Chemical Reaction Engineering 1 (Homogeneous Reactors)

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Lecture No 24

Gas Phase Homogenous reactions

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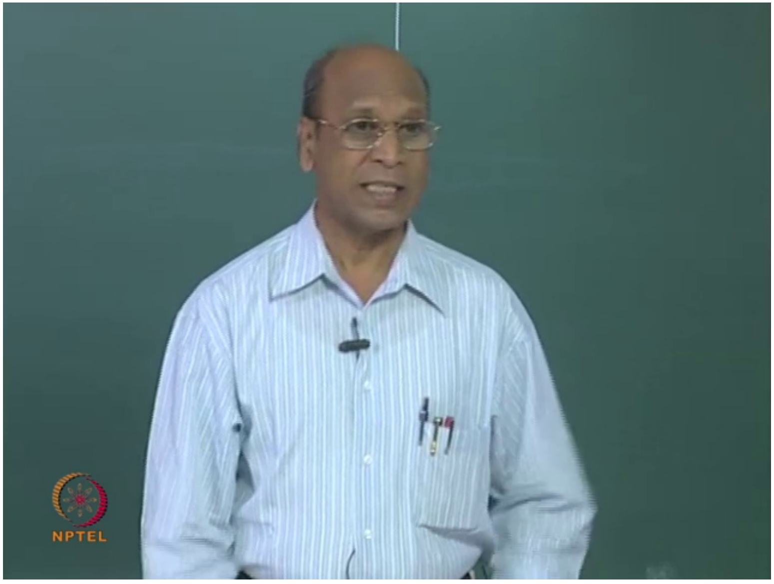

So I think this is very important for you, you know to solve all those problems, Ok. I told you now; I have to give one derivation that is very nice derivation. That is for, till now we have talked about only liquid phase reactions.

If you have gas phase reactions, what do you do? Because you were taking sample of a gas phase reaction, whatever reactor you may use, you may use batch reactor even for gas phase but taking sample is very difficult. Normally how do they analyze gases?

(Professor – student conversation starts)
Student: Gas chromatography
Professor: Yeah.

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That is what, where did you use this?

Student: Heard.

Professor: Yeah, gas chromatography is one

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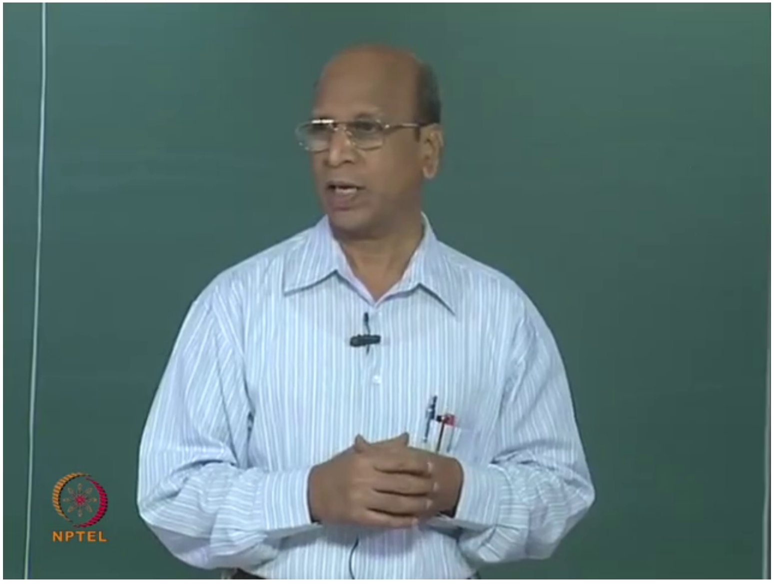

but gas chromatographs are very, very costly normally. So then you also cannot take the sample. Of course you can take sample and then again inject but nowadays if you want online gas chromatographs I think they are 50 lakhs, 40 lakhs,

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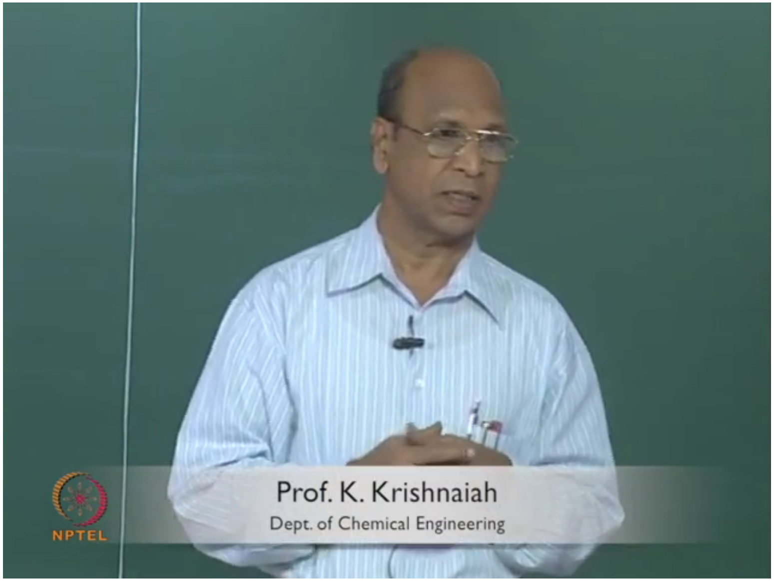

so like that you have the cost.

(Professor – student conversation ends)

So as engineer I told you no, without anything how do you measure. That is the greatness of an engineer if he is able to really measure it. Without anything how do you measure? So that is what your ultimate motto, right.

So when you have gas phase, how do you really find out the kinetics and how do you first of all take the samples or analyze the concentration or measure the concentration? So gas phase reactions, gas phase, Ok homogeneous again, Ok so how do you get the rate for gas phase homogeneous reactions. The question

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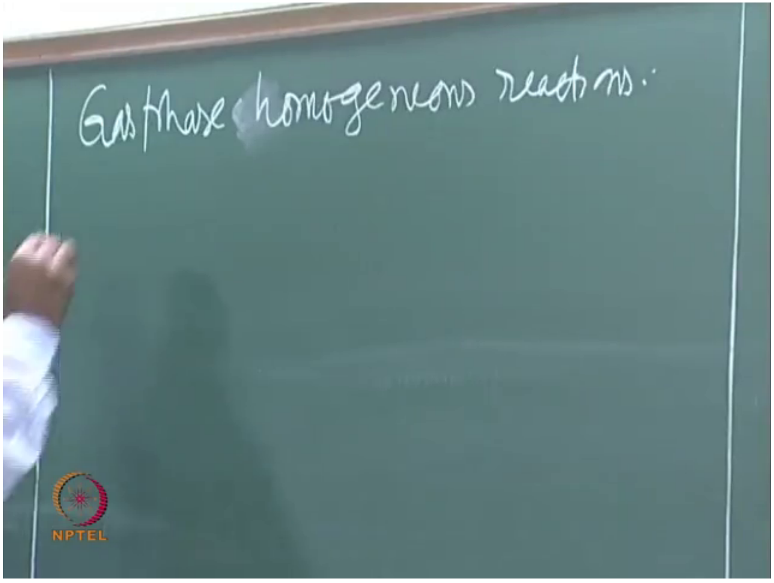

is minus r A, how do you get, right?

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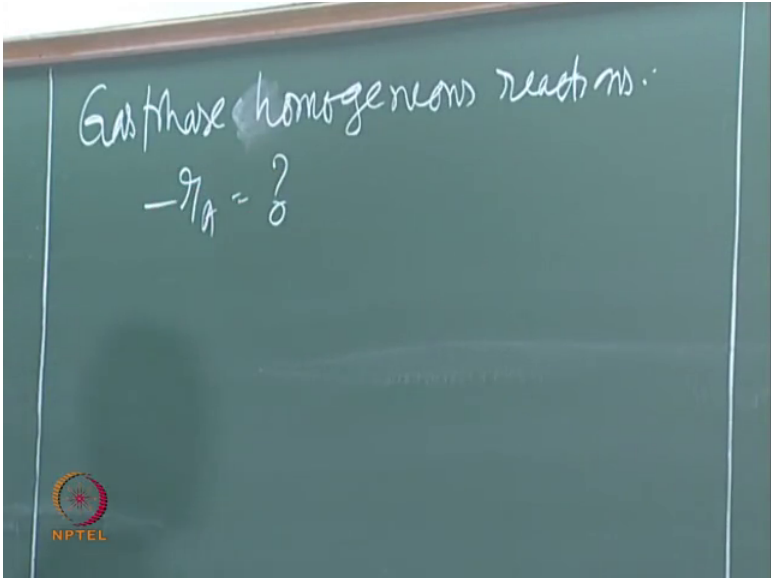

So that is why those who are familiar with Levenspiel book, I think Levenspiel is one of the greatest engineers I can appreciate any time. Because his concepts are simple, his explanations are extraordinary and his clarity is fantastic. Ok so that is the reason why many, many complicated things he makes it very, very simple. That is why the complicated chemical engineers won't like him.

Because some people deliberately want to, you know make things complicated, right, for example starting with a tensor and a vector. Ok, dead! I think the moment we say tensor and vector, 90 percent of our brains closed. Ok, then when you put the del then the remaining 10 percent also closed.

(Professor – student conversation starts)
Student: (laugh)
Professor: I mean you see that experience. Ok.
(Professor – student conversation ends)

So now mathematics is a beautiful language provided you are thorough with the concepts. That is a beautiful language. I mean, representing in the form of that del is a wonderful form, simplest form. Any complicated equation can be written in 1 or 2 words that is all. I think when you expand only you know what are the complications there.

But that has to come when you are really thorough with the phenomena that is going on. That means the moment we say del x, you should know what is del x and then how it is representing, what kind of physical phenomena that is representing in a process. Then it is fantastic. Ok. So that is why, as engineers if you write only mathematics, I think nothing will happen, right?

That, those things are also required because you know, again do not use your sub routine thinking that Krishnaiah does not know mathematics that is why he is telling that. Ok, and always our subroutines work very fast in the brain. Ok. So I am not telling that. You know, as engineers how do you make things very, very simple? For example gas phase reactions, how do you measure the gas concentration?

(Professor – student conversation starts)
Student: Partial pressure
Professor: Ok, yeah how do you measure partial pressure? See always questions. Always questions. You see it is very simple to say no, partial pressure. How do you measure partial pressure? Have you thought anytime about that?
(Professor – student conversation ends)

Ok, how do you measure total pressure? So I have taken a batch reactor where, Ok I may put a stirrer also, still I mean gases will move easily, still I will put a stirrer. Then close this entire thing. This gas fellow is highly movable. So that is why it will easily try to escape. So that is why you have to have perfect seals and all that and then put inside that closed vessel; that we call as reactor.

And then you start stirring. If you want to maintain temperature and all that, again you should have a jacket and all that, Ok, this is coolant in, coolant out. Ok, C in,

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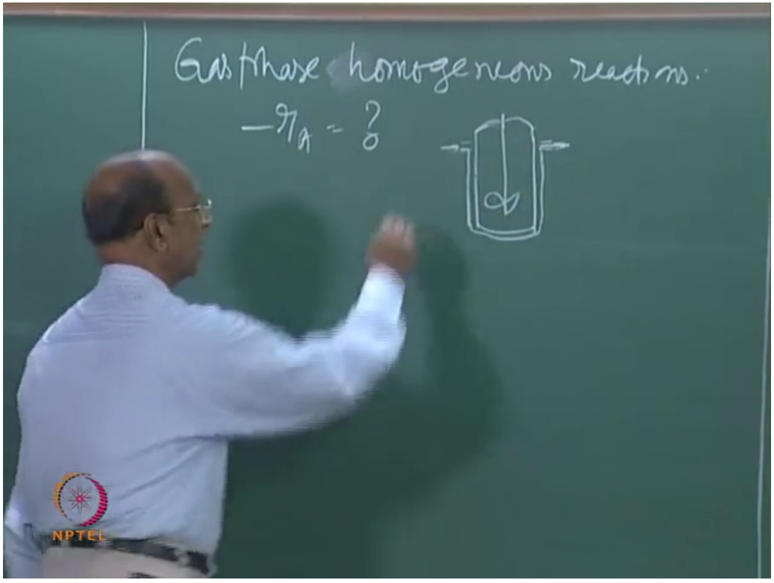

C out, coolant means that is, Ok. C means not concentration. So how do you measure here the pressure first of all? How do you measure temperature?

(Professor – student conversation starts)
Student: Thermocouple
Professor: That is very easy. Thermocouple or thermometer, Ok. Yeah, thermometers cannot be 2 meters, 3 meters long. So that is why we put the thermocouples very easily.
(Professor – student conversation ends)

So I should have a temperature sensor here, so may be somewhere here. This will give me temperature and here I should have a hole and then that inside pressure should reflect there. There is a

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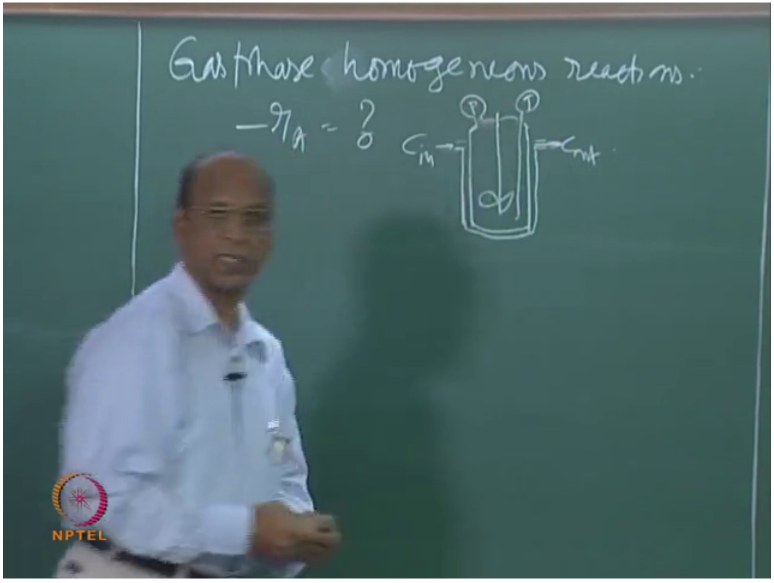

pressure gauge. That is why I do not know whether you have read course on instrumentation where pressure gauges and all that are taught, Ok. So those things are very important, those things are required, right.

So this is the pressure what we can get. Now if you get total pressure, how do you get the partial pressure?

(Professor – student conversation starts)
Student: Mole fraction
Professor: How do you get mole fractions?
Student: Total number of moles...0:05:47.5
Professor: yes?
Student: From the conversion 0:05:48.4

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Professor: Conversion, yeah, right. I mean if you know the conversions then you know each and every, composition of each and every reactant and also products,

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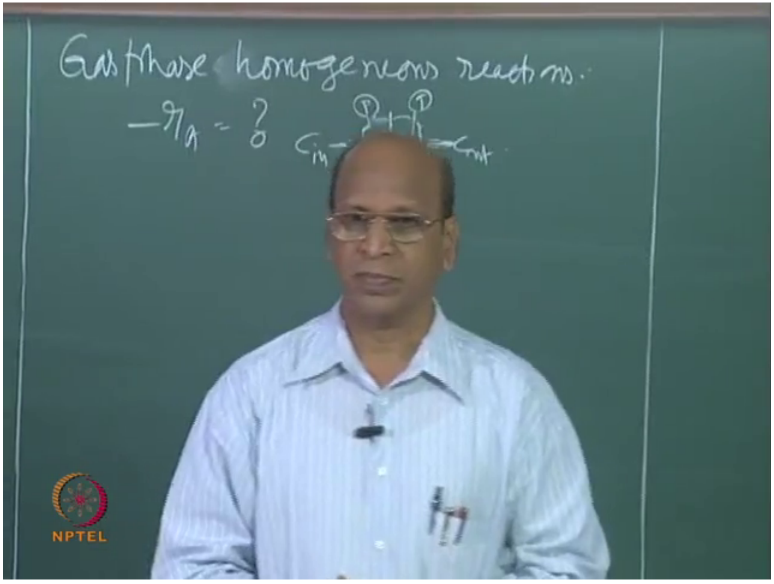

because again mole balance, simply mole fraction and mole balance, right, total number of moles and also, that particular component, what are the number of moles that divided by total number will give you mole fraction, Ok, so like that.

(Professor – student conversation ends)

So that is the reason why the gas phase reactions, the moment we started thinking about how do you measure gas phase reactions, it is not that easy, right? So that is why Levenspiel has beautifully used these two concepts. If I have variable volume or constant volume, so that means variable volume if I have, what will change? Variable volume, the answer itself in the question, what will change?

(Professor – student conversation starts)
Student: Volume
Professor: Volume changes. So now if I have a reactor where the volume is expanding or contracting, then if I am able to measure that, total volume change, so then I have to find out how the individual molecules, you know contributing for this total volume change, you can convert that into concentrations or partial pressures. How do you get concentration from partial pressure?
Student: C A by R T
Professor: C A by R T, Ok, that also we know.
(Professor – student conversation ends)

So that is why either this or that if you have, you can convert one from the other particularly for gas phase but liquid phase there is no meaning of converting one from the other, Ok. There is no meaning in that. If you want, you can do it but there is no meaning. Ok, so variable volume is one method.

The other method is constant volume. This is constant volume batch reactor, V constant.

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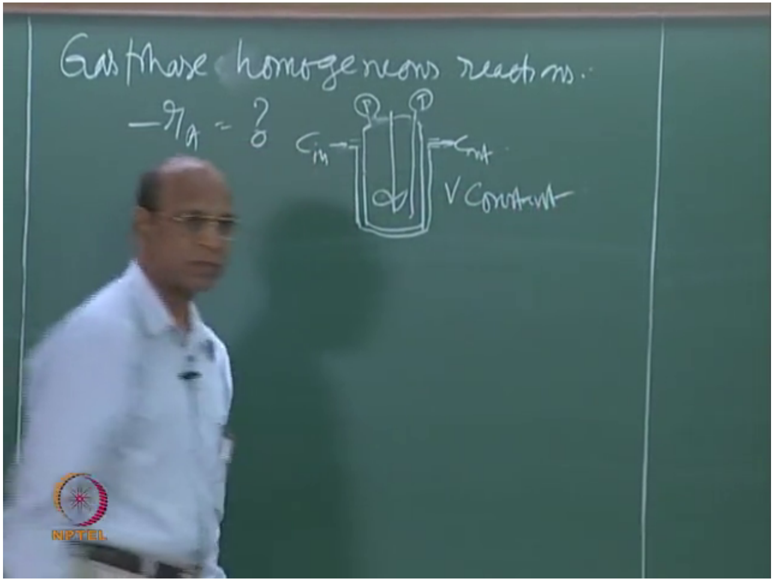

Ok, so now if I have a reaction here, right so then let me say, simply A going to R,

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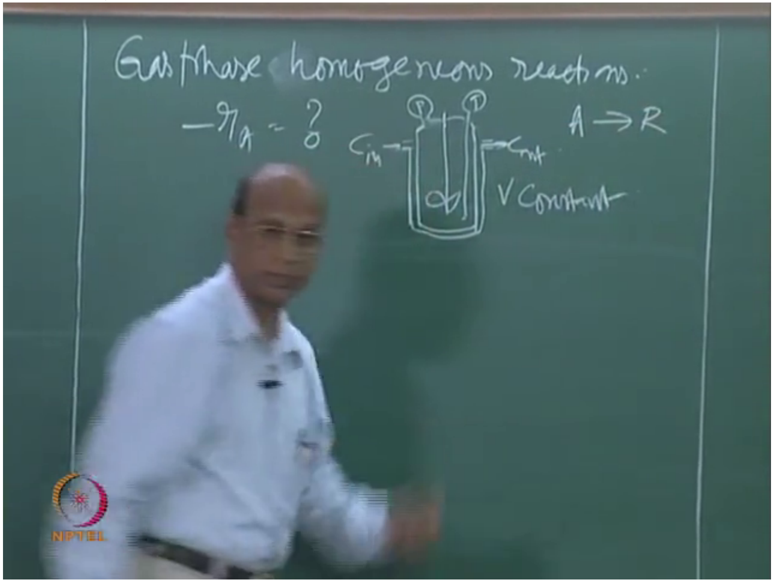

Ok, so now if I want to use constant volume means pressure should increase, right?

Volume is constant. P V equal to R T. I am keeping only one temperature, temperature is constant. R anyway we know it is a constant. Constant only no, R? Ok. So then if all that constants then only pressure should change.

But unfortunately when I have A going to R there is no pressure change, then how do you find again concentration? This is why gas phase reactions are very, very difficult. What we do in this case when we have one mole going to one mole or when there is no volume change, Ok then you have to use, as she suggested as gas chromatography. Ok.

You have to take samples or you have to analyze continuously, if you are very rich person you can buy very costly online gas chromatograph and then allow the samples to go continuously and then again return. So somewhere here you put a small pore and put the gas chromatograph and again return back, Ok.

So it draws some sample

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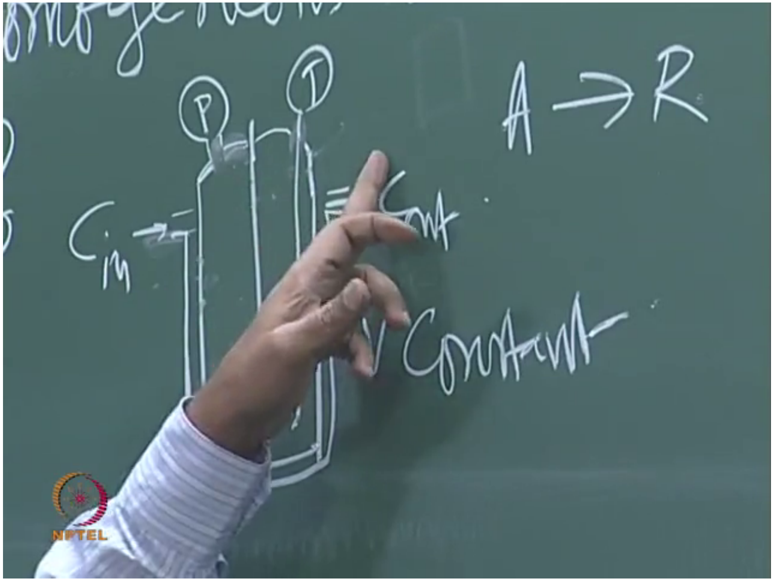

and now everything is computer controlled. So 1 second, 2 seconds, 3 seconds, 4 seconds you can program on the computer and it sucks at 1 second, 1 sample, quickly analyzes and afterwards because you know, you cannot throw out all the time. If you throw it out all the time, nothing will be there inside, inside the reactor after some time. So that is why again you have to send it back.

But now you see the response time and analysis time all these things should be very, very fast, right. Otherwise you cannot have another reactor somewhere here. That is you know

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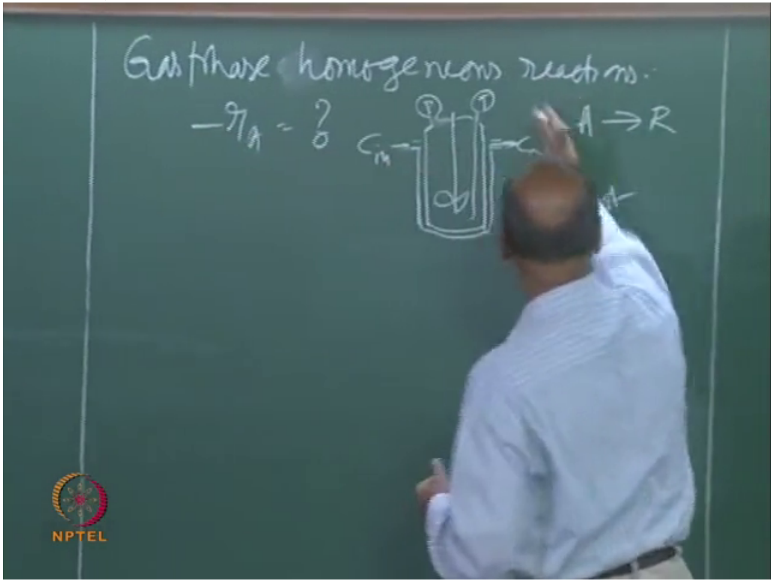

gas chromatograph. So this is what is the thinking you have to do before starting the experiment. Ok, now I have gas phase reaction. How do I analyze the samples? What kind of reactor I use?

What temperature and pressures you use and all that from thermodynamics you know you will get it. Whether reaction is reversible, irreversible and all that, Ok, good. So under these conditions

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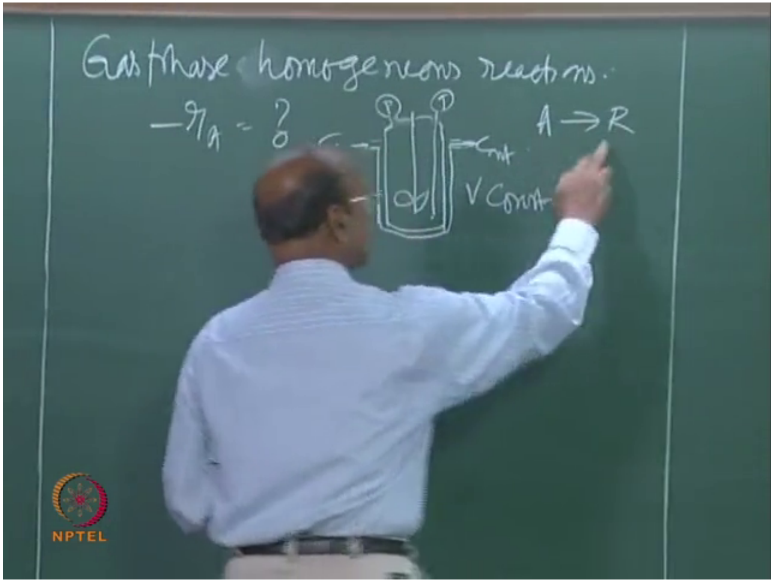

we do not have a choice. We have to use sophisticated instrumentation, right.

Otherwise for simple cases, if I have volume change how do we solve that problem? That is what what we discuss now. How do we solve the problem when I have actual changes in the moles during the reaction? We will take a very general reaction where I have a A gas plus b B gas giving me, it can be reversible also but anyway let me take first r R gas plus s S gas,

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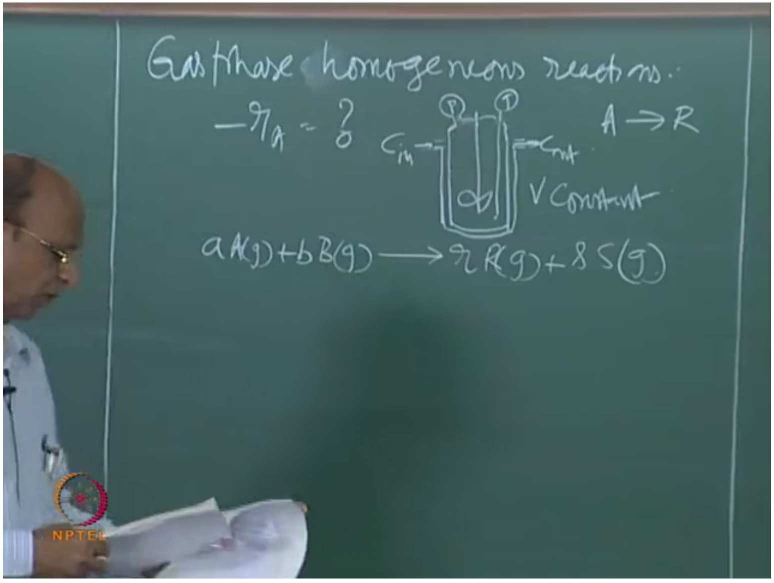

Ok. It is a gas phase reaction.

So I think I know, definitely this A plus B and you know R plus S must be different. Otherwise both are same means again no there is no volume change, Ok good. So initially at time t equal to zero, I will have here N A naught, N B naught, N R naught, N S naught, Ok, those are the initial number of moles which you fed into the system.

So after time

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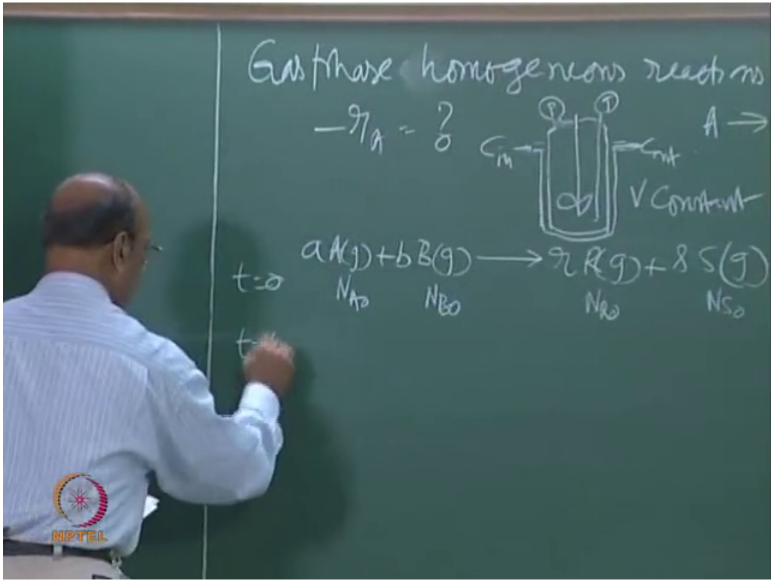

t equal to t, I have here, some reaction has already taken place and from your process calculations you know that, that number of moles that are there at a particular time t is N A naught minus yeah, I, I use another word, A into xi, where xi is extent of reaction, please write that,

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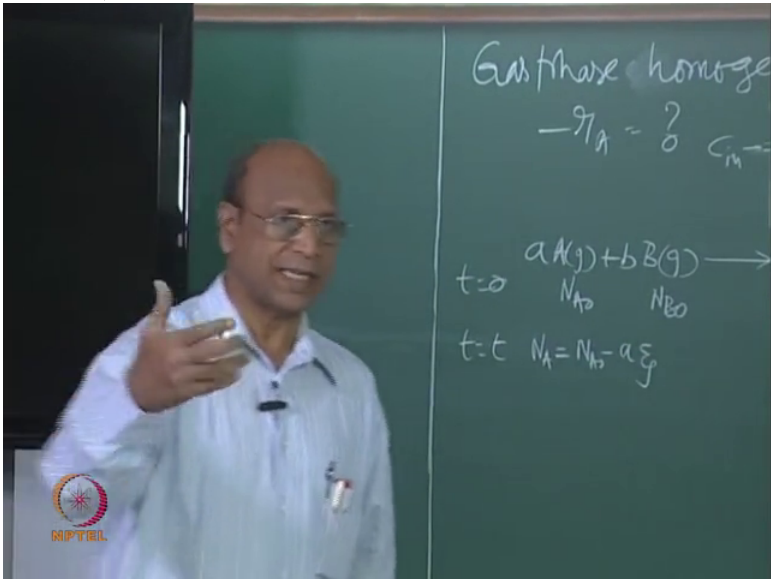

where xi is extent of, it is not conversion. It is not conversion, Ok, yeah I think I will just comeback to that.

So N B also equal to N B naught minus B xi and N R naught, sorry, N R equal to N R naught plus, this is plus because it is product, so xi and N S equal to N S naught plus S into xi. Ok, why we are using xi is xi is more, a better parameter because that is universal parameter. If x is, if I am using x, I have to use only for A, one of the components. But xi is a general one. What are units of xi? Does xi has units?

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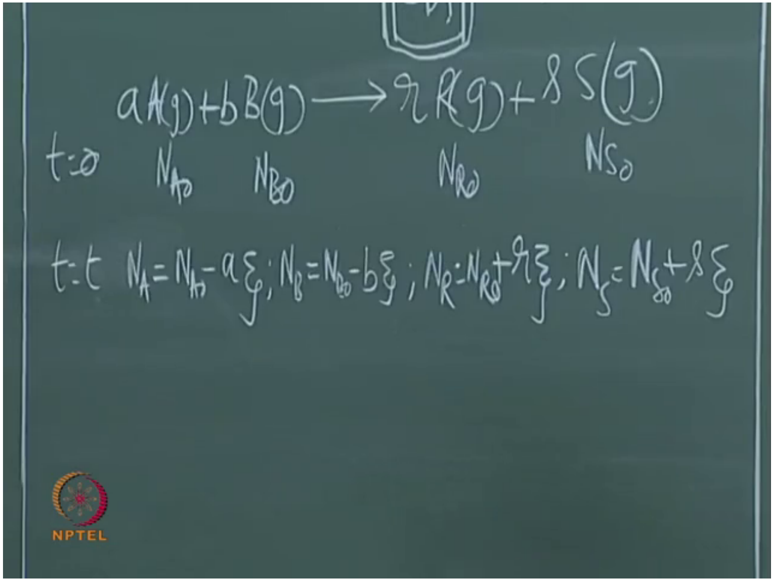

$$aA(g)+bB(g)\longrightarrow rR(g)+sS(g)$$

$t=0$ $\quad N_{A0} \quad N_{B0} \quad N_{R0} \quad N_{S0}$

$t=t$ $\quad N_A=N_{A0}-a\xi_j;\ N_B=N_{B0}-b\xi_j;\ N_R=N_{R0}+r\xi_j;\ N_S=N_{S0}+s\xi_j$

(Professor – student conversation starts)

Student: Dimensionless

Professor: xi?

Student: It is moles per...

Professor: You can take this

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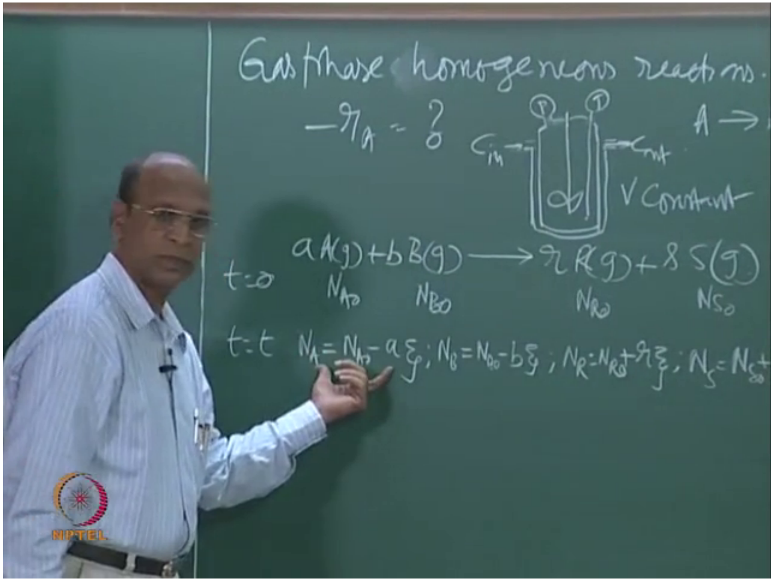

Gas phase homogeneous reactions.

$-r_A = ?$

$$aA(g)+bB(g)\longrightarrow rR(g)+sS(g)$$

$t=0$ $\quad N_{A0} \quad N_{B0} \quad N_{R0} \quad N_{S0}$

$t=t$ $\quad N_A=N_{A0}-a\xi_j;\ N_B=N_{B0}-b\xi_j;\ N_R=N_{R0}+r\xi_j;\ N_S=N_{S0}+$

Student: Moles per

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Professor: You take this,

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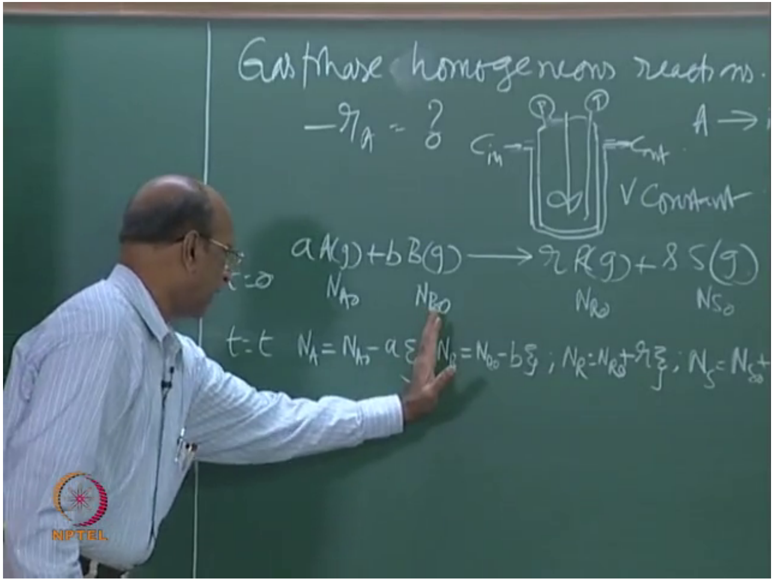

yeah, so anything we say, xi or x you cannot say it is unit-less,

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you know, not dimensionless. Because you have to see. Now you can define xi in fact. xi equal to N A naught

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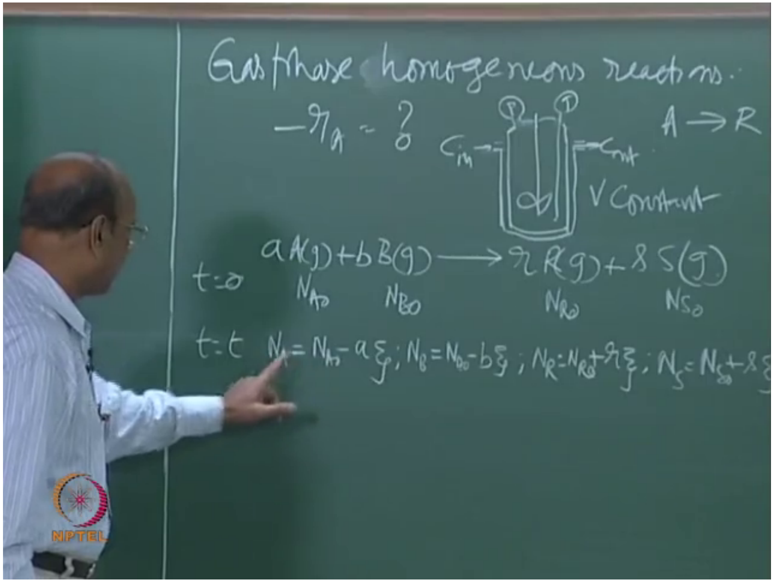

Gas phase homogeneous reactions:

$-r_A = ?$

$A \rightarrow R$

V Constant

$t=0 \quad aA(g) + bB(g) \longrightarrow rR(g) + sS(g)$

$N_{A0} \quad N_{B0} \quad N_{R0} \quad N_{S0}$

$t=t \quad N_A = N_{A0} - a\xi; \; N_B = N_{B0} - b\xi; \; N_R = N_{R0} + r\xi; \; N_S = N_{S0} + s\xi$

minus N A by A, and also N B naught minus N b by B and like that, you know here also. (Professor – student conversation ends)

Right, that is N A minus N R naught by R, Ok N A minus N R naught. So all these things are there for xi. xi definition you know, already. This is what is the parameter used by that Aris I told you know, Aris book, that is the parameter what he uses. There are some advantages with that. There are nice advantages with that.

So this is the xi where it is extent of reaction, equal to extent of reaction. Yeah, so

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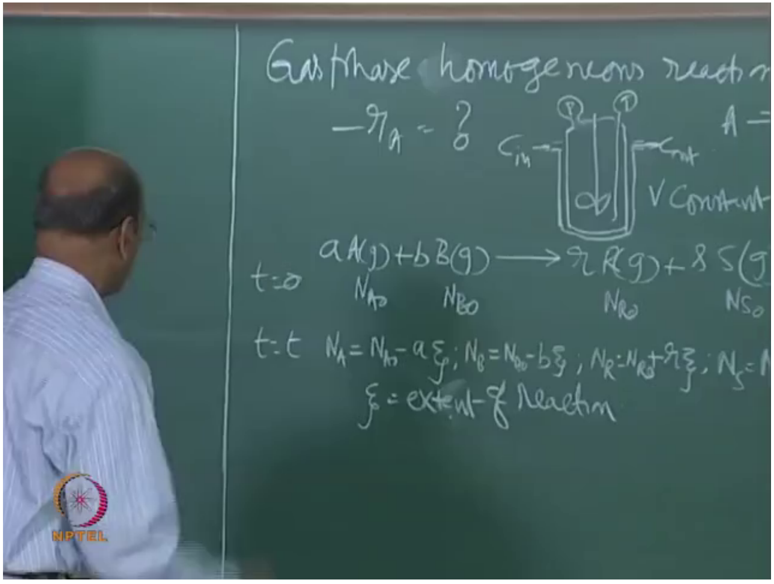

I would like to have the total number N t naught, N t naught is total number of moles at time t equal to zero. So all that will be N A naught plus N B naught, N R naught plus N S naught, Ok.

So equations if I start giving, yeah I think I can start from here only, 1, yeah so

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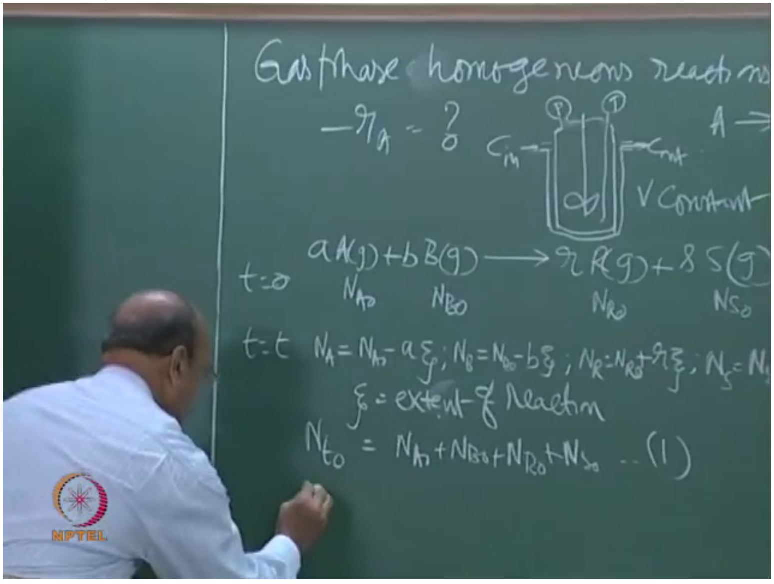

N t, N t is N A plus N B, N R plus N S. So that I can also write, Ok so this one, I have already these things, right? I have already all these things there. So it is N A naught, let me write patiently all this, plus N B naught minus B xi plus N R naught plus R into xi plus N S naught plus S into xi, this is equation number 2.

So now can I write

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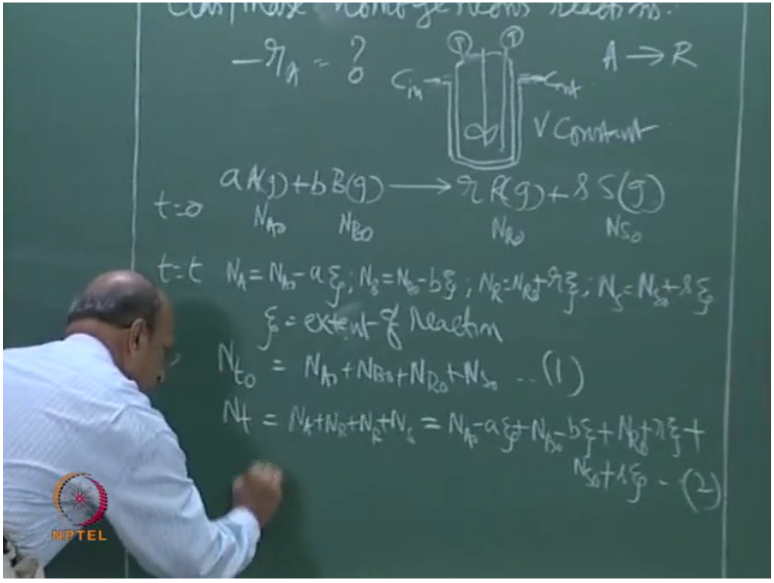

$-r_A = ?$ C_{in} C_{out} $A \rightarrow R$

V Constant

$aA(g) + bB(g) \longrightarrow rR(g) + sS(g)$

t=0 N_{A0} N_{B0} N_{R0} N_{S0}

t=t $N_A = N_{A0} - a\xi$; $N_B = N_{B0} - b\xi$; $N_R = N_{R0} + r\xi$; $N_S = N_{S0} + s\xi$

ξ = extent of reaction

$N_{t0} = N_{A0} + N_{B0} + N_{R0} + N_{S0}$ ..(1)

$N_t = N_A + N_B + N_R + N_S = N_{A0} - a\xi + N_{B0} - b\xi + N_{R0} + r\xi + N_{S0} + s\xi$ - (2)

this N t equal to N t naught plus delta N xi,

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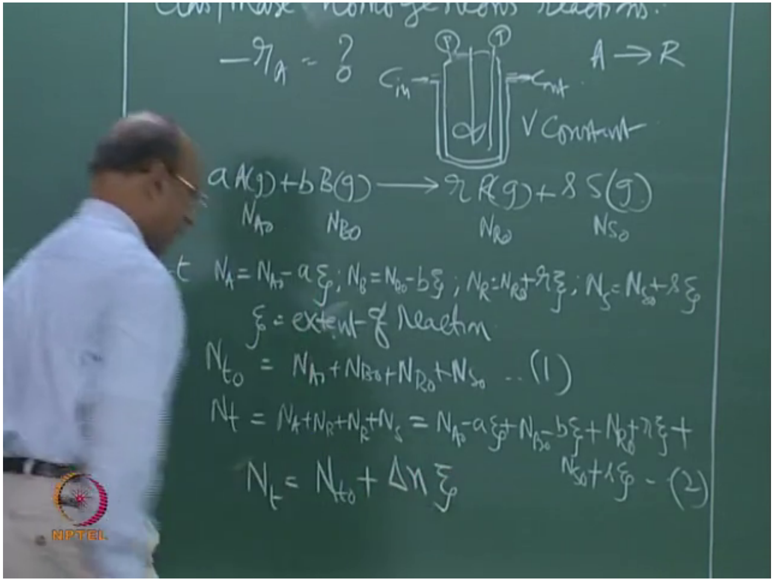

$-r_A = ?$ C_{in} C_{out} $A \rightarrow R$

V Constant

$aA(g) + bB(g) \longrightarrow rR(g) + sS(g)$

N_{A0} N_{B0} N_{R0} N_{S0}

t $N_A = N_{A0} - a\xi$; $N_B = N_{B0} - b\xi$; $N_R = N_{R0} + r\xi$; $N_S = N_{S0} + s\xi$

ξ = extent of reaction

$N_{t0} = N_{A0} + N_{B0} + N_{R0} + N_{S0}$ ..(1)

$N_t = N_A + N_B + N_R + N_S = N_{A0} - a\xi + N_{B0} - b\xi + N_{R0} + r\xi + N_{S0} + s\xi$ - (2)

$N_t = N_{t0} + \Delta n\,\xi$

this is equation 3, where delta n equal to, excellent, minus a minus b. So that is the stoichiometric coefficients, you know, coefficients,

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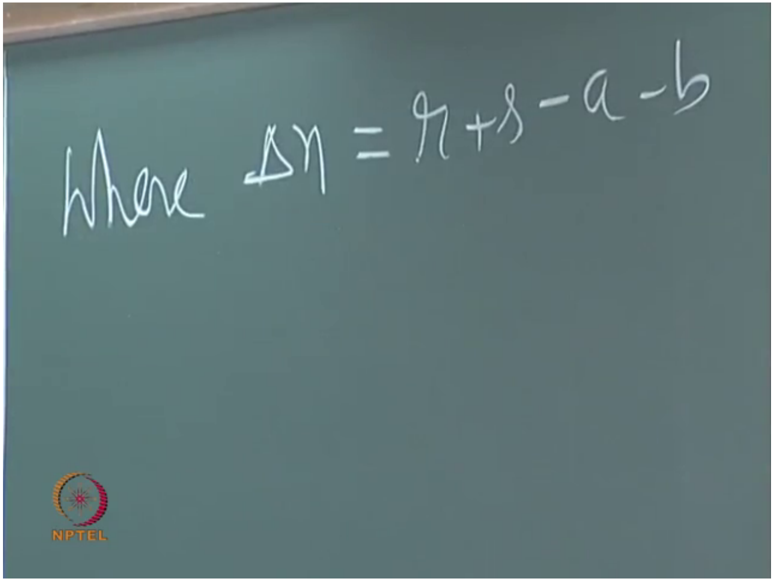

the difference of stoichiometric coefficients between products and reactants, ok. That is the one, delta n.

So now N t by N t naught, Ok that is total, moles at any time divided by total moles at t equal to zero is now 1 plus, I am just dividing this by N t naught, so I have delta N by N t naught into, N t naught into xi, Ok. So this is equation number, this is 4, this is 5.

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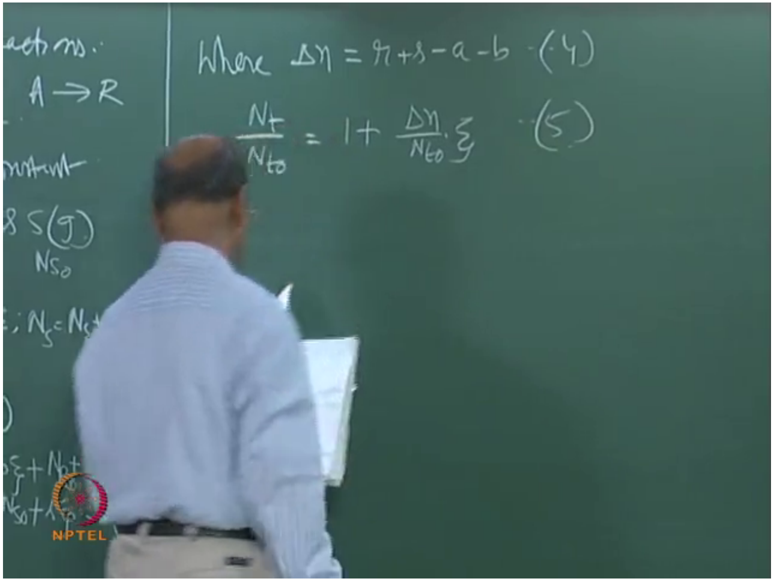

xi definition you know.

(Professor – student conversation starts)

Student: Sir, what is 0:15:40.8

Professor: Why?

Student: 0:15:47.3 how it has been converted to

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Professor: I know, number of moles how much is converted, that is best parameter for me. Number of moles is much more important for me than the concentration.

Student: Using the same convention, 0:16:06.4

Professor: Yeah, does not matter, actually that is what I require.

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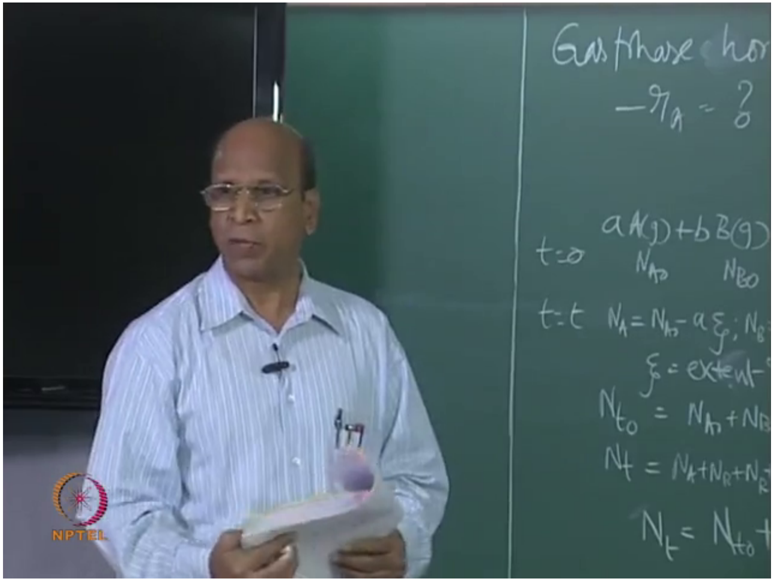

Because if I am able to use that, that is very good for me. Because I do not differentiate whether I have N A or N B or N S or N R, because everything is same.

(Professor – student conversation ends)

That is what, always university or any academic institution wants this unification. Always industry wants differentiation. Really. That is why periodic table has come because that is unification of all the properties in one place. Why should you remember 103, how many are there, 103, 104, 105? 118?

(Professor – student conversation starts)
Student: 189
Professor: 180?
Student: 9
Professor: 109? That is what you are telling?
Student: 0:16:48.0 118
Professor: 118?
Student: 108
Professor: So many new ones were not there
Student: Sir, 109
Professor: Yeah, I think, I remembered till 104. After I do not have (laugh), I do not want to remember. So why should I remember these 104 or 105 or 106 or 107 independently all the properties? Ok.
(Professor – student conversation ends)

So instead of that I put in the periodic table, you know that means you know the horizontal rows and vertical rows because now I can unify all these elements in this row will have or in this column will have some properties or in this row will have some properties. Beautiful unification, who did it?

(Professor – student conversation starts)
Student: Mendel

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Professor: All of you? Jyoti? Mendeleev. Where is he

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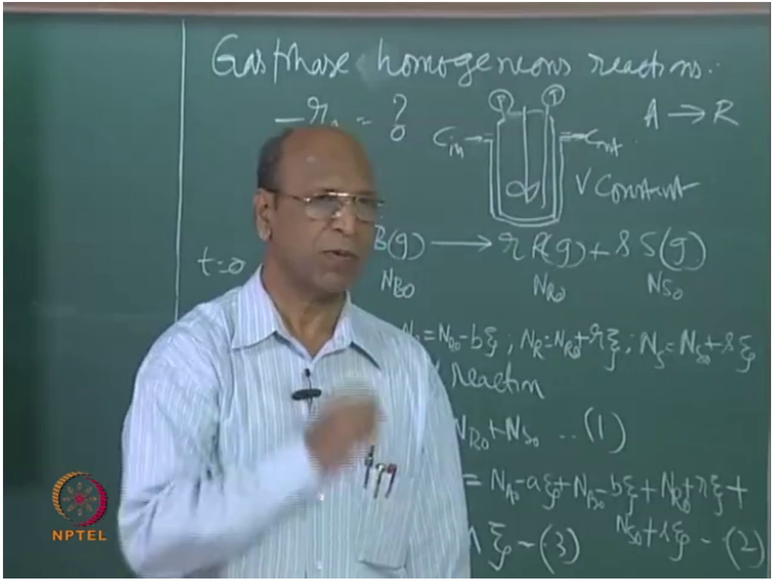

from or where was he from?

Student: Russia.

Professor: So that is the one.

(Professor – student conversation ends)

Whereas industry, they want differentiation. Why? Because if they want to produce hydrogen, all of them are interested only in the properties of hydrogen. They do not want to look at any other element. That is why it is a wonderful statement when I said you know, industry always lives or thrives on differentiation. And academic institution always thrives on unification.

Because for anything, even if you do P h D, definitely one of the examiners at any point of time or in your interviews also, they may ask that Ok, what is the generality? You have done only on this system. How do you generalize, they ask.

So that means your work which you have done in this laboratory, is it valid only for that specific purpose? Can you also extend for other systems? Ok. I mean in terms of temperature, pressure, or flow rates, can you extend further? So that is the kind of thing. So that is why please remember

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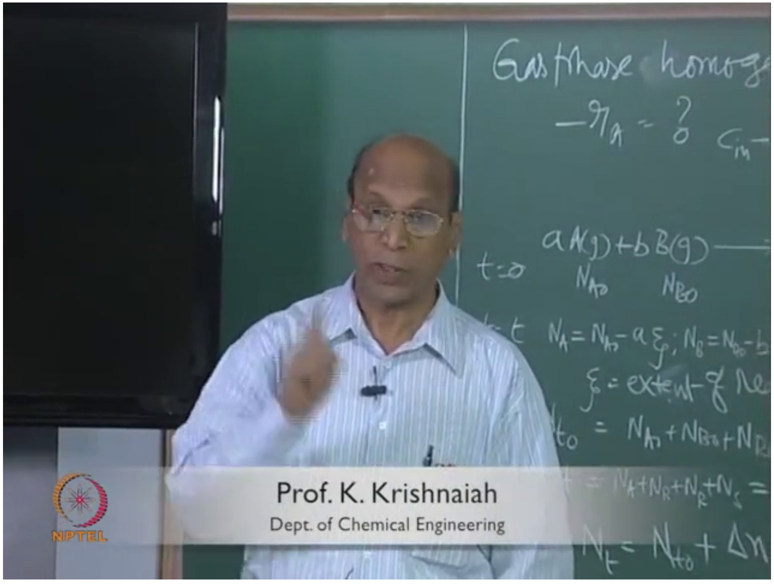

industry always thrives on differentiation. And academic institution thrives on only unification.

So that is why xi you have to really appreciate. You should question me, Sir why are you using X A, conversion. Ok, conversion because these things, you know these things when you learn first time, that is why you say, you know love at first sight, you know and first time love all these things we say, because first thing, anything you do first time, you remember always.

That is why whatever you learnt in high school only you remember. Because that is the first time you started writing, you know, alphabet and all that. So beyond that I do not know really how much we learnt. When you come to the Graduate School like B Tech and all that, I think we are not learning much.

You check yourself, I say. You check yourself. In the school how much knowledge you have retained here? Knowledge means not degrees. How much is retained? At any time what you can recall, what you learnt in school only you can recall.

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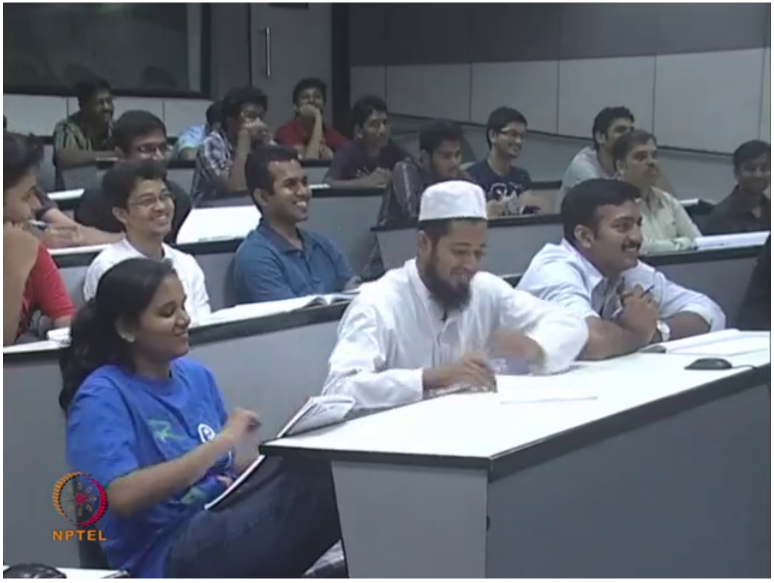

So now this is the equation what we have where xi definition,

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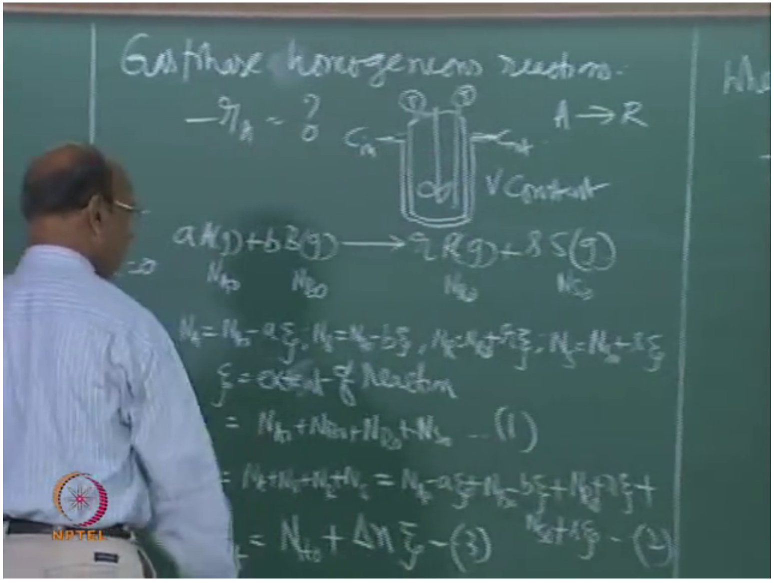

I think, Ok let me write xi equal to N A naught minus N A by A which is also equal to N B naught minus N B by B which is also equal to N R minus N R naught by R, also equal to N S minus N S naught by S, Ok, good. So this is the general definition of xi, that is no problem. I think this equation I can call it as 6,

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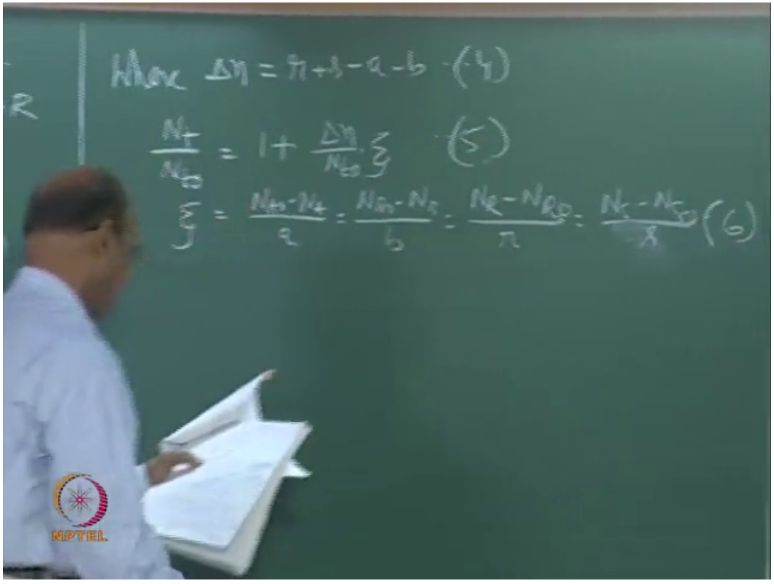

Where $\Delta n = r + s - a - b$ (4)

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}}\xi \quad (5)$$

$$\xi = \frac{N_{a0}-N_a}{a} = \frac{N_{b0}-N_b}{b} = \frac{N_R-N_{R0}}{r} = \frac{N_S-N_{S0}}{s} \quad (6)$$

good.

So now we take this equation and we will try to just manip/manipulate, just try to manipulate that equation. So this N t by N t naught, what is our ultimate aim? To measure the pressure or volume, Ok, yeah. So N t by N t naught equal to 1 plus this 1. What I do here is, delta N by N t naught, N t naught and this one, for xi, I will take, you know for xi, next is xi I have,

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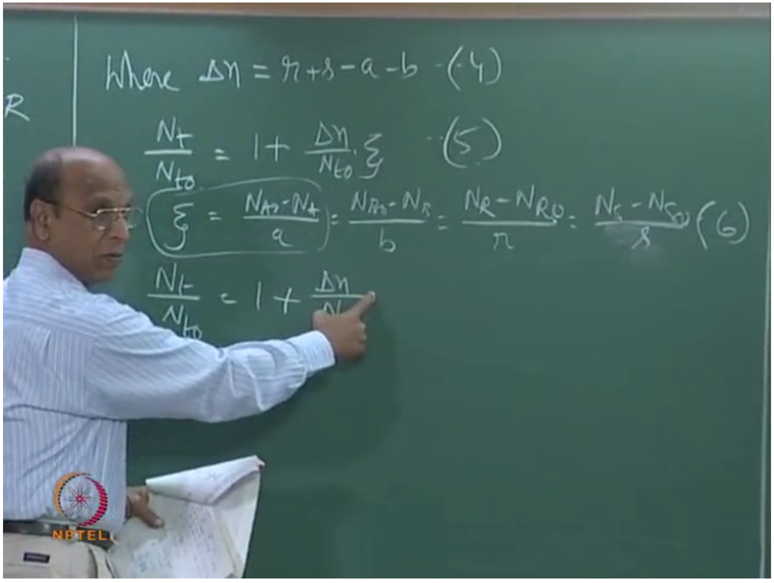

right, for xi I will substitute here N A naught minus N A by A, Ok.

I will further simplify this one. I think I will come to 0:20:45.7, I want to satisfy 0:20:45.7 by writing that, so this is delta N by N t naught, N A naught, N A naught minus N A by N A naught, what do you get?

(Professor – student conversation starts)
Student: 0:21:07.3 of N A
Professor: Correct? Check.

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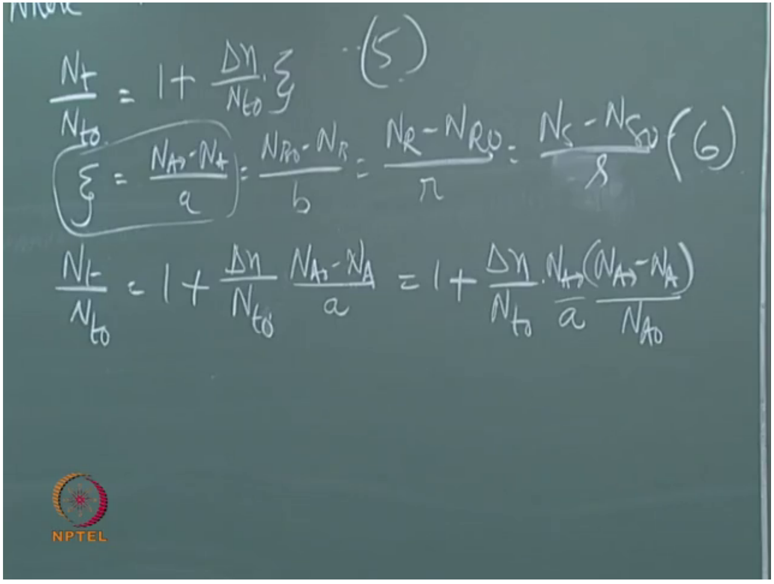

Correct no, N A naught, N A naught I can cancel out. So then I will get only this. So why I have written this one is to satisfy 0:21:25.4

Student: (laugh)

Professor: Ok. So delta N by A, so this is N A by N A naught, correct no? Sorry N t naught, N A by N t naught, then what I have, into,

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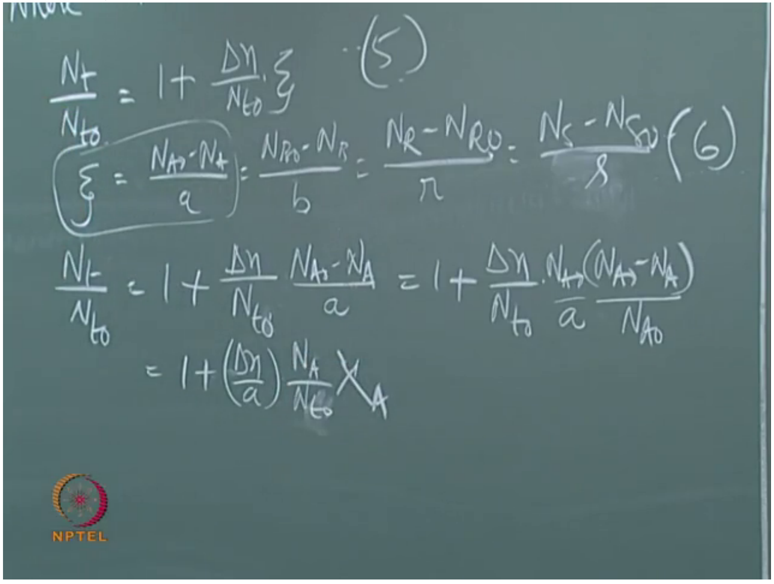

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}} \xi \quad \cdot(5)$$

$$\boxed{\xi = \frac{N_{A0}-N_A}{a}} = \frac{N_{B0}-N_B}{b} = \frac{N_R-N_{R0}}{r} = \frac{N_S-N_{S0}}{s} \quad (6)$$

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}} \cdot \frac{N_{A0}-N_A}{a} = 1 + \frac{\Delta n}{N_{t0}} \cdot \frac{N_{A0}}{a} \frac{(N_{A0}-N_A)}{N_{A0}}$$

$$= 1 + \left(\frac{\Delta n}{a}\right) \frac{N_A}{N_{t0}} X_A$$

0:21:49.3 are you happy? N A naught minus N A by N A naught.

Student: Numerator it will be N A naught

Student: Sir numerator will be N A naught

Professor: Where is N A naught?

Student: del N into N A naught

Professor: This one, no?

Student: No Sir, the next one.

Professor: this one

Student: Next line.

Professor: This one

Student: Sir, next line.

Professor: oh, this one, Ok.

Student: Numerator will be N A naught.

Professor: Delta N I have given here, Oh this one

Student: No, no.

Student: Numerator

Professor: Thank you, thank you, N A naught. Good. So N A naught, yeah N t by N A naught into X A, very good. Thank you. I think you have not stopped, you have not started sleeping. (Professor – student conversation ends)

So yeah, this one now, N t by,

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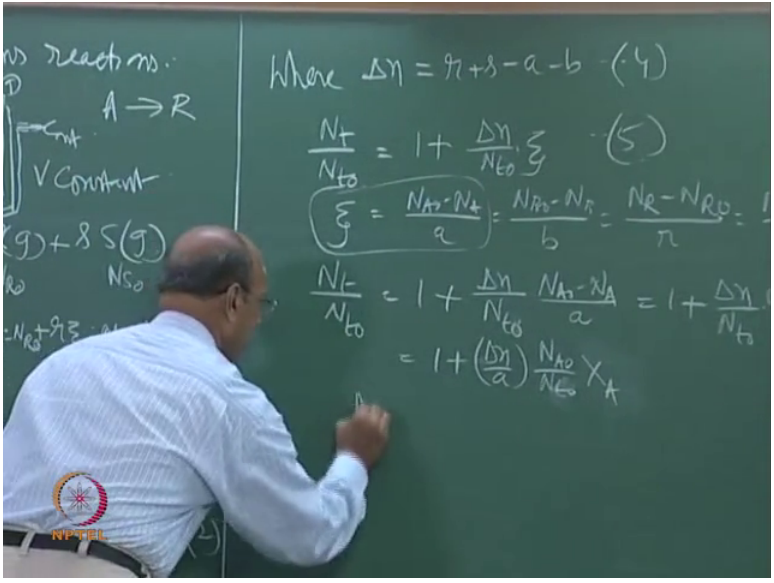

N t by N t naught, I can now write as this one as delta A into Y naught, by the way, N A naught by N t naught what is that? Mole fraction. Correction no, initial mole fraction at time t equal to zero. Mole fraction of A, mole fraction of A.

So y A naught, this is the one, Ok, so these two into X A where this equation equal to 7, where delta A equal to what is that

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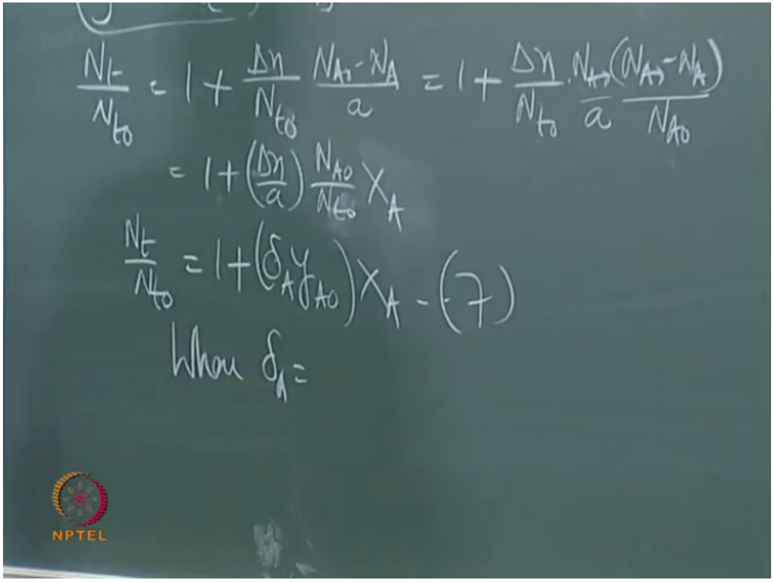

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}} \frac{N_{A0}-N_A}{a} = 1 + \frac{\Delta n}{N_{t0}} \cdot \frac{N_{A0}}{a} \frac{(N_{A0}-N_A)}{N_{A0}}$$

$$= 1 + \left(\frac{\Delta n}{a}\right) \frac{N_{A0}}{N_{t0}} X_A$$

$$\frac{N_t}{N_{t0}} = 1 + (\delta_A y_{A0}) X_A \quad - (7)$$

Where $\delta_A =$

delta n by A and Y A naught equal to N A naught by N t naught, Ok,

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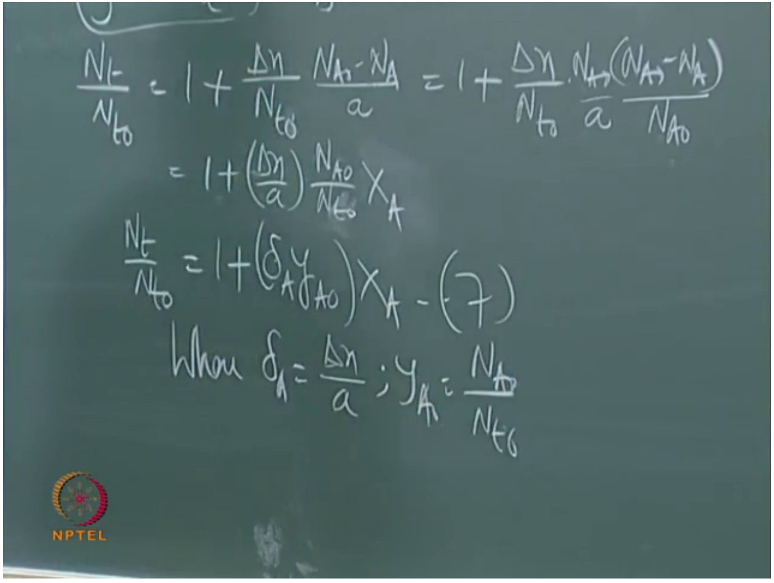

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}} \frac{N_{A0}-N_A}{a} = 1 + \frac{\Delta n}{N_{t0}} \cdot \frac{N_{A0}}{a} \frac{(N_{A0}-N_A)}{N_{A0}}$$

$$= 1 + \left(\frac{\Delta n}{a}\right) \frac{N_{A0}}{N_{t0}} X_A$$

$$\frac{N_t}{N_{t0}} = 1 + (\delta_A y_{A0}) X_A \quad - (7)$$

Where $\delta_A = \frac{\Delta n}{a}$; $y_A = \frac{N_{A0}}{N_{t0}}$

good. You know, you may not remember now. This delta A into y A naught is, in fact, epsilon, Levenspiel epsilon. Ok, yeah.

So this also can be written as N t by N t naught equal to 1 plus epsilon A X A where epsilon A this equation is 8, 8, where epsilon A equal to, delta A into yeah, delta A into y A naught. Ok.

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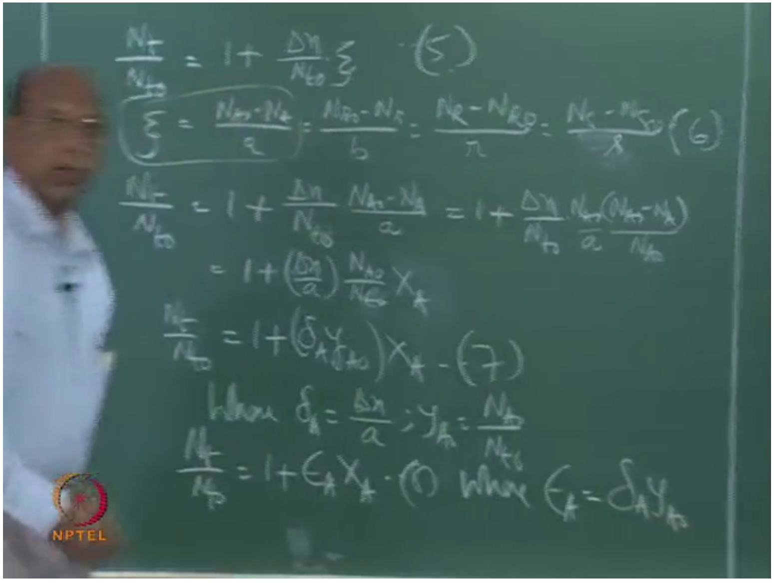

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}} \xi \quad (5)$$

$$\boxed{\xi = \frac{N_{A0} - N_A}{a}} = \frac{N_{B0} - N_B}{b} = \frac{N_R - N_{R0}}{r} = \frac{N_S - N_{S0}}{s} \quad (6)$$

$$\frac{N_t}{N_{t0}} = 1 + \frac{\Delta n}{N_{t0}} \frac{N_{A0} - N_A}{a} = 1 + \frac{\Delta n}{N_{t0}} \frac{N_{A0}}{a} \frac{(N_{A0} - N_A)}{N_{A0}}$$

$$= 1 + \left(\frac{\Delta n}{a}\right) \frac{N_{A0}}{N_{t0}} X_A$$

$$\frac{N_t}{N_{t0}} = 1 + (\delta_A y_{A0}) X_A \quad (7)$$

where $\delta_A = \frac{\Delta n}{a}$; $y_A = \frac{N_{A0}}{N_{t0}}$

$$\frac{N_t}{N_{t0}} = 1 + \epsilon_A X_A \quad (8) \quad \text{where } \epsilon_A = \delta_A y_{A0}$$

So now normally we define epsilon A as volume at, yeah, volume at 100 percent conversion minus volume at zero point

(Professor – student conversation starts)

Student: By zero

Professor: By, Ok, yeah, you know that mug up is there in your mind,

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that is no problem. That is the definition of epsilon.

(Professor – student conversation ends)

But the real meaning of epsilon A

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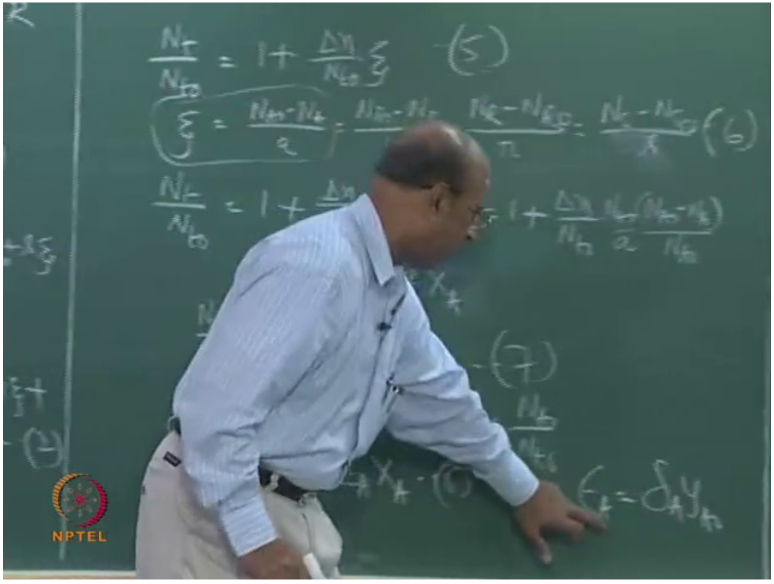

is it is the stoichiometric ratio, delta N by A, Ok, delta N by A, that is why you are writing epsilon A. One can write also for epsilon B and all that. With this derivation, whatever you want, epsilon B also one can write, right? And this equation can also be written in terms of X B.

Only thing is correspondingly wherever you have to substitute,

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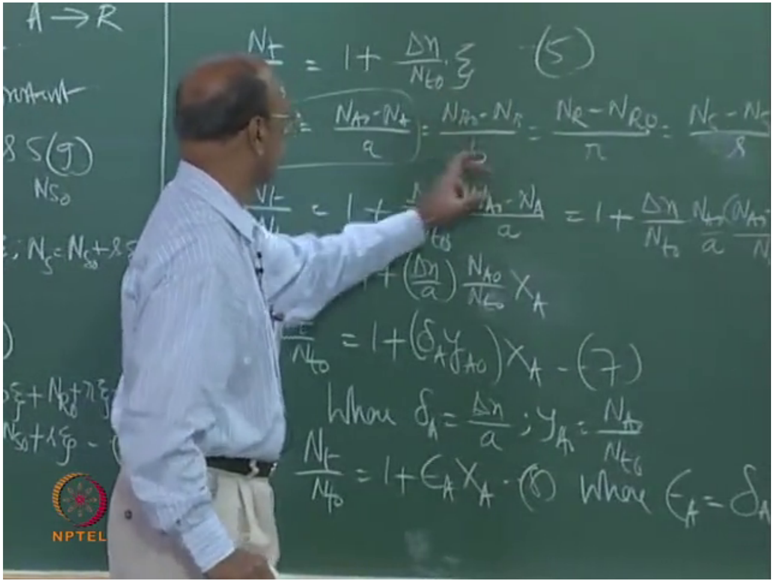

for that xi you have to substitute here. Ok, so this is more general expression, yeah. So do you

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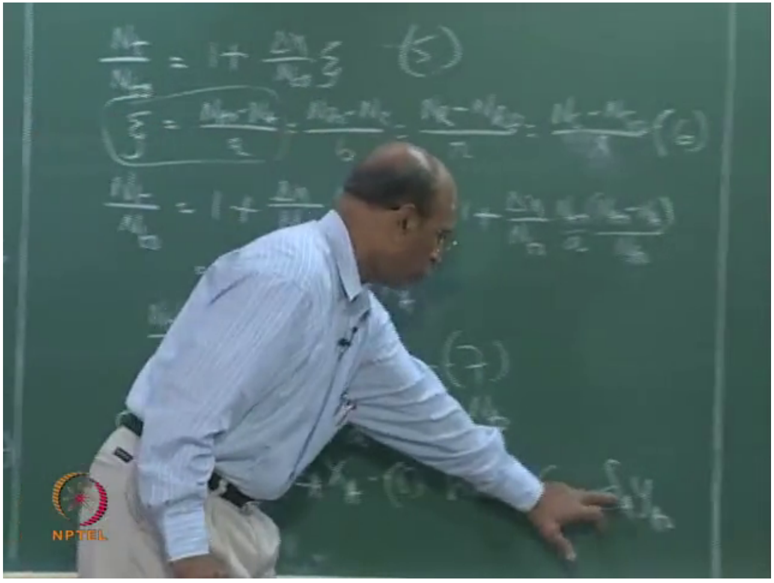

know this delta? delta is delta n by a. Do you know that in the beginning itself, before starting the reaction? Yeah how do you know? Stoichiometry, I say.

You should sometimes tell me Sir, you are asking stupid questions. We already know this.

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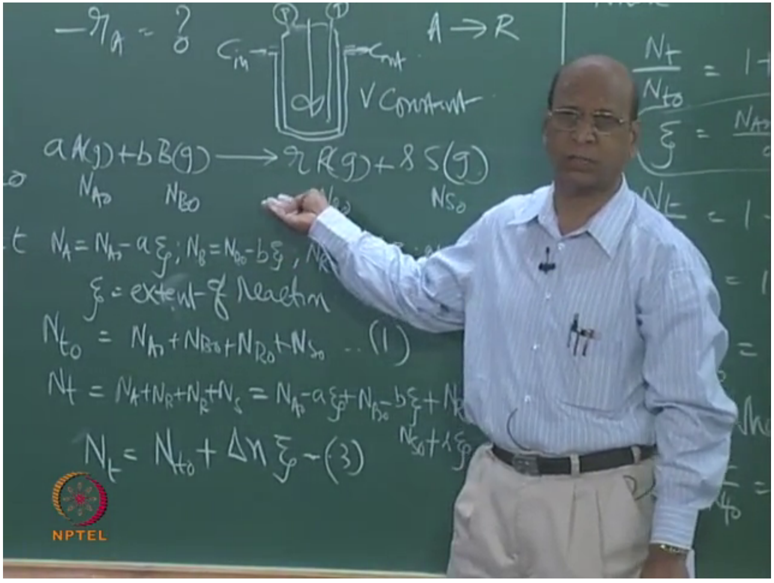

That, you will have to tell me that. Then I stop asking that kind of questions. Ok, because I think you know this delta N I have written here clearly. But those people who are sleeping, I want to wake them up. That is why I am asking again that question, Ok. So delta N I know in the beginning itself.

Because stoichiometry is one of the requirements for me to start with the, my entire reactor design. Ok, that is the first requirement, stoichiometry. So I know, what are the stoichiometric coefficients. So that is why I know delta A. And y naught do you know?

(Professor – student conversation starts)
Student: Yes, yes
Professor: You definitely know. What is y naught if I have pure reactant?
Student: 1
Student: 1
Professor: Yes, pure reactant means if I have only A?
Student: 1
Professor: Yes, if I have A plus B? Just A plus B only, yeah point 5.
(Professor – student conversation ends)

So that is why you know that information. So you do not have to go and write volume at 100, volume at 0 divided by volume at 100 and all that, you do not have to write. Because from stoichiometric equation itself you know all that information. Epsilon A you can calculate.
And by the by, this is the definition given by Levenspiel and he has propagated this way of thinking. So that he can formalize this epsilon A; that volume change, whether it is increasing or decreasing in terms of an equation, that also I will just derive.

But there is another school of thought

(Refer Slide Time: 26:51)

by you know Carberry. Have you heard of name Carberry, James Carberry? James Carberry, he has also Chemical and Catalytic Engineering. In fact the next course is based on only his own

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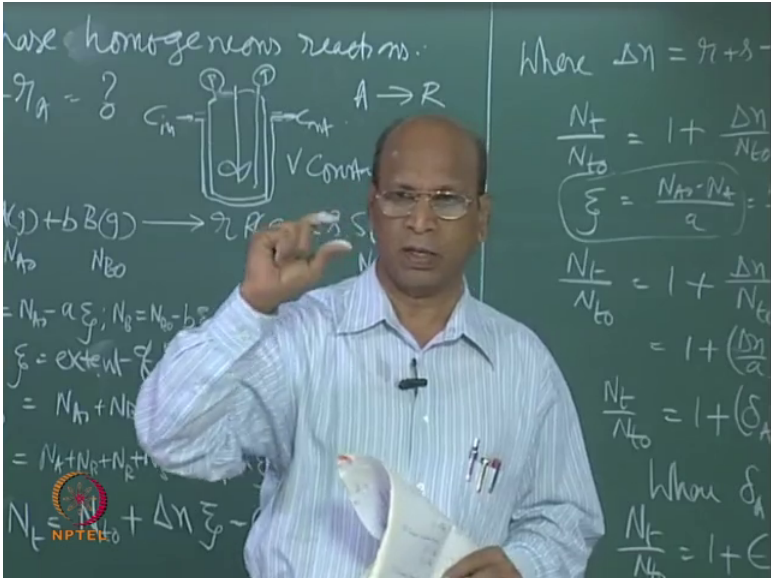

book title.

He wrote a book called Chemical and Catalytic Reaction Engineering, Carberry. In fact, it is J J, James J Carberry, Chemical and Catalytic Engineering, that is the title. I think this is McGraw Hill; McGraw Hill, New York, N Y we write, I think may be 77 but anyway. I think I just put question mark, you will tell me afterwards, Ok.

So that is how you write the textbooks

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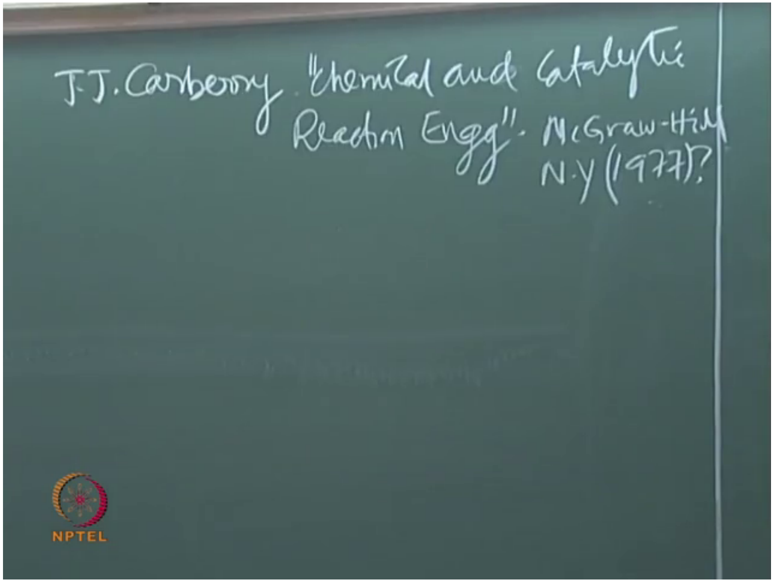

J.J. Carberry "Chemical and Catalytic Reaction Engg". McGraw-Hill N.Y (1977)?

whenever you are writing, Ok. So J J Carberry and yeah, Carberry and Smith, James Smith also, James Smith, Chemical Engineering Kinetics and he is also McGraw Hill publication. New York is the place and yeah, I think his first book was in 1951 or 52, James Smith. So then whatever you see, the current book is actually third edition, I think 1983 or so, Ok. So three volumes, I think he has contributed a lot.

For example his Smith and van Ness, Thermodynamics book, so even now it is a wonderful book and I think when it completed 50 years there was a big celebration also for that book. Because really it was one of the books that are available for chemical engineering thermodynamics. Title also is wonderful, Chemical Engineering Thermodynamics, even though the best book is Denbigh, Chemical Equilibrium, Ok. But this one is straight for the students. That one is for

(Refer Slide Time: 28:49)

philosophers, you know Chemical Equilibrium, right?

What is that, Pooja tell me.

(Professor – student conversation starts)

Student: Y V C Rao's basic book Fundamental Thermodynamics.

Professor: Why we see?

Student: (laugh)

Professor: Y V C?

Student: Y V C Rao.

Professor: Oh Y V C Rao, Ok. I think that is latest generation. Because I think you know Ipad 5, or Ipad 6 or something

Student: (laugh)

Professor: Yeah, these generations later, that is zero. (laugh). So that is why, yeah I think this is another problem no? I think

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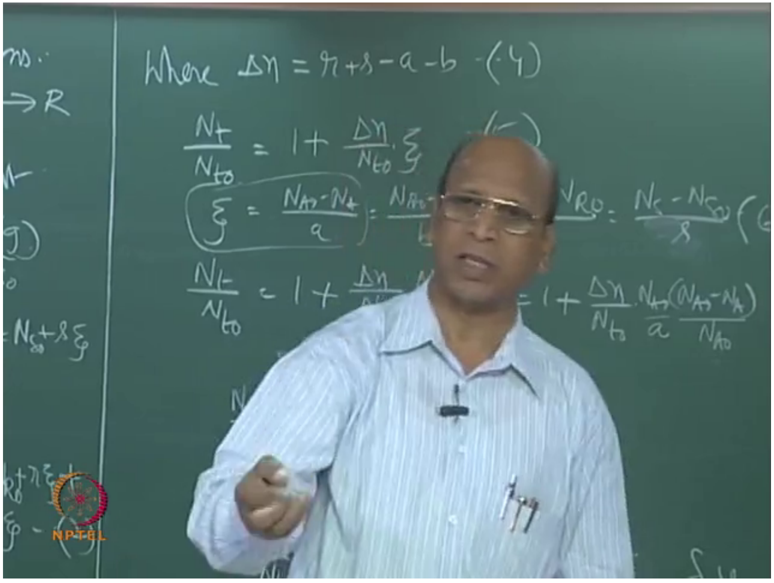

most of the people now, they are following you know...In our time we do not have any Indian books. It is good. We have some Indian books also. But it is not only Indian books that you have to read. Because you do not get the other exposure.
(Professor – student conversation ends)

All our books were foreign books. And we were proud when we were doing our B Tech because only chemical engineering people were using all imported books. Civil Engineering, Mechanical Engineering like Theraja, Theraja.

(Professor – student conversation starts)
Student: (laugh)
Professor: Ok. Bharati Bharati. Ok I think you know that kind of thing. Or Heat Engines by some Shukla Shukla. So that kind of books are only there for them.
(Professor – student conversation ends)

But for us, you know Levenspiel, right, Smith, James Smith also you know Thermodynamics

(Refer Slide Time: 30:00)

and Fluid Mechanics by I think McCabe and Smith, McCabe and Smith. All our books are only foreign books. Ok, Treybal, yeah, Fogler was not there. He was not born even when I was studying.

Ok, so those are the books what we had, you know

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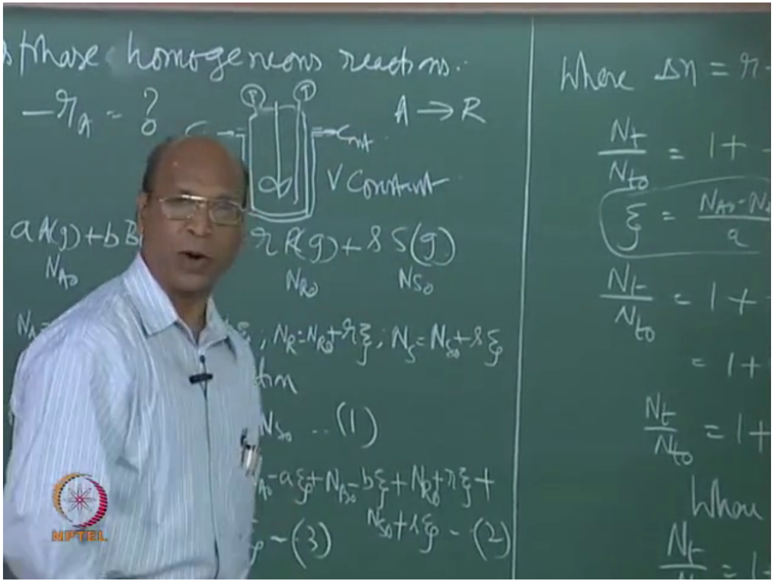

at the time, we were really proud. But now you do not know all those books. You know only Y V C Rao and who is that person who writes many books, Pande? Panda? What is that, Gavhane?

(Professor – student conversation starts)

Student: Yes
Professor: Gavhane is expert in all subjects.
Student: (laugh)
Professor: Ok, so I think he should be given Nobel Prize, I say. It is not possible to be expert in all subjects. Right, I think we do not have Nobel Prize in India. So we should have given that.
(Professor – student conversation ends)

So that is the kind of things what we have. Ok and you should also remember, you should definitely see, this is the time to see, all these books are there in our library. At least for the sake of seeing, that you have satisfaction of, I have seen this book. Ok. So I think, Perry you have seen no? Or the Indian book is there? Gavhane. Handbook of Chemical Engineering by Gavhane is there?

(Professor – student conversation starts)
Student: (laugh)
Professor: No, not there? I have never seen that book. I do not know. But somehow I think, many people I think, my students used to tell me, Ok, good.
(Professor – student conversation ends)

So this is the equation. That is why, epsilon that is the blind definition what he has given, Levenspiel simply by V at some time, and V, not time, conversion no, yeah 100 percent conversion and all that, good, so this is the equation. Now this equation we can write also in terms of volumes and pressures. Because N t by N t naught.

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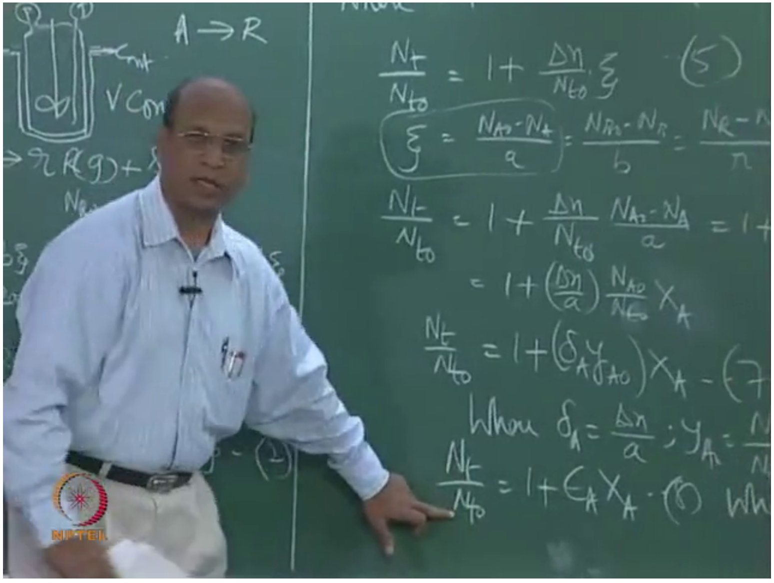

So I will go to now my ideal gas equation, P V equal to n R T, Ok n, n is the number of moles that is, this will come there. So I will have this equation P V equal to N t R T, that is one equation. And another equation is P naught V naught N t naught by R T, Oh this is T, T naught, right.

Now you divide N t by N t naught equal to, N t by N t naught equal to P, yes Ok, P by P naught, correct and T naught, what about V, V by V naught into T naught by T, R will get cancelled, no.

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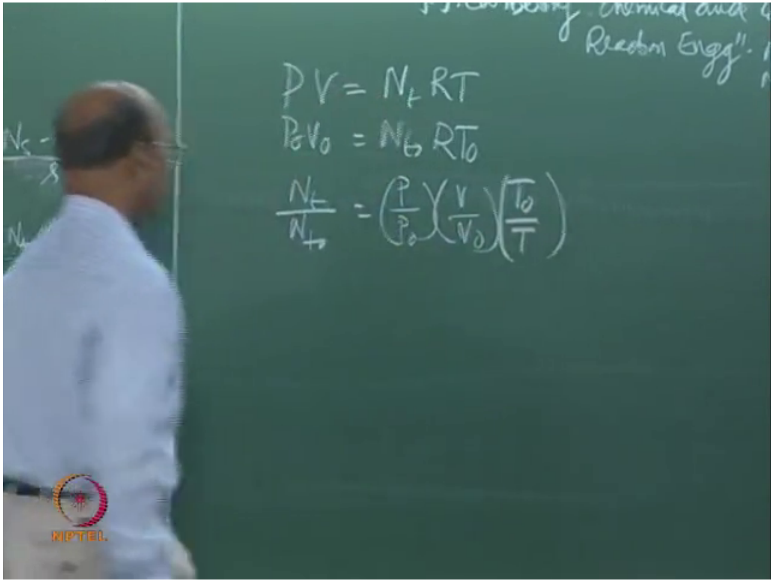

Yeah. So now this is equal to,

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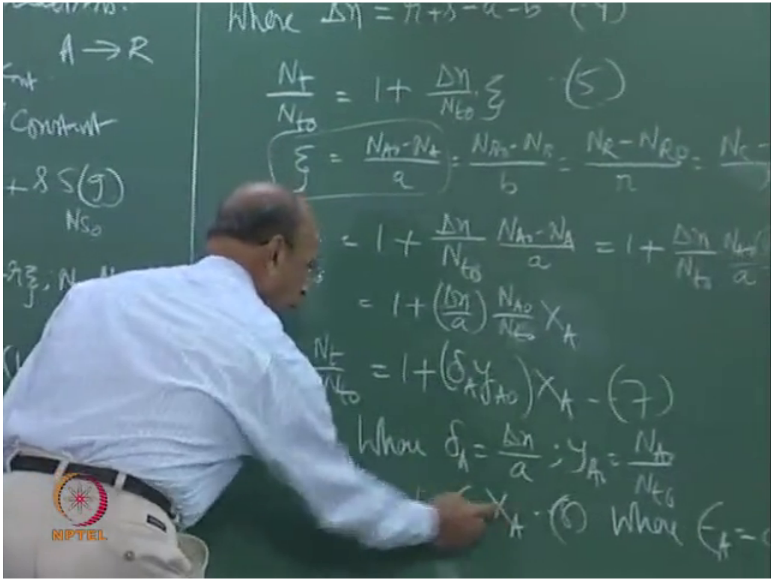

I have 1 plus

(Professor – student conversation starts)

Student: Epsilon

Professor: This is equal to 1 plus epsilon A X A, yeah, Ok 9.

(Professor – student conversation ends)

Now I can write this equation

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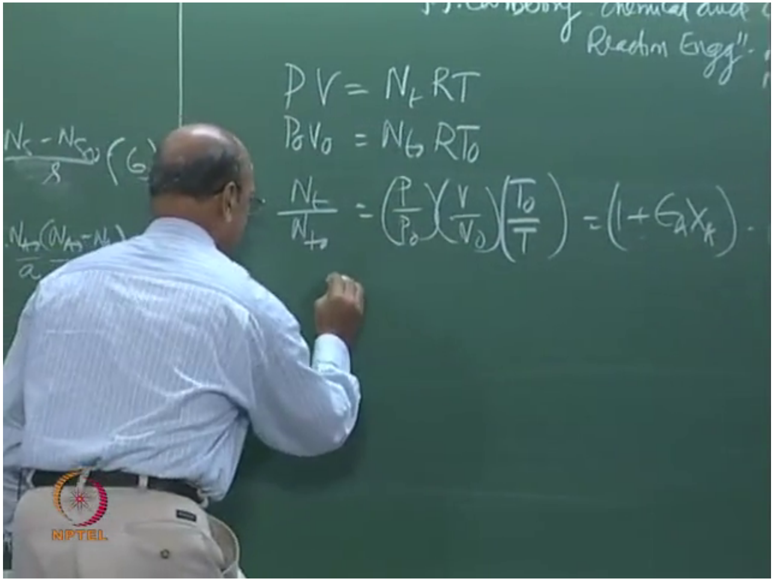

as P by P naught, Ok, first I think I will write the familiar form. So V by V naught equal to 1 plus epsilon A X A into P naught by P, if I write wrongly please tell me, T by T naught, correct? T by T naught.

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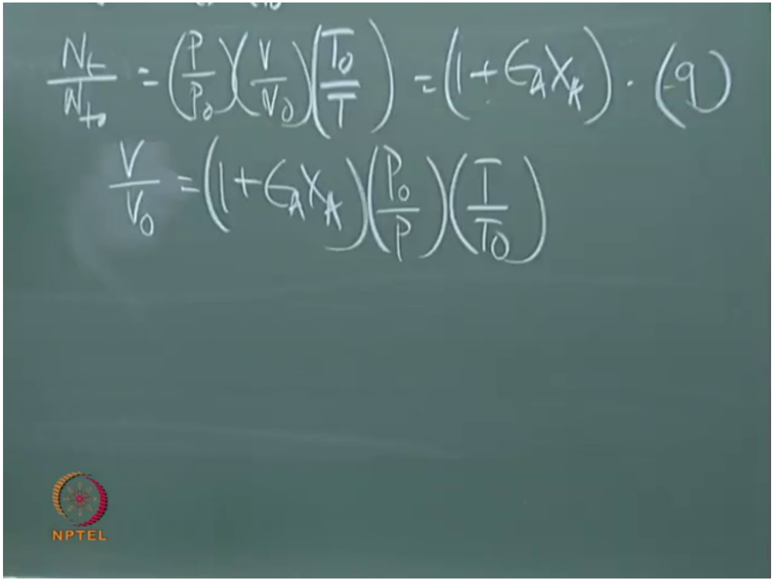

$$\frac{N_t}{N_{t0}} = \left(\frac{P}{P_0}\right)\left(\frac{V}{V_0}\right)\left(\frac{T_0}{T}\right) = \left(1+\epsilon_A X_A\right) \cdot (9)$$

$$\frac{V}{V_0} = \left(1+\epsilon_A X_A\right)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)$$

If I have a constant density system. That means variable volume. Yes variable volume and if I have isothermal case. What is the equation?

(Professor – student conversation starts)

Student: 0:33:35.0

Professor: What is the condition? I have constant...

Student: Constant

Professor: Yeah, constant temperature, and also variable volume that means pressure is constant

Student: Constant.

Professor: That means P equal to

R P naught

Professor: P naught, variable volume. When you have

(Refer Slide Time: 33:53)

variable volume pressure must be constant.

Student: Constant

Professor: That means P equal to

Student: P naught.

Professor: P naught. So for variable volume, variable volume P naught equal to P, variable volume and isothermal, isothermal and T equal to T naught

(Professor – student conversation ends)

Ok what is the equation we get, V by V naught equal to...yeah, now, now at least you remember what is this equation? This is 10, this is 11, this is what is the definition of Levenspiel

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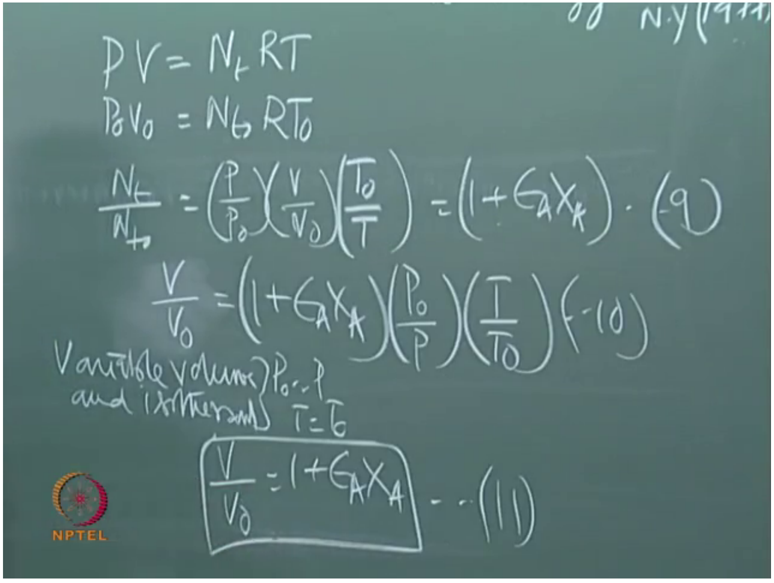

N.Y (19

$$PV = N_t RT$$

$$P_0V_0 = N_{t0} RT_0$$

$$\frac{N_t}{N_{t0}} = \left(\frac{P}{P_0}\right)\left(\frac{V}{V_0}\right)\left(\frac{T_0}{T}\right) = (1+\epsilon_A X_A) \cdot (9)$$

$$\frac{V}{V_0} = (1+\epsilon_A X_A)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right) (\cdot 10)$$

Variable volume) $P_0 = P$
and isothermal) $T = T_0$

$$\boxed{\frac{V}{V_0} = 1+\epsilon_A X_A} \cdots (11)$$

under strict conditions like variable volume, that means pressure is constant, temperature is isothermal conditions so temperature is same that is why you get this equation, Ok, good.

So now you have to use this equation to define conversions and all that. Let me write that pressure equation and then we can decide, yes tomorrow...we cannot run immediately. So then the other equation in terms of constant volume, constant volume and isothermal case what do you do? Constant volume yeah, and isothermal. Constant volume means

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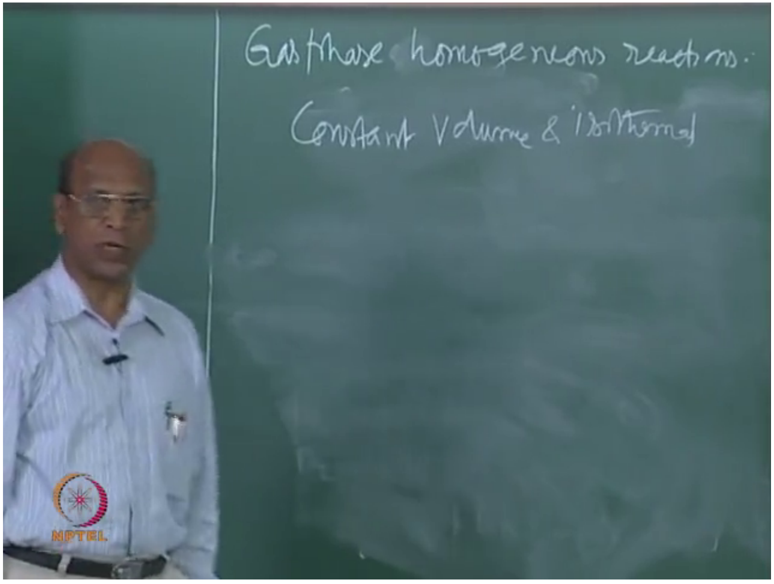

Gas phase homogeneous reactions:

Constant volume & isothermal

V equal to

(Professor – student conversation starts)

Student: V naught

Professor: V naught and T equal to T naught. Now tell the equation?

Student: T naught equal to 1 plus epsilon A X A

Professor: P by P naught equal to

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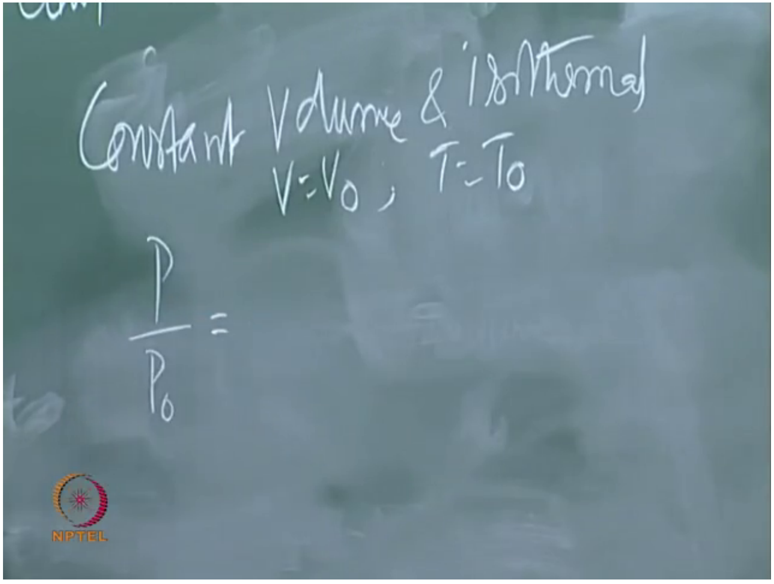

Constant Volume & isothermal

$V = V_0 \; ; \; T = T_0$

$$\frac{P}{P_0} =$$

Student: 1 plus epsilon A X A

Professor: 1 plus

Student: Epsilon A X A

Professor: Correct,

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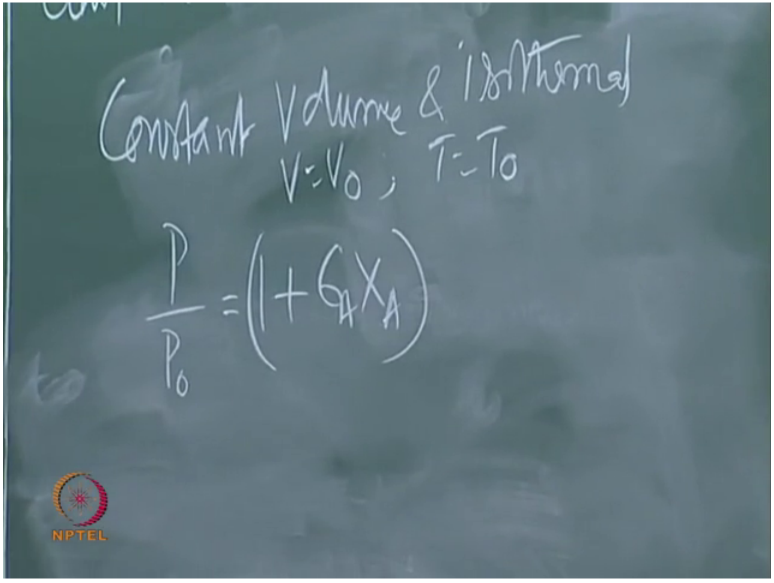

Constant Volume & isothermal

$V = V_0 \; ; \; T = T_0$

$$\frac{P}{P_0} = (1 + \epsilon_A X_A)$$

P by P naught, yeah good. So now this equation you are familiar. But from this equation you have to get the partial pressures.

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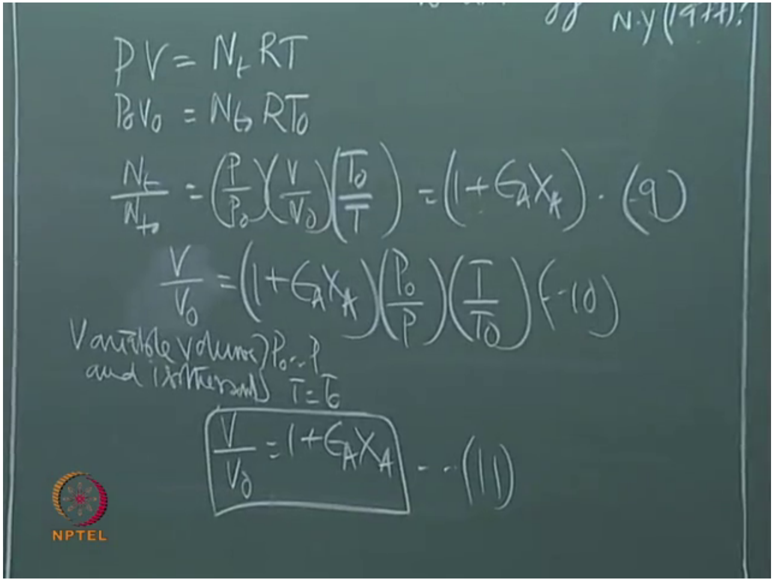

N.y (1977)?

$$PV = N_t RT$$

$$P_0 V_0 = N_{t0} R T_0$$

$$\frac{N_t}{N_{t0}} = \left(\frac{P}{P_0}\right)\left(\frac{V}{V_0}\right)\left(\frac{T_0}{T}\right) = (1+\varepsilon_A X_A) \cdot (9)$$

$$\frac{V}{V_0} = (1+\varepsilon_A X_A)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right) (10)$$

Variable volume } $P_0 = P$
and isothermal } $T = T_0$

$$\boxed{\frac{V}{V_0} = 1+\varepsilon_A X_A} \ldots (11)$$

(Professor – student conversation ends)

Ok, so from one equation we are able to get two of the Levenspiel's you know, derivations, two derivations he has done. I mean he has not derived that, actually he gave the definition, no derivation there. Right.

What we have to get is, you have an equation which you have seen in third chapter, P A equal to P A naught minus A by delta N, P minus P naught, see. This one, even if I write like this, this is the total pressure. When I write, somewhere here it is partial pressure, Ok.

So this is the equation which you are familiar with, you know, when you see Levenspiel book. Third chapter, in fact third chapter

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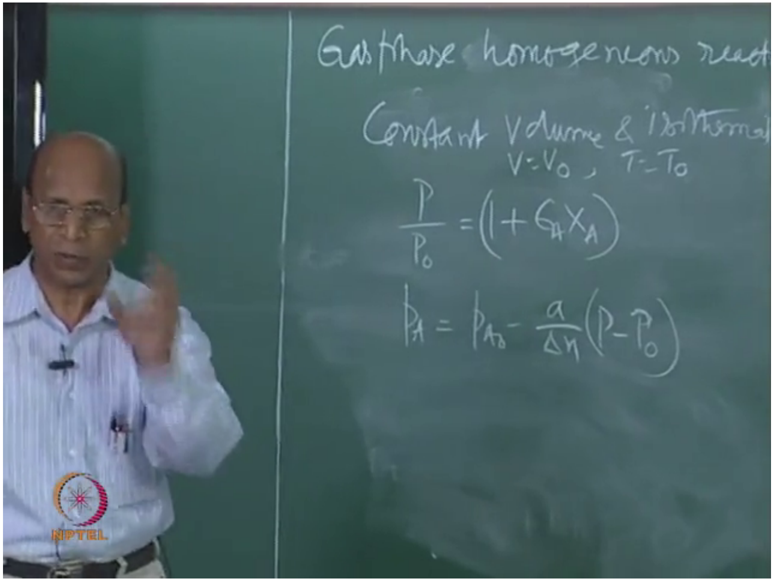

first derivation is this, right. So can you get this, this from this? That is equation number 12. This is 13 and I will put question mark, how do you get this?

In fact, from this you can also get this. I will just leave it to you, that one how do you get. In fact, you can get this one for not only P A, P R you can get, P B you can get, P S you can get, all that. Can you get this from this?

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Ok, you have all the definitions.

You have what is

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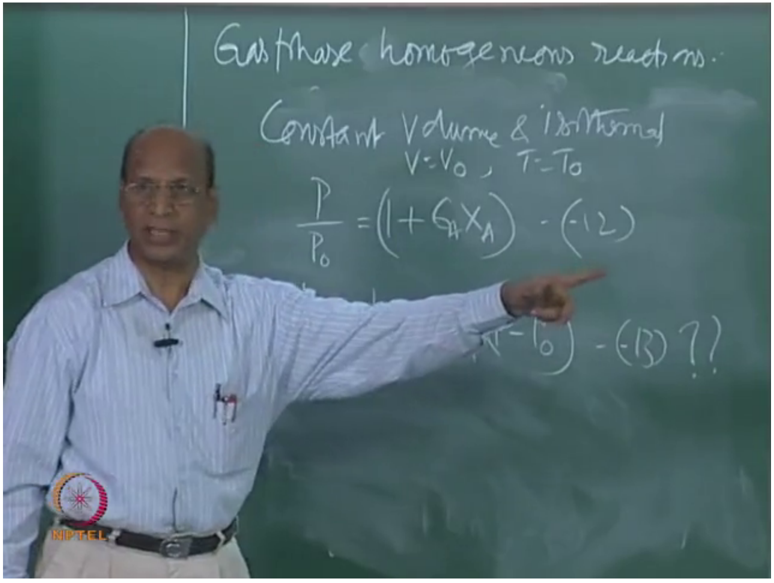

epsilon A, right

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and you know what is x A, here in this equation there is no X A also.

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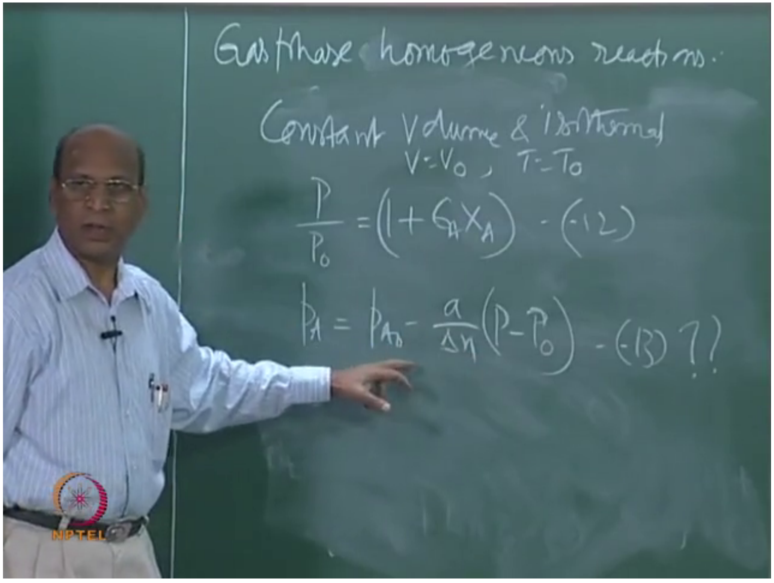

X A is nothing but N A, that is Ok but in terms of partial pressures, how do you write? Because it is constant volume. Constant volume, in terms of partial pressures how do you define X A?

(Professor – student conversation starts)

Student: P A naught

Professor: That is all. P A naught minus P A by P A naught.

(Professor – student conversation ends)

So you substitute for X A, that.

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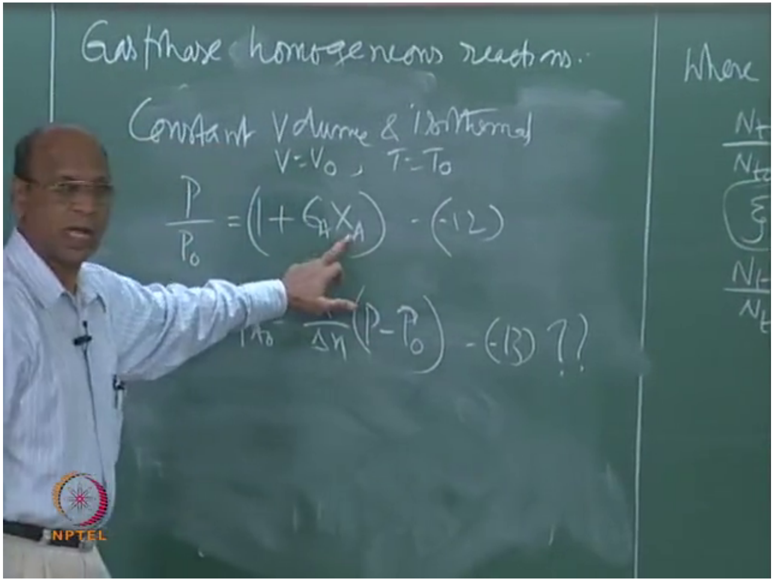

And epsilon A you know, right. And then you arrange that equation you will get this. Because you have that mole fraction and all that no, y naught is mole fraction, right, so that is why I leave it to you, That you derive on that. So that I have one for separate test. I will tell that, Ok derive this equation. Right. It is not difficult no? All of you are Ok or 0:38:13.6?

(Refer Slide Time: 38:13)

(Professor – student conversation starts)

Student: It is Ok

Professor: Ok, no problem. Yeah, this is very simple derivation only, it is not that difficult provided if you use these

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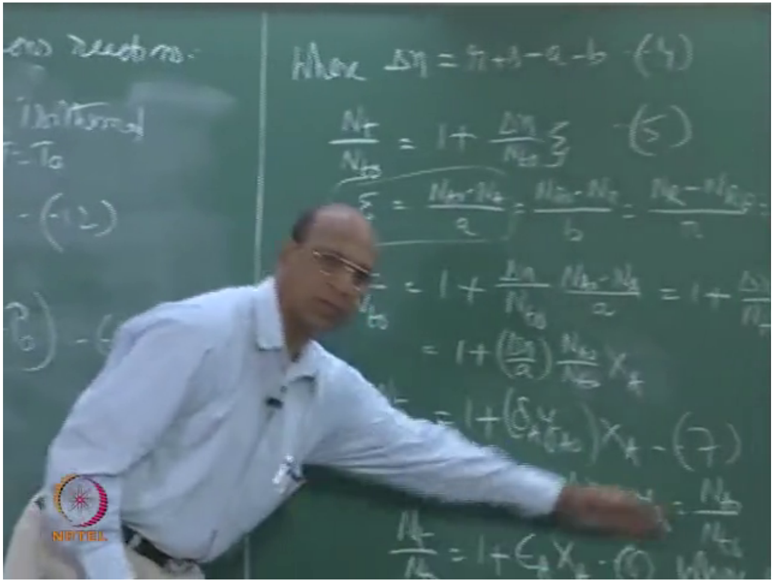

equations, you can easily derive this from this,

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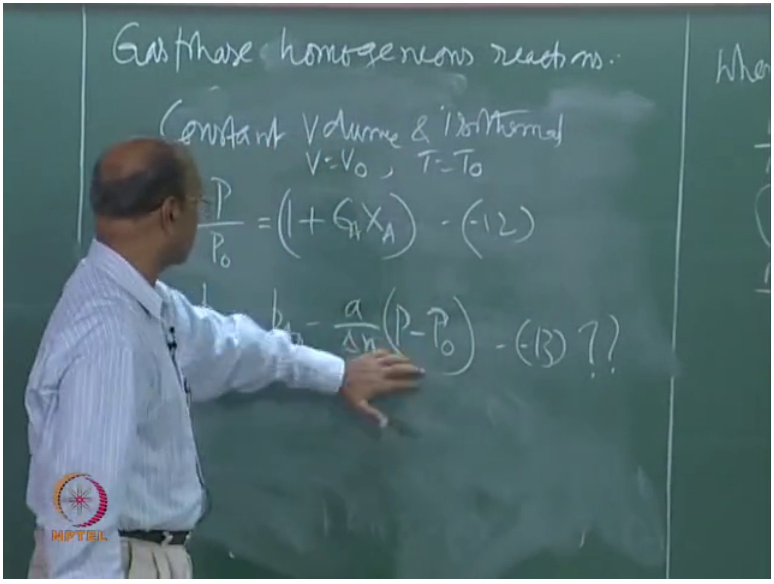

Ok this from this, Ok this from this. Ok.
(Professor – student conversation ends)

This is nice one because I think from the same equation we are able to get the two things. Now you have lot of work to do. Because now third chapter is over and fifth chapter is over, Ok. That fifth chapter is reactor design. That equations we have.

Actually second chapter is T and all that, you know Arrhenius equation, mechanisms of reaction and all that. That also we have discussed. So first chapter is introduction, anyway. So third chapter is now what we have discussed. Now I cannot derive each and every equation.
Now it is for you at this point of time, you derive all the equations.

Now our idea is to go to that final diagram. What is that, input, output, contacting, kinetics. Now you have the contacting. Contacting means any reactor when we have to choose, what is the design expression, that part you know. And in that design expression, you have minus r A, right minus r A. That minus r A now you know how to get. Right? So what you do is, once you get this P A,

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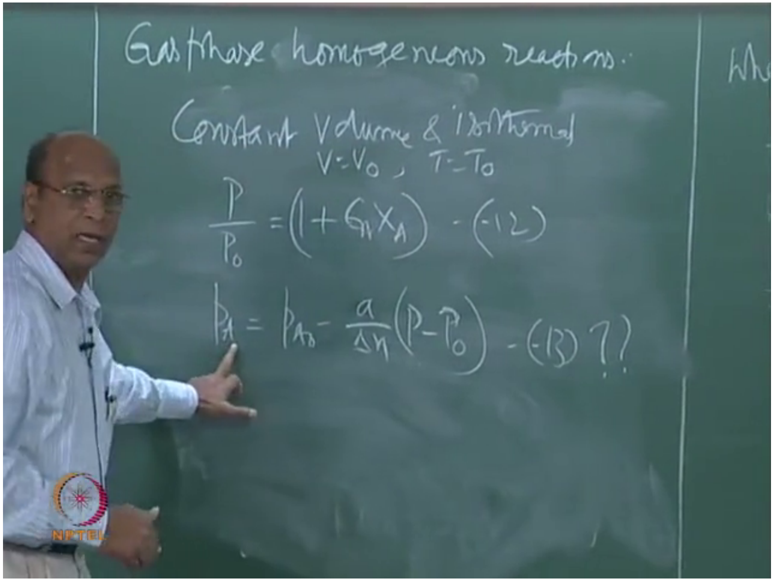

P B, P B also you can have another equation, P R , P S, those are the concentrations for us. Now that versus time will be given,

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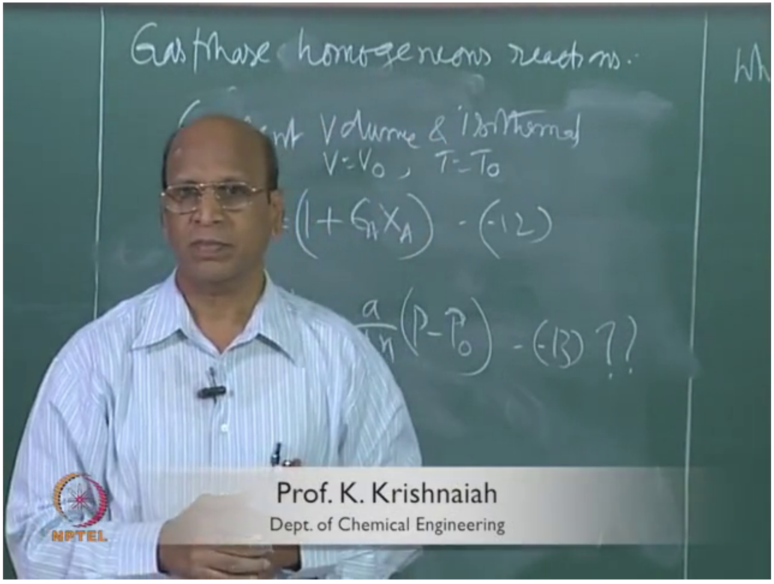

right? Otherwise you can also convert this into concentrations by dividing by R T, R T, R T. Then you have.

Now what you have, concentration versus time, or partial pressure versus time. In fact I would have given also, Sushmita you have seen all the problems? In the assignment, I think if I remember correctly I also gave in terms of partial pressures, 1 or 2 problems. Ok. So that is why.

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Unless you also move with me by spending time in your room

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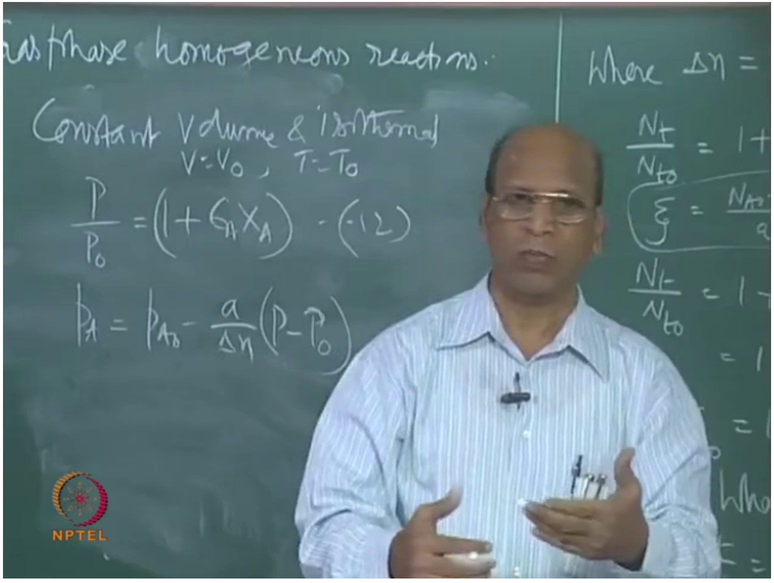

you will be lost. And otherwise you will not be comfortable in the subject. In the class you feel that everything will be clear. But the moment you start solving problems, you will have many doubts. So at that time you have to discuss with your friends.

If they are not able to clear, you have to come here. We will discuss and then we will completely try to learn this subject as deep as possible, Ok. We will stop here and tomorrow morning at 9 o'clock we will start the class, thank you.