
5	0.22	0.041	10.8	0.32
6	0.17	0.051	7.9	0.43
7	0.22	0.041	15.8	0.19

Now, you can do this same kind of experiments at other temperature; say let us say T equal to 210. So, I just write down the data here serial number 1, 2, 3, 4, 5, 6, and 7; then, you have y A 0 is 0.12, 0.28, please bare with me; because this is important that is why I am just writing it down. So, do not be impatient; we will shortly this just few minutes I will be with you y A 0. And, then you have how much of you know; the total molar flow F t o is moles per minute that also given that let we write that down 0.071, 0.032, 0.023, 0.032, 0.041, 0.051, 0.041 is it all right.

Then, you have temperatures activity you have time sorry; time is 0.0, 0.4, 10.2, 3.4, 10.8, 7.9, 15.8. And, then activity is 1.0, 0.96, 0.35, 0.70, 0.32, 0.43, 0.19.

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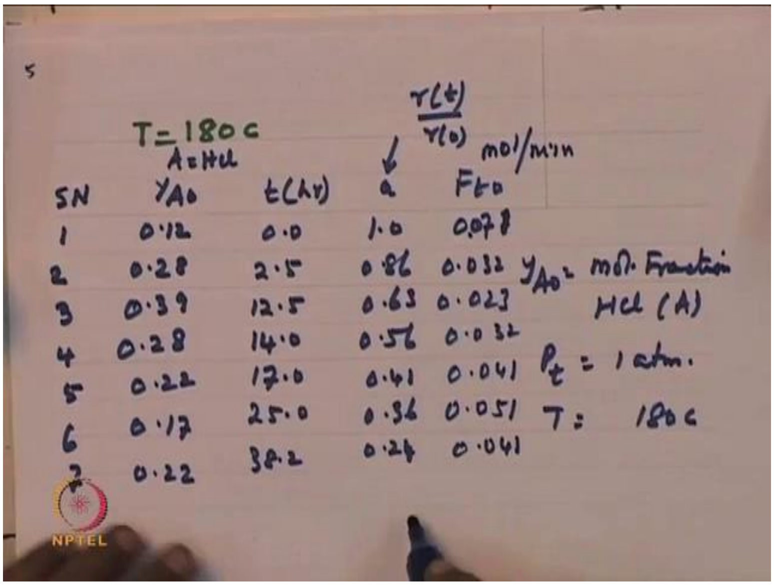

T = 180 C

A = HCl

$\frac{r(t)}{r(0)}$ mol/min

SN	y_{A0}	t(hr)	a	F_{t0}
1	0.12	0.0	1.0	0.078
2	0.28	2.5	0.86	0.032
3	0.39	12.5	0.63	0.023
4	0.28	14.0	0.56	0.032
5	0.22	17.0	0.41	0.041
6	0.17	25.0	0.36	0.051
7	0.22	38.2	0.24	0.041

y_{A0} = mol. Fraction HCl (A)

P_t = 1 atm.

T: 180 C

Now, please bear with me; in the previous data I have not menti1d this F t 0 I forgot to write down. So, let we just write down 0.078, 0.032, 0.023, 0.032, 0.041, 0.051, 0.041; so, I have got this mole per minute. So, I have data and then I have calculated the activity using the relationship r of (t) divided by r of (0). So, this is how can calculate all right.

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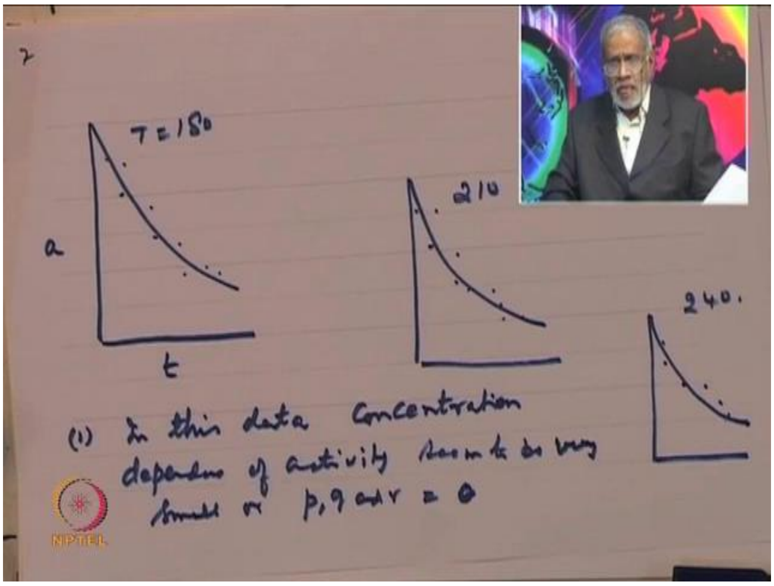

(1) In this data concentration dependence of activity seems to be very small or p, q and r = 0

Now, we have data; now, at 180 we have data, now at 210 we have got 2 set of data. In this particular case; fortunately, we have little bit more data and the context of having telling; this is that see you need to be able to determine the activation energy you need minimum data at 3 temperatures. So, this is the instance where we have no choice about to do experiment minimally at 3 temperatures. So, we have serial number y A 0, F t 0 activity time. And, activity so 1, 2, 3, 4, 5, 6, 7; 0.12, 0.28, 0.39, 0.28, 0.22, 0.17, 0.22, 0.071, 0.032, 0.023, 0.032, 0.041, 0.051, 0.041. Now, 0, 0.9, 1.9, 5.8, 2.8, 1.5, 0.6; activity is 1.0, 0.84, 0.62, 0.30 0.44, 0.70, 0.86.

Now, what is this we got? We have got from our experiments data at 3 temperatures. So, we have data at 3 temperatures 1 2; let us say 3 this is T is 180, 210 and 240. Now, when make a plot of a verses t u get a plot like this, plot like this, plot like this; and interestingly the concentration dependence is not to be seen. On the other words even though we have d1 this measurement different flow rate and different composition as you can recognize from the data given; that is the activity verses time data at the 3 temperature does not seems to reveal any serious concentration dependence. So, the first thing we can conclude is that in this data concentration dependence of activity seem to be very very small or p, q and r equal to 0; it seems like that it seems that p, q, r are 0 is it clear.

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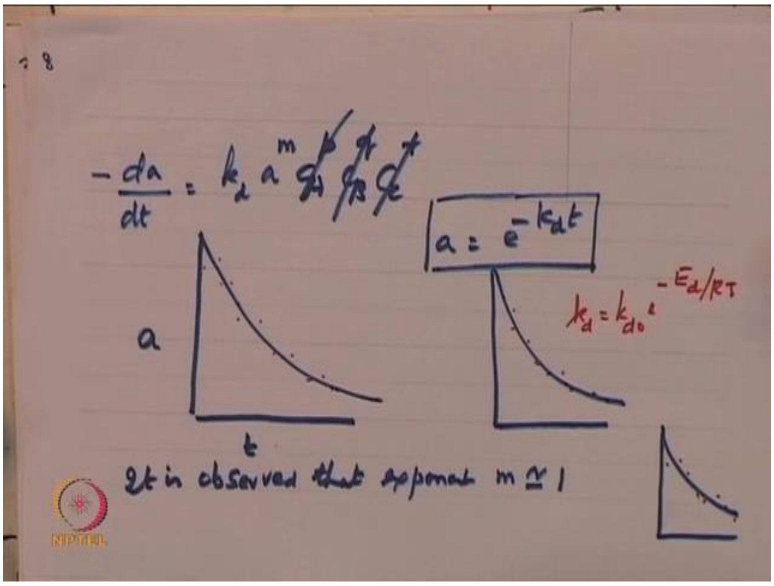

$$-\frac{da}{dt} = k_d a^m \cancel{C_A^p} \cancel{C_B^q} \cancel{C_C^r}$$

$$\boxed{a = e^{-k_d t}}$$

$$k_d = k_{d0} e^{-E_d/RT}$$

It is observed that approx m ≃ 1

Now, if moment we recognize the p, q, r are 0; therefore, all we have to do is to solve. Now, the only thing that we have is to do that of d A times d t equal to k d times a to the power of m; and then C A to the power of p c B to the power of q c c to the power of r. All the dependence are not there; therefore, we have to only solve this equation. Now, if you look carefully at the data a verses time; then, you notice that this dependence is exp1ntial it is observed that the exp1nt m is nearly are showing that a equal to e power minus of k d times t.

So, what we are saying is that from the data that is given it appear that activity d k is exp1ntially. How did you come to this great conclusion? We first plotter the activity verses time; and we found that it was not showing not much of temperature concentration dependence. So, then we decided that let us take data and then determine what is the value of m which is exp1nt of activity. So, we simply assumed to be 1 and then therefore, we plotted a verses time. And, then we find a verses time when you plot a verses time; we find that our data something looks like this at each temperature; you understand what I am saying? What I am saying is that the data seems to suggest that the exp1ntial decay is valid and this rate constant k d for different temperatures can be absorbed from the data given. So, you can determine k d is equal to what? k d 0 e rise to power of minus E d by R T energy for deactivation.

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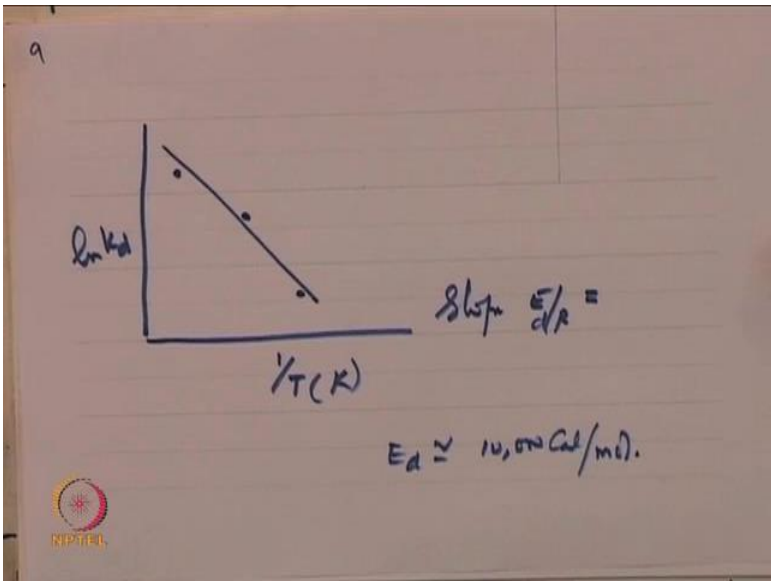

So, if you have data for k d at 3 temperature; then, you can plot them and find out what is the activation energy for deactivation. So, let us see how it looks like; so we can make a plot 1 by t verses l n of k d. So, what is the plot expect to see? What shall we except to see k d should be? So, this should be a line at 3 temperature is that correct; so this slope s gives E by R is that clear what we are saying. So, in this we plot the data k d verses y t, t is in Kelvin. So, then we get a stated reasonably good straight line and slopes we can call this as E d turns out to be approximately 10,000calories per mole what is absorb from experiment this is clear.

Now, you can compare this E d 10,000 calories per mole with varies other kind of data is simple data which people would like to compare is the heat of vaporization of mercuric chloride. Now, the fact remains is that the heat vaporization of mercuric chloride is much much higher than 10,000. And, therefore we should not be unduly whether the fact that out activation energy is so different from the thermodynamic property. Please recognize that activation energy is a kinetic property; therefore, it is only give kinetic information it does not give you any information.

Therefore, do not try to compare the activation energy data with heats of vaporization. The heats of vaporization of mercuric chloride etc are thermodynamic property. And, here even though the deactivation may be very strongly related to the evapourisation of mercury. But the activation energy for that process may be quite different from the activation energy that you see in what is called as vaporization and condensation. Vaporization and condensation involves heats of condensation which is around 17, 18, 19, 20,000 and so on. So, this is very different from heats of vaporization; so this is pointed wanted to get a question.

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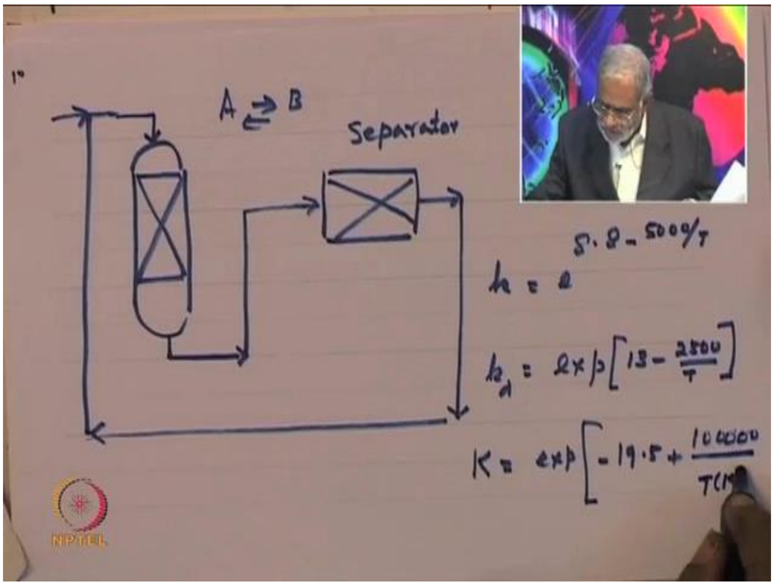

Having said this let us look at more challenging problem in front of us is the following you have a reactor all right; it is got an catalyst all right. Now, it goes to a separator this is separator; so it goes to separator from there it comes out. Now, frequently what is an interest to us is that we do not want to waste the product; so, it is recycled, it is recycled is that clear. Now, what is being said is the following you just write down; you have some data k the reaction A goes to B, B goes to A and so on.

So, k value equal to exp1ntial of 8.8 minus 5000 by t ok; k rate constant k, k d equal to exp1ntial 13 minus 2500 by T. Equilibrium constant K equal to exp1ntial minus 19.5 plus 10,000 divided by T is function of k.

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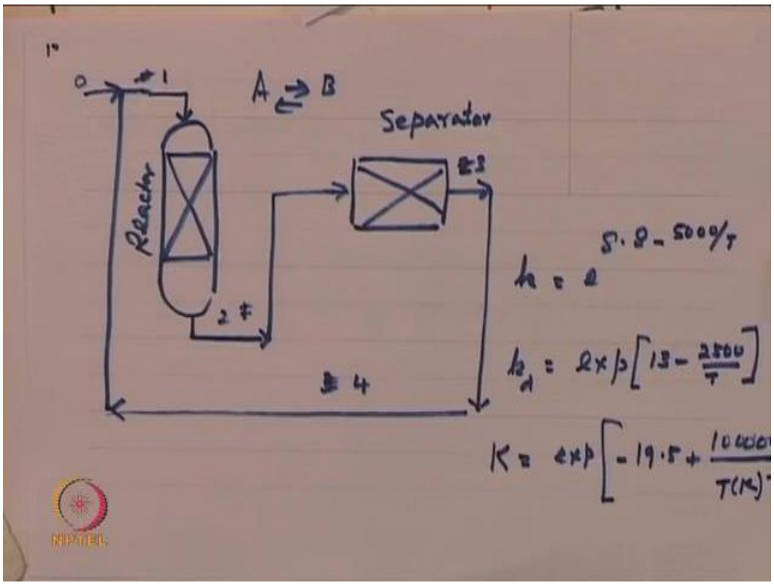

So, the question in front of us is the following first 1 question is obtain design equation for the process is that clear. What is meant by design equation for the process? It should relate conversion to the residence times to temperature to vary feature; that is in our hand when we do a design. So, first what we want is that obtain the design equation for the process having d1 that this is the first question. Second question is since catalyst deactivates; what is the reactor temperature of operation this is clear. We have 2 question first question is process design? And, then since catalyst deactivates what is the reactor temperature of operation? After, let us say after put some time after 30 days; some numbers.

So, because you should know how you should run the plant with time; so, this is the idea how do you do this? This is a reactor; so, I will call this is 0 1, 2, and 3 sorry this is 0. This is 1, this is 2, this is 3, this is 4; I am sorry. Now what we are trying to say is that what is the process design means that we should be able to relate conversion to some variable which is in our hands. Let us first do that and then address various questions that might arise first let us do that. We want to relate conversion to various operating variables; let us do that first and then all the rest will become quite easy.

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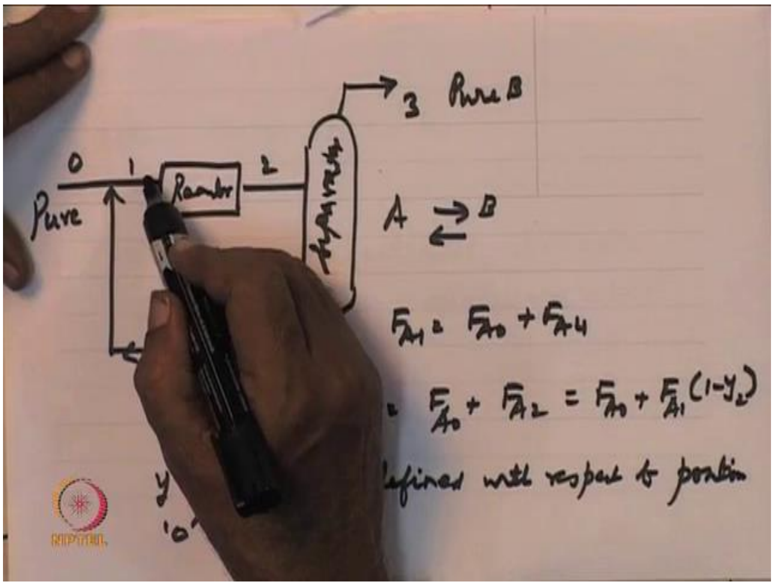

To do this I draw this once again we have a reactor, we have a separator; so, it is 0, 1, 2, 3, 4, A goes to B. And, A this is the reaction and this is pure B; therefore, see this is pure A do you understand this why this is pure A? Because here it is pure A and due to reaction you will find a mixture here. But record all the pure B; therefore, only pure A comes here. Therefore, the concentration here must be C A o this is quite obvious all right. F A 1 is F A 0 plus F A 4, F A 1 equal to F A 0, F A 4 is same as F A 2 that is equal to F A 0 plus F A 1 times 1 plus minus of y 2; y is conversion defined with respect to position 0.

Please; let us understand this fully what I we saying we have this process and it is a time a dependent operation that also we have explained. And, in this the time dependent operation what we have to find is that appropriate this is the reactor. So, we have to find a way by which we will operator the reactor correct this is a separator. So, the whole time dependent activity here is that how do we change the temperature of the reactor? So, that we can get what we want; this is the point that we are trying to get a cross. So, before we start with this problem what we said is that we will do some elementary stoichiometry and setup all the relationship; so, that we can deal with them as we go along.

So, F A 1 is F A 0 plus F A 1 minus of y 2; where say y 2 it is meant it is conversion at position 2. But in this case conversion position 2 assuming that position 1 is the reference; that conversion at position 1 is 0 that is the example this is only a reference. So, I do not think to should worry too much to brought this all right we have d1 that.

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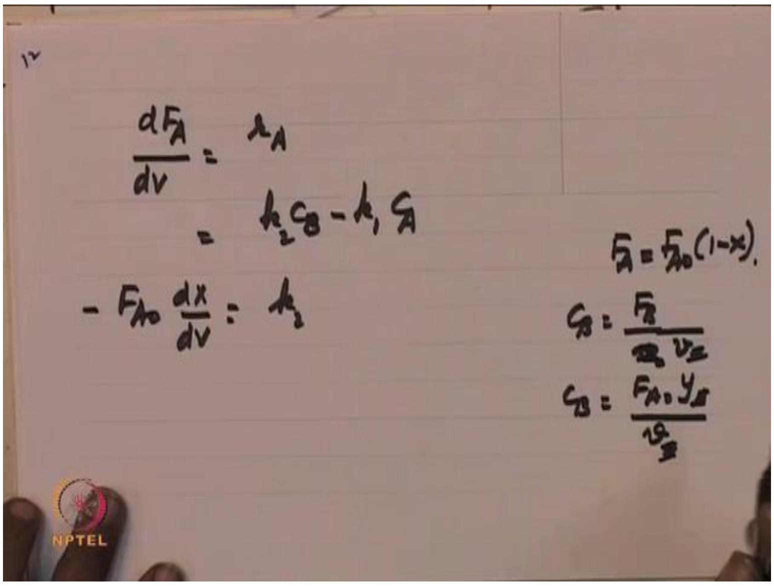

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$$\frac{dF_A}{dV} = r_A$$

$$= k_2 C_B - k_1 C_A$$

$$-F_{A0}\frac{dx}{dV} = k_2$$

$$F_A = F_{A0}(1-x)$$

$$C_B = \frac{F_B}{v_E}$$

$$C_B = \frac{F_{A0}\, y_E}{v_E}$$

Now, what we have now we have to be able to write the design equation after all we want to write the design equation for the reactor. Let us write the design equation for the reactor what is it? This is a plug flow reactor; so, what is d F A by d v equal to r A what is r A by definition? Rate of formation of correct this is rate of formation of a and rate of consumption of A. So, the left hand side becomes F A 0 d x by d v F A 0; notice that A equal to F A 0 times 1 minus of x this we know.

Now, this is because in this negative sign here, I will put negative sign here; then k 2 what is C B? C B equal to F B divided by v. So, C B equal to F B is what F A 0 times y 2 correct exit F B Z the exit. What is V? That is important what is V? V equal to that I have d1 here. Let me just see that is V; let we write have equal to V at the outlet V at the inlet. This is V at the naught, V 0 is naught V 0. This is C B exit; means it should be V 2 is it all right.

See concentration in a reactor; what comes out the volumetric flow is V 2; and therefore, this is C B at any position therefore, V at any position. So if you want C B at any position; it is F A 0 y by C B. Similarly, C A at any position is equal to have d1 all this thing; let we just write 0 down instead of doing it again and again let we write it down.

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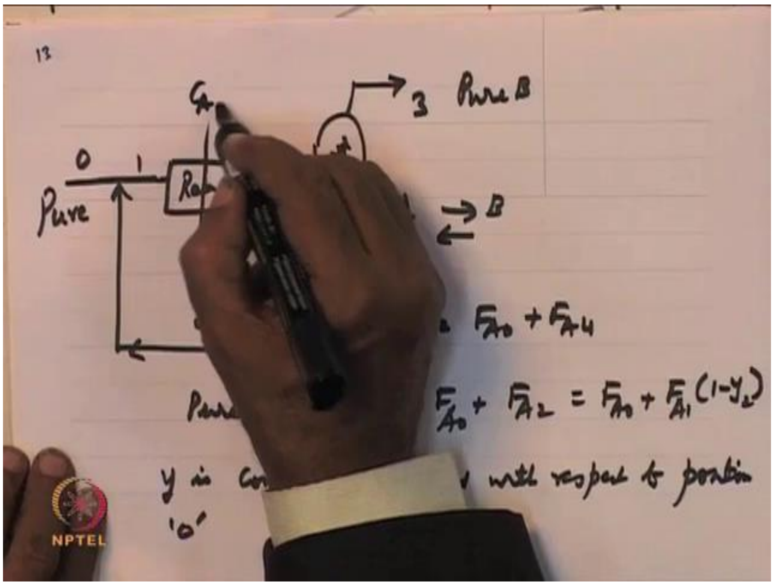

You will first calculate what is F A 1 equal to F A 0 plus F A 4; please recall this figure F A 0 plus F A 4 equal to F A 1, F A 4 equal to F A 2. And, F A 2 is F A 1 multiplied by 1 minus y 2. So, we will write that is equal to F A naught plus F A 2 that is equal to F A naught plus F A 1 multiplied by 1 minus y 2. So, this becomes F A naught divided by y 2 F A 1 is that clear. Now, what is C A? C A 4 we said C A 4 is same as C A naught; because B is fully recovered. Therefore, here you get pure A only; therefore, C A naught C A 4 is equal to C A naught.

Now, we said V 4 what is V 4? Please, notice here V 4 volumetric flow at this point V 4 by definition is what? V 4 is equal to F A 4 divided by C A 4; that is F A 2 divided by C A 4 equal to this is F A 1 into 1 minus y 2 divided by C A 4 is C A0. What is F A 1? F A 1 is F A 0 into 1 minus y 2 by y 2. Now, what is V 1? V 1 is equal to V 0 plus V 4.

Notice here V 1 equal to V 0 plus V 4 and we will be say this in a volume balance are not correct. But if the densities are the same for all the streams this is ok; that is why the volume balance we used.

Now, this is equal to V 0 plus just a moment F A 0 I forgot C A 0 here. So, it is V 0 into 1 minus of y 2 divided by y 2; that is equal to V 0 by y 2 is that clear. So, we will got V 1 which is V 0 of y 2. Therefore, we are now in a position see after all why we have d1 all these things; we want to say write the design equation for this reactor. To be able to write the design equation for any reactor; we should see know the concentrations at various positions. Now, if you want to write the concentrations at any positions; and then you should able to understand how to define conversation.

So, have we define conversions with respect position 1; therefore, we need what is concentration at any point? What is C A here? Which is C B here? This we should be able to tell once you are able to tell that in a we are in a position to write the design equation for the equipment so what is let us write everything quickly; now, without losing too much time.

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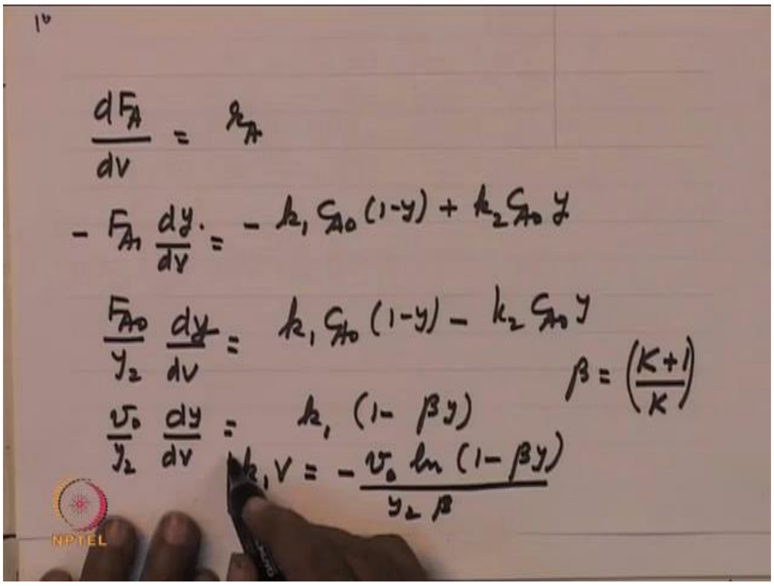

$$\frac{dF_A}{dV} = r_A$$

$$-F_{A0}\frac{dy}{dV} = -k_1 C_{A0}(1-y) + k_2 C_{A0} y$$

$$\frac{F_{A0}}{y_2}\frac{dy}{dV} = k_1 C_{A0}(1-y) - k_2 C_{A0} y$$

$$\beta = \left(\frac{K+1}{K}\right)$$

$$\frac{v_0}{y_2}\frac{dy}{dV} = k_1(1-\beta y)$$

$$k_1 V = -\frac{v_0 \ln(1-\beta y)}{y_2 \beta}$$

So, we have C A equal to F A divided by V. By definition at any position in this reacting equipment we notice that V 1 equal to V 2 there is no volume change. And, v 1 is equal to V 0 by 2; therefore, v 2 is also equal to V 0 by 2 any positioned flow V 0 by 2 correct that we already d1. So, this therefore, F A at any position is equal to F A 1 into 1 minus of y divided by V by V 0 correct. V at any position is V 0 by y 2 all right. That is equal to F A 0 by y 2 divided by V 0 by y 2 multiplied by 1 minus of y; that is equal to C A 0 into 1 minus of y. similarly, C B equal to C A 0 times y.

So, what we have got we have got the concentration at any point. Therefore, now we have write the design equation and find the process design equation for the reactor that what once we know that everything; let us quickly do that. So, we have the please recognize we write the process design equation for the reactor; keeping in mind the fact that the concentration A and B are given by fairly simple relationship ok. So, we have d F, d F A by d v equal to r A; so, F this is written as minus of F A 1 d y d v equal to r A which is minus of k 1 C A 0 1 minus of y plus k 2 C A 0 y is that clear.

Now, F A 1 is we know F A 1 is F A 0 by y 2 d y d v. So, minus sign goes off; therefore, it becomes k 1 C A 0 1 minus of y minus of k 2 C A 0 y or we can write this as d y d v, V 0 by y 2 equal to. We can simplify this and write this as k 1 times 1 minus of beta y; where beta y equal to k plus 1 by k. I will not show the detail; but it is very obvious take some common and comes nicely like this.

So, we can integrate this and then the integrated form I just write down the integrated form; so that we can go back look out the problem of interest; because we are going away from and then doing same. So, the integrated form of this equation I will write it here itself why going to k 1 V equal to minus of V naught l n 1 minus of beta y divided by y 2 times beta. So, this is the integrated form I will just box this; so that you know we know what we have done. Now, the rest is fairly straight forward and we cannot text also we have not forgotten and so on.

So, what we have got here is that we have a deactivating catalyst. And, therefore we have got the design equation for this reactor and then it is separator and so on. Now, the question that is in front of us is the following it says this catalyst deactivates; which means what? This particular k 1 which contains the activity. So, frequently it is better actually that is why we can put an alpha here which is the activity; so that this is an alpha. So, basically what we got here is this term is k 1 times alpha; where, k 1 is rate constant alpha is the activity. Now, what did we say that this activity decays? And, this activity decays function; we have determined that is what we said that in the example that we illustrated we found out from our experiments how activity decays with time.

And, then we said that what is that said that dependence on concentration in that example we said the concentration dependence not there.

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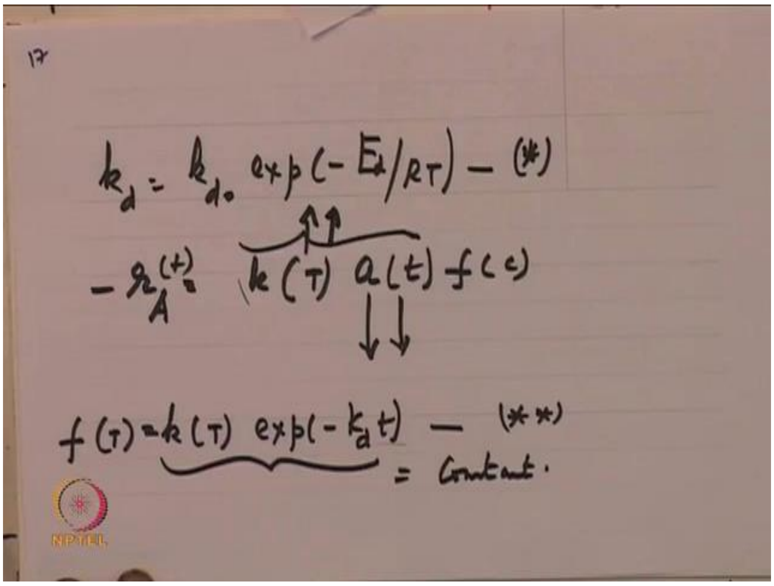

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$$k_d = k_{d0} \exp(-E_d/RT) \quad - (*)$$

$$-r_A^{(t)} = \overbrace{k(T)\, a(t)}^{\uparrow\uparrow}\, f(c)$$

$$\downarrow\downarrow$$

$$f(T) = \underbrace{k(T) \exp(-k_d t)}_{} \quad - (**)$$

$$= \text{Constant}.$$

Therefore, we determined the deactivation rate constant k d as a function of temperature. So, what we got let we just put it in the context; what we got was the following, we got from our experiments k d equal to some k d 0 exponential of minus of E d by R T this we got from our experiments. So, essentially what we have got all the data we have got from our experiments what is being our tuff is that how do you run this process? On other words we want this product to be produced at a steady rate; which means that as this catalyst deactivates even then this the amount of product B does not change with time.

How do you manage this? We said yesterday that if you look at this rate function r A is typically which is a reaction velocity. And, that is activity function that is function of time. And, of course, our rate function will have a composition what we point out yesterday is that we want to see that this term which is function of time this should not change. As this activity keeps on going down and how do you manage this? We manage this by ensuring that this product does not change with time. How do you ensure this?

We ensure this by looking k T what is k T? k T is which some exponential of minus of k d times T; where, k d is given by this equation.

Let us say star on other words; if I say this star, star and star. So, I have to keep this function; let us say the function of temperature this should be constant as temperature change. This should be equal to constant value how to you do this? We do this by changing the temperature at which will see the process. That means we will change the temperature at which we run the process; so that this product is always a constant. And, if you do that this function remain a constant. And, therefore the composition at position 2 does not change. And, this is how we take care of running process that involves catalyst deactivation.

Recognized the incorporating the rate function into this r A which recognize k d times at can be kept constant. How do you keep constant by changing the temperature of the process? Actually, increasing the temperature; this temperature is increase because this is decreasing. As, this goes on we keep on increasing this; so that this product is kept constant. And, that way we can ensure that this process runs; so that the amount of this product that is produced at position 2 does not change with time even though this is a time dependent operation; the reactor is time dependent. But we adjust the temperature; so that the time dependent is not seen at position 2. Therefore, this is not seen in our separator; therefore, our process runs as though it does not recognize the effect of deactivation activity.

Thank you