Chemical Reaction Engineering 2 (Heterogeneous Reactors)

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Lecture 20

Industrially Important Catalytic Reaction Models

So yesterday we have discussed, I told you that we have to give some industrially important reactions so that you will have an idea what kind of rate expressions they use. Industrially important catalytic reaction models, okay. The first very famous one is ammonia synthesis all of us know that, okay. So the rate expression, okay, first of all the stoichiometric equation is 3 H 2 gas plus N 2 gas giving us 2 N H 3 gas so catalyst is iron, okay.

So the rate expression for this, r equal to some constant k partial pressure of N 2. I may write sometimes partial pressure sometimes I think concentration also depending on which I got from the temperature. Partial pressure of H 2 to the power of 1 point 5 divided by P N H 3. This is one term, minus k 1 dash partial pressure of N H 3, 1 point 5. This is one equation.

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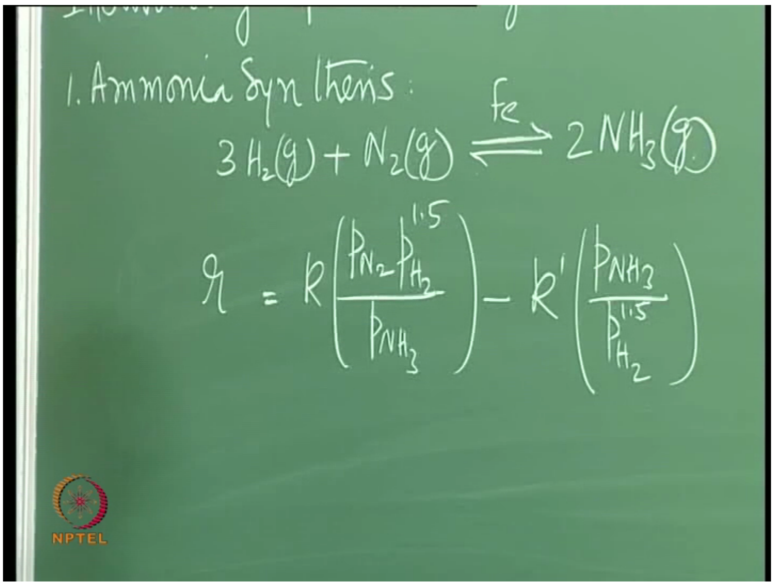

So next one again most of the time I have been telling this is sulphur dioxide, oxidation of sulphur dioxide, good. Reaction is S O 2 gas plus half O 2 gas S O 3 gas and you know V 2 O 5, vanadium pentoxide. The rate expression for this that is available, there are many types of rate expression for this, is some other constant k partial pressure of O 2 divided by P S O 3 whole to the power of point 8 minus k dash partial pressure of S O 3 by partial pressure of S O 2 to the power 1 point 2. So this is equation 2, good.

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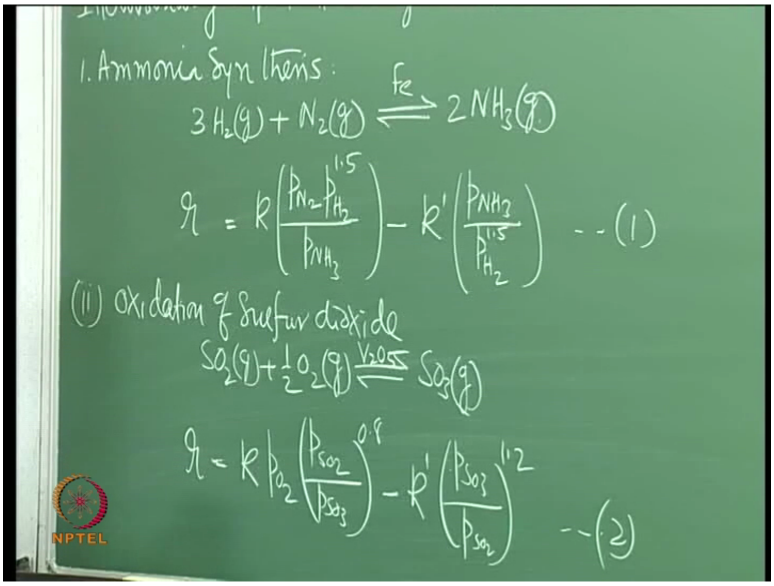

So, then third one which you may not know that much is oxidation of nitric acid. Yes, so the reaction is N O gas plus half O 2 gas giving us N O 2 gas. Catalyst here is silica gel, okay. Yes, N O nitric oxide.

Student: Nitric acid.

Professor: Oh, oxide I said. Good, I am happy you have not slept. You are alive, okay good. So this is the one. For this the reaction is r equal to partial pressure of N O square, partial pressure of O 2 divided by, okay, I think I will write a plus b partial pressure of N O square plus c some other constant, partial pressure of N O 2. Yes, where a equal to point 005834 and b equal to 23 point 63 and c equal to point 03268. So this is 2, this is equation 3. Another example is, okay, ethylene chloride. From ethylene and H c L.

Yes, so equation is C 2 H 4 gas plus H c L gas giving C 2 H 5 c L. Now here the catalyst is zirconium oxychloride. You see things are getting complicated on silica gel. So I have to write separately, okay. Catalyst is zirconium oxychloride on silica gel, okay. So the rate expression correspondingly for this is , okay, C 2 H 4 as A and H c L as B. Otherwise in the subscript I have to write all this that is why. And C 2 H 5 c L as let us say R, okay.

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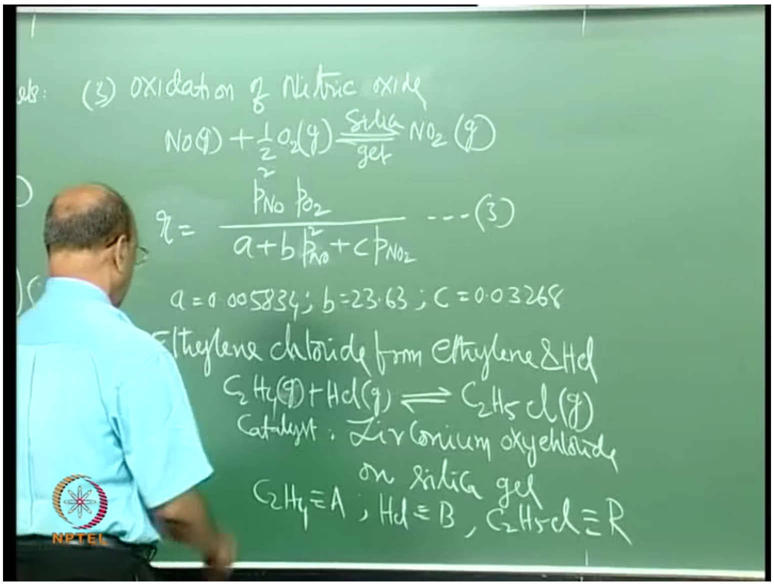

Now the equation will be r equal to some constant P A P B minus P R some other constant whole thing divided by 1 plus capital K A P R by K P B plus K B P B plus K R P R plus inert, yes. That is the equation. So this equation is 4. Good, so one more 5 is, okay, catalytic hydrogenation of C O 2 to methane. Catalyst is not known but the reaction is C O 2 gas plus 4 H 2 gas giving us C H 4 gas plus 2 H 2 O gas.

The rate expression is, catalyst is not known, some constant k partial pressure of C O 2, partial pressure of H 2 to the power of 4, 1 plus K 1 partial pressure of H 2 plus K 2 partial pressure of C O 2 to the power of 5. Very peculiar equation, yes. So one more also I will give you for S O 2 because to tell that if the catalyst is changed, rate expression also will change, okay. So for sulphur dioxide oxidation again I think there are some values also given here.

So this reaction is at very high pressures. Pressure is 30 atmospheres, yes and temperature is 314 degree centigrade. You see how accurately and of course some values are given for k, 7. Of course corresponding units we have to take depending on atmospheres there. Then just to give you an idea K 1 equal to 1 point 73 and K 2 equal to 0 point 3, okay good.

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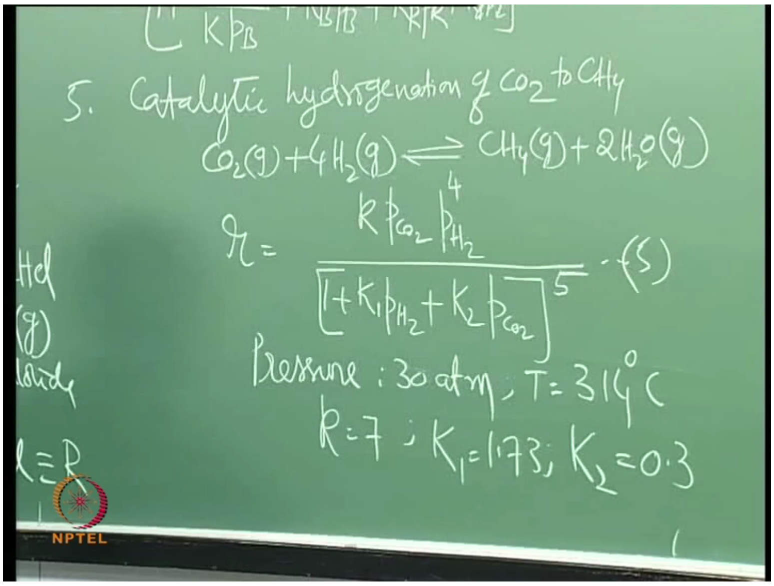

So next one is sulphur dioxide oxidation again. This is 6, S O 2 oxidation same reaction but this time it is platinum catalyst. S O 2 gas plus half O 2 gas, this is platinum giving S O 3 gas. So rate expression is some constant k, partial pressure of S O 2, partial pressure of O 2 divided by 1 plus K 1 partial pressure of O 2 to the power of half. Do not get sleep because next (())(14:34) maybe all this, okay. So that is why if you sleep then again tomorrow you will feel bad. K 2 P of S O 3.

We have another term here P of O 2 again half. So this is equation 5 equation 6, okay. Another one again for S O 2 oxidation, okay. This is one of the oldest equations that are used. Directly I am writing rate as k 1 partial pressure of S O 2 to the power of half, partial pressure of O 2 minus k 2 partial pressure of O 2 to the power of half, partial pressure of S O 2 minus half. So this is equation 7.

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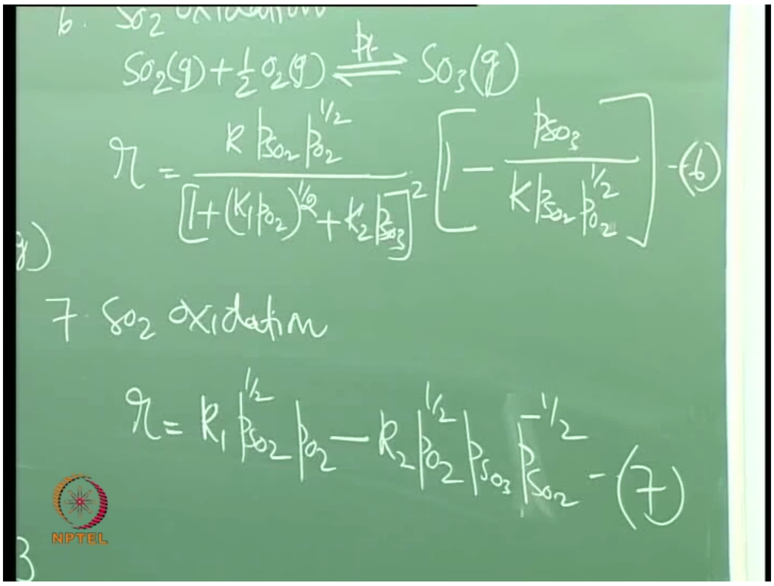

And you may get bored with all these writing but I think you have to really appreciate. It is like heat transfer course where most of the time we write the correlations. Student may get bored but I think behind every correlation there is a big story that you have to appreciate that story, okay. So similarly here we have written all the equation. You may be feeling bored that why this fellow is writing all these equations, right? But behind every equation there is tremendous amount of work, right?

For example you see for oxidation of sulphur dioxide S O 2 to S O 3, there are three. First of all if you change the catalyst your rate will change, okay, rate equation. Then totally there is no relationship between equation 2 and equation 6 and also equation 7. That is purely empirical. That is what yesterday I have been telling you, purely empirical the bottom one. That is one of the oldest one given by one professor called Calderbank. I think he is from Finland or so, okay.

So like this you have to develop the equations and then what you learnt here is there anything coming? Out of all these equations what you learnt the methodology? So the moment you have this particular reaction then we have to write the mechanism. That mechanism is your imagination. Model is always your imagination please remember that. Model is in the mind and the experimental data is real and you know every persons mind will be different. So the way I imagine for a model you need not imagine.

So that is why unless model is proved with the experiment no model is right, okay. It has to be proved by the experiment at the end. So that is why you may have thousands of models but finally few data points must be necessary to validate the model. This is American education. You know they write thousand models and one data point. And Japanese are totally opposite. They are also opposite other side, okay. They are west and these people are east and you know they have almost zero models and infinite data, Japanese.

So that is why their industry and all that is based on solid you know experimental data. Germans also like that. They do not worry first about the models. First they worry about the experimental data how accurately you take and then depending on your capacity you can have any type of model. Model is a physical representation but there are models where from first principles you develop. That no one can change. We all developed say that must be same. First principle means taking the basic phenomena into account.

What is really happening? It cannot be different when I look or when you look or when someone looks. It should be the same. So once you know the phenomena then start writing the equations. Like simplest example is same thing what we are doing. You imagine what is happening. How the reaction is taking place? Then you write step 1 mass transfer, step 2 diffusion step, 3 reaction, okay. Whoever observes definitely there is a mass transfer step, definitely there is a diffusion step, definitely there is surface reaction step, right?

So mass transfer equation there is only one whoever writes, right? Only constants may change depending on conditions and all that. And diffusion again same, always we take only fix. If it is multi component diffusion then you go for?

Student: (())(19:59)

Professor: No, the other famous one. Formality component.

Student: Maxwell.

Professor: Maxwell and before that who was that? There is (())(20:11) , okay. So, that you use. And surface reaction again our imagination. Surface reaction is nothing but all this, okay. So that is why I think modelling of this LHHW kinetics for catalytic reaction is one of the really toughest jobs. And there are people who specialise only to evaluate those constants.

Again you need many mathematical techniques and then I tell you from the beginning chemical engineering was a science and the first engineering magazine which is science is chemical engineering science. I do not think any other civil engineering science was not there. Recently they started but from the beginning 1950 itself they have started chemical engineering science journal.

I do not remember but (())(21:03) also was there for long time as an editor. The first editor I do not know. So that means everything is based on science but you know scientific engineering, okay. We have engineering scientist and scientific engineers. You know the difference Swami? Hello, you are in the class?

Student: Yes.

Professor: Okay tell me, yes because it is madness you just sit down and then you look at me but you are there somewhere, okay. Only thing is this chord is missing what they put here. What it is say first of all? Unfortunately I have a good psychology. Looking at the people I can interpret many things. Unfortunately I am right.

Yes scientific engineers, engineering scientist what is the difference? Yes Siddharth? Calculating? Scientific engineers and engineering scientist, okay. Ashok Kumar? He is not looking at me. You are seriously thinking? Tell me the difference between these two.

Student: (Enginee) Engineering science means engineer with whatever science. (())(22:34)

Professor: Okay good. Engineers who use lot of science are called scientific engineers and scientists who use lot of engineering, yes engineering scientist.

Student: Sir, which one are you?

Professor: That is difference. I do not know. I do not know somewhere in between, okay. So that is why from the beginning I think you know why I told this one was lot of mathematical techniques are first used only by chemical engineers because you know civil engineering is most of the time empiricism. Even now because even though they beautifully calculate all the things using structures and all that, by the time it goes to that mason all the theory goes.

Whatever he believes he has to do, he will do it. So you cannot go and tell stress is different here strain is different here all that. You will say this fellow is mad and then he may throw us out also, okay. So that is why I have been telling also I think they use lot of factor of safety. And the other extreme is aerospace engineering, okay, where they cannot use much factor of safety. But in between we are somewhere but we are towards aero, okay.

Really I think you know how many beautiful plants have been constructed based on total theory. For example fluidized bed and all that unless you understand theory you cannot design, okay. You cannot design. You can run. You can put some solids and then send some gas till it fluidizes and then you can use it but scientifically running the plants, okay. That is why I just wanted to tell you all these equations are very tough to evaluate, okay.

And these constants evaluation is one of the really toughest jobs. I think good book for this also is chemical engineering kinetics by J M Smith. You heard of that Kavya? Used it? What is that book again tell me I will write here.

Student: Chemical engineering kinetics.

Professor: By whom?

Student: J M Smith.

Professor: Who is J M Smith by the way?

Student: J M Smith.

Professor: J M Smith. Has he written any other book?

Student: Unit operation (())(25:01)

Professor: That J M Smith is different. He is not J M Smith anyways. Yesterday you told one name.

Student: (())(25:10)

Professor: Smith and Van Ness. That Smith also is J M Smith. He is good in thermodynamics and then kinetics. Both are connected most of the time and that his book is very good book. Very good book taking the real industrial problems and solving whereas (())(25:26) book is like Indian movies. All fiction fantasy wonderful problems that is why we like it, okay. And unfortunately J M Smith book is like (())(25:38) movies.

No one will see because he again shows only the same hut and lighting will not be there and people will not have anytime clothes, okay. Only minimum clothes that are possible, okay. So this is the kind of movie she shows because anyway every day we are seeing that. Why should again we see the same movie? That is why people will not go. Whereas here I think you know Rajnikanth the moment he moves his hand like this hundred people flying, staying there for some time, no gravity, okay.

Gravity is also is hit by you know Rajnikanth. Gravity also is afraid of Rajnikanth that is why it will not allow people fall. They will stay there for some time. Only when he says like this they fall all of them. Wonderful fantasy you know, yes. That is the kind of fantasy what we have. I think similarly in (())(26:32) book he gives wonderful problems like that. I do not know you used (())(26:36) only right? The remaining little bit you used.

Student: Formulas.

Professor: Oh formulas, okay. I think there are wonderful books. Sherlock Holmes problem also is there in (())(26:47). Yes, fifth chapter and there is one (())(26:51). Yes who is a betting guy, okay. He bets and then he wants to win and all that. So there is a French and UK I think war that is naval fight, okay. That is between I think UK and who wins and all that. That comes in multiple reactions.

So that is why this book is very good. J M Smith I think if all of you know that that is fine. I do not have to write and it seems always J M Smith is very sad and also tell it seems my book no one uses, (())(27:31) book everyone uses, okay. That is why recently also someone was telling me always. But I think thermodynamics book is excellent book and this book also reality wise and particularly the catalytic part he has done wonderfully work, the catalyst chapter.

Not only catalyst chapter, most of the heterogeneous chapters are very good there in that book. So that is why please see that. I may also give some problems on that, okay good. So this is the one what we have and yesterday also I have been telling you that, okay, there are some more things here. This equation can you check whether it is according to the actual theory, equation 5.

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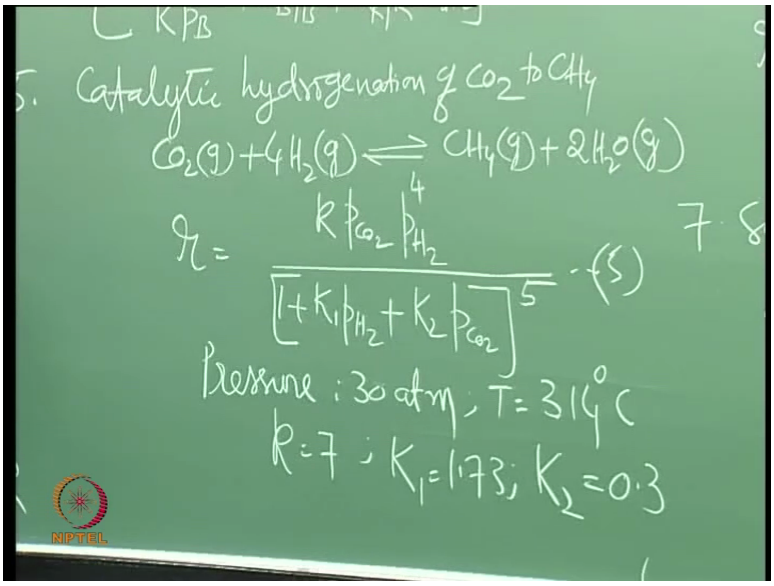

Professor: Only thing is it is not, it is not what?

Student: Reversible.

Professor: It is not reversible. It is only irreversible reaction even though we have shown it there the reverse.

Student: In equation 4 the denominator is square, right?

Professor: The denominator is?

Student: Square.

Professor: Square will not come there because that is what next one I just want to ask you because if square is there you will not get this kind of equation, okay. Today also you could have got similar one, okay. There will be simple plain K A, K B, K C or K 1 K 2 K 3 like that only. So that means it is not reaction control, okay. So like that we can get some ideas.

Some ideas we can get. In fact I told you the Nobel laureate Ertl I think three years back 2008 2009 2010. Maybe 2009 or 2008 he got a Nobel Prize for the surface chemistry catalytic reactions where he has given mechanisms for the you know what is that C O oxidation, C O to C O 2 and also ammonia. His ammonia model is fantastic. Ammonium model is very complicated because hydrogen when it goes and sits on the active side, it again dissociates. It becomes H plus or so.

I think I do not remember exactly. H dot or something they put. That entire mechanism he has given. Ertl, if someone is interested if you go to his website he has given all this data, all these models, okay. E R T L, I also have that paper with me. I think if you are interested I can send it to you. Otherwise that becomes e-pollution. Unnecessarily you have to store and then keep it there, okay. E R T L Ertl is his name.

We also wanted to invite him to our institute but I think trying because now we want to start now Nobel laureate lecture series. I am looking after that. I think you know we are not able to get. This February itself we are supposed to get one person but no one accepted. Of course we only started December end so that is why probably they are busy. So every year we would like to have two Noble laureates on the campus who will stay here at least three to five days, okay. They are busy.

I think 5 five they may not stay that is why we also attracting them telling that you know you can also come with your spouse. Yes, trip. So spouse means they may stay one more day or two more days, okay. Here so I think right now no one accepted but Ertl also we would like to invite him, okay, because I think that at least we thought that that will enthuse our students when I think the program is that the Noble laureate has to discuss even with students, okay.

And faculties separately and faculty students together and one general lecture we will invite even outsiders from the city. That is popular lecture. Popular lectures I think some people will give beautiful lectures, Nobel laureates. So that is why I think I really like that. Of course he is not a Nobel laureate. Stephen Hawking Brief History of Time, I think you have read it. Yes you read it? Yes I think after reading it definitely I changed my style of teaching, okay. In the sense that anything can be described in words like a story.

He is like Denbigh, the way he writes. Wonderful simple examples and the way he expresses, okay, it is fantastic. I think I read Brief History of Time at least six or seven times and it is like a novel. The moment you start you cannot stop till you finish it, so thrilling. Yes second book Grand Design also I read. And before that that also I have right now. I have to read that now. So I think you know that kind of great people when you the read definitely we change our attitude of how to present things.

And another person who changed me was you know he would have not known but by observing, okay. There was one person I think he has authority in the world on heat exchanges, Schlunder from Germany. Schlunder, he is excellent in heat transfer and mass transfer and he has got this big book on heat exchange and design, okay. He came here and then he started giving lectures for I think on drying one week. We also attended. That was long time back. I think maybe 15 years back or so. We attended.

Actually that was for industry where in Savera hotel. So in Savera hotel they have conducted this course for three days for industry. So I think he came here first and then he was with us for some time and then he was also casually telling why do not you also come and sit. So we went. In fact myself and professor A R Balakrishnan and also another two people. Professor Verma that was another person, professor Subbarao, these two people retired.

Four and one more I think yes mechanical engineering Professor Srinivas Murthy was there. Now he is (())(33:53) professor. He retired last year. So all five of us went. Really I loved that the way he was explaining. He is German and he was speaking English. I think the three days he has not uttered not even by mistake one German word. That is the kind of control he has on the subject, okay. That means you know the concentration. Otherwise if I go to Delhi now and then try to speak Hindi, Tamil words with come, okay.

And I know also Tamil. That is also there, okay. So that kind of thing we have you know that concentration is not that much for me. I am telling myself. So he was always trying to take one single particle and then trying to find out the drying kinetics for one single particle and then extend to larger cases. Very small books in Germany has written heat and mass transfer books not more than 70, maximum 100 pages. I have that books with me.

The way he explains things and till then I was thinking that I think drying experiment we know only taking a pan, hanging it and then trying to find out what is the drying rate curve for single point particles. And then this single particle is extended for it can be beautiful exchange you know pepper drying in Kerala. That is one of the biggest problems. I mean we pray solar system and sun and then we just try to do the solar drying. I do not know now also solar drying is done or technically they are drying now.

Yes, so in this pepper drying very interesting thing is that if you dry too much in a dryer you know the pepper oil also will evaporate and he has shown mathematically with single particle and all that how to dry without losing much pepper oil. And this is true for not only pepper. You have that clove you know. Yes so that drying all that, so wonderful. It is a really fantastic person and suddenly I met him in Germany when I went last time I think that is 2003. He came to that Institute for giving a lecture.

See he was retired but still very active. Then I asked him sir how are you, you may not remember me but I think I attended your course. You have to come to IIT Madras. IIT Madras he remembers and then I was asking sir what you are currently working on. He now says that drying is very interesting phenomena. You see last 30-40 years only drying for him, okay. Apart from general heat and mass transfer and then he says that now when you take a porous particle and it is drying, it seems inside that pores you have convection.

What is the size of the pore and then you know you can imagine that what kind of convection you will have in that pore and that it seems influences the drying rate. Now I am working trying to develop a theory for convection within the pores. See that interest I say. That is the passion for them. And when compared to them where are we? In our country we do not have that passion. We do rituals. From children onwards we know how to do rituals, correct?

Without understanding going to temple and breaking coconut and if someone ask why are you breaking coconut I do not know because it breaks I am breaking, okay. So that kind of arguments you know like that. We do not know mother father. Mother father we know. Grandfather grandmother and all that we know but every time we go and put something to them even after death and we do not know the logic. So like that you know our mind is never allowed to think, allowed to grow, allowed to question.

This is the problem. That is why we are not able to create good you know academicians in this country because from the beginning everything you are told I know even when you are writing the examination mother and father tell you how to write the examination. And they will choose our subjects. They will choose our food. They will choose our clothes, okay. And they will tell us how to walk, how to talk, everything and you become clones of them because original thinking is not there.

That is why you see even the cow or buffalo after the birth that calf will never stay with that. Only till milking period that is all. After the milk is over this is separate, that is separate. Afterwards it cannot even recognise I do not know whether it recognises or not mother father. We should also be like that. After milking throw that fellow away or throw that girl away. So they have to come on their own. When they are coming on their own then they become something. No it is too much.

That is the reason I think you know that freedom is not there for mind that is why we are not able to do anything. Yesterday there was a good discussion on NDTV also about I think what is wrong with Indian science or something. I think that is the title. Yes, I think it is everything starting from childhood onwards. It seems after Ram there is no Nobel Prize in this country, okay. I mean people who went abroad they got it. That is different. They are the citizens there, okay, Indians.

One person was telling I think he is very good. I think he may be journalist. He was telling that it seems only in our country Ram and that spectrum has never been commercialized. It seems all other countries they have commercialized, they have earnt lot of money because many equipment was developed based on that and we did not do that. We do not know how to do that also, okay. And again same thing I think you know what I told also people were telling that you know we have to give freedom to our children.

We have to find out their talent and allow them to you know go in that direction. But no, for everyone for us our family always either engineer or doctor. As if there is nothing else existing in this world, correct? If both of them are not there then something else, okay. That is why that minister seems to be intelligent person. I think I forgot his name. Science and Technology minister. Not then (())(40:11) someone else maybe one science minister. He was talking some Kumar I think or something.

Yes, he was telling the same thing you know. We never allow our children to grow and I think this has to change a lot in the country. And he was telling that there is a lot of money and now it seems only point 83 percent GDP we are using for research which is very small, okay. And China is using 2 or something like that yes. And we also want to copy China and then you know we are also trying to use next plan 2 percent GDP. That is lots of money. Even now we have lots of money but where is a passion? Passion is not there but money is there. Yes?

Student: Increase the stipends.

Professor: Yes, I think you know desperately I am trying to get increase of stipend particularly for MS. PhD they have increased already almost 18-20000, okay. 20000 is a good amount in hostel, okay.

Student: 8000 is not.

Professor: 8000 is not but I think MHRD is not willing to increase that. Not now, last two years desperately I am trying. Even two weeks back I talked to director when he was going to Delhi, sir please to talk to them. But unfortunately what happened was only MS is only in IIT

Madras and IIT Delhi, it is not a general problem of all IITs. That is why they are not increasing. They treat this one as another M Tech equivalent so that is why 8000-8000 equivalence is there, okay.

So that is why that passion you know sometimes also I talk about this, the reason is, where is the passion for you? After coming here would you like you know Anurag, anytime after coming here your thought that you want to be an excellent chemical engineer? Tell me very frankly. Why sometimes?

Student: I feel like it.

Professor: When do you get motivation?

Student: When I like something and I am reading something. When I am reading something and I like it.

Professor: You see life is not that every day is thrilling. Some days it will be boring and some days it will be thrilling. But only on the day when you are thrilled then if you say that you know I like it then the next moment if you are not writing exam some other subject you say I hate this subject because you have not written the exam. So that is not the one. Whether you are able to do well or not well, passion remains as passion. That kind of passion I am asking. I do not think even 1 percent of all of Indians I am talking, I am not talking about you, we have that passion.

But whereas that passion is there for movie actors, artist and players like again cricket is up and down I think but again tennis players that passion is there. You can see that musicians. You know Sania Mirza how many hours per day she practices? You do not know. Go and see some TV sometime back about her it came. It seems 7 hours 8 hours also she practices every day. If you read 7 hours 8 hours every day, my God I think you know you can get everywhere yes, okay.

Do you do that? We never, 8 minutes is very long time for us to read per day. 8 minutes I can tell you with concentration, okay. Chess players for example, how many hours they play? And musicians and you would have seen no musicians like that you know Bhimsen Joshi that kind of people. They come to stage and then just sit down, okay. They just look like that and then go to that world that is all. They close the eyes. They forget everything and then you know they will be singing days, months, years also if you do not stop them.

That is the passion. Where is the passion for you to sit down before CRE book and then till I come and pull it out you are still there before CRE book, impossible. So that is why I like that movie Avatar. Avatar all of you have seen but I saw some good things there. You know Abhinav, Avatar you saw? What did you like in that picture? Again passion is not there. Even for movies you should have passion.

One thing I liked there is you know thus pigtail, USB port yes, that pigtail taking and then putting into whatever they want you know either horse or the tree, okay. Or the bird. Bird also automatically you know join together that bond. That is fantastic for me. I mean I would like to do that you know. There is a book called (())(45:01), very tough book you know chemical reaction engineering book. Introduction to chemical reactor analysis. That book is very tough.

If I have that I would like to go and then put it there, okay, because so that I will become part of it. That is what you have to do. The moment you entered IIT if you are a chemical engineer we should have chemical engineering as a port, okay. All of you should come and then take this and then attach there. Then you will become part of it. Then only it is possible. That is the kind of passion. That is why I like really that movie you know fantastic. I do not know how this fellow got that idea James Cameroon.

Wonderful idea he got, yes because that much time is required you know for that passion you know because another 10 years also you would have worked for that and also he said that you know the technology was not enough for that movie to be taken when he first thought about that. That is why he waited. Do we have that kind of ideas about thermodynamics, about CRE or about mass transfer anything? I mean I have this problem I would like to solve this, okay. And in the class that fellow lousily explain so let me solve this.

That kind of passion do you have? No, absolutely not. Happily taking you know text book before one night then afterwards writing the examination. Next day feel as if you are a total stranger for that subject. No, all of students, it is not only you or me you know. All the students I am telling, okay. So that is why I think at least that passion I think I do not know how many people I have changed but I think I have been telling this many times, okay. But they enjoy and then go out and then again forget, okay.

We will stop here and then in the next class we will have this step 1 and step 2 mass transfer step, okay. Film control or film transfer and diffusion control both of them we will take and then see how to develop the equations for that and combining those equations with this equation, okay.

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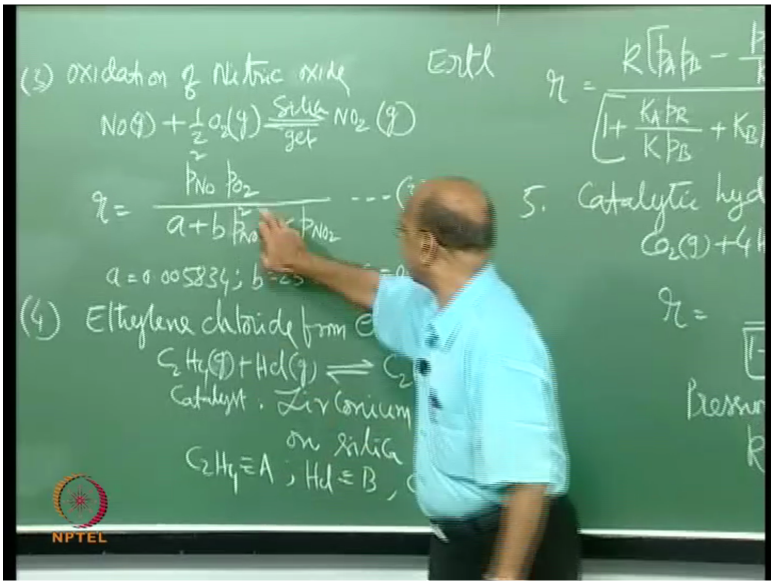

This is the equation. This equation also called intrinsic rate equation because there is no mass transfer or heat transfer coming into picture, okay. So now using this intrinsic equation how do we develop equations if mass transfers are controlling. Two mass transfer steps, okay. That we will do next class. Good, thank you.