Fundamentals Of Combustion – (Part 1)

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Lecture – 19
Chemical and reaction kinetics

So, let us start this lecture with the thought process.

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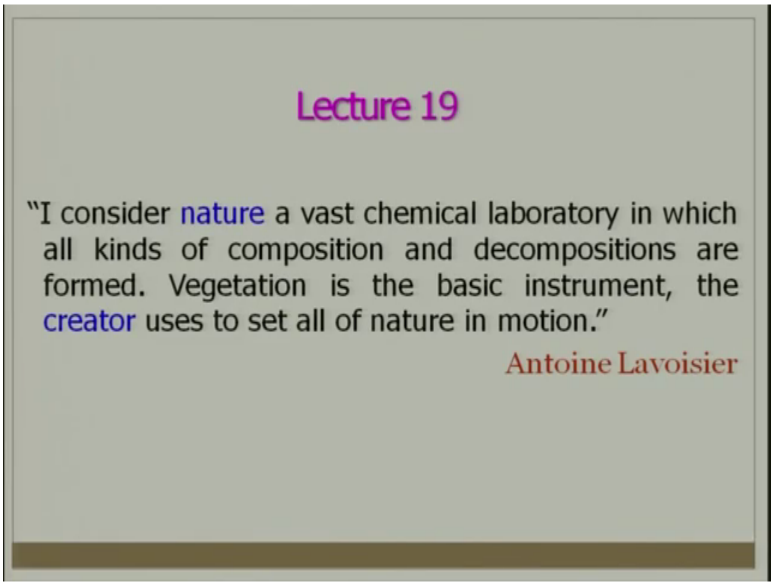

Given by; Antoine Lavoisier which is a great chemistry "I consider nature a vast chemical laboratory in which all kinds of composition and decompositions are formed. Vegetation is the basic instrument, the creator uses to set all of natures in motion."

Actually similar statement particularly last one is being talked about in our literature, in people may not be aware about our scripture last statement is similar, what Lavoisier has talked about ok? And also they look at it. So, if you look at in last few lecture we discuss about how to handle the chemical equilibrium in other words how to estimate the.

Chemical equilibrium along with adiabatic temperature right and if you consider that, there also we looked at the chemical reactions right. Today, we will be learning the basically chemistry of the combustion chemical reactions, how to handle those things will be doing if you look at that in equilibrium, what we did?

We basically looked at extent of the chemical reaction, what is taking place right? Yes or no, we are not bother about the, what will be the rate of reactions right? We looked at only the extent of which the; it will be the reaction will be proceeding for that also we consider the chemical reactions and in combustion therefore, we will have to look at extent of rate of chemical reactions because why we will do that we need to.

Find out what is the heat release rate? Right. So, for that we will have to consider the chemical reaction; let us consider few reactions for example, two moles of hydrogen reacting with one mole of oxygen going to the product.

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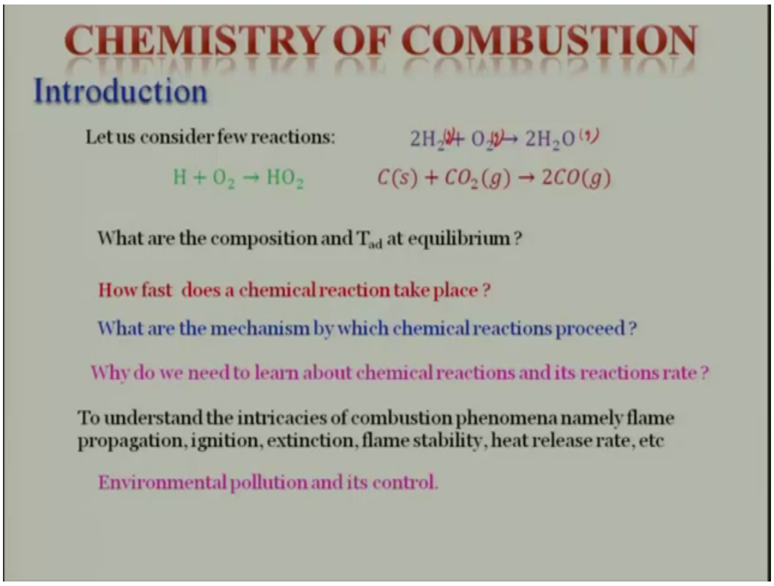

Two moles of water right and here what we are considering we are considering basically all this are gas right we are considering of course, the water can be gas it can be also liquid we have already discussed that and this is the reaction whether it possible in nature or not that is a questionable right is it really possible this reaction to occur right that is a question we need to ask.

Why not the question might be coming in your mind and let us look at a H is reacting with oxygen is going to the H O 2 right, and there might be another reaction which will be considering the carbon reacting with carbon dioxide going to the 2 C O is a very nice thing you know what you will do we are having. So, much of carbon dioxide in the air like we have increasing the carbon dioxide in every year tons of carbon dioxide why every year every day tons of carbon dioxide do emit then, why do not you take it out.

And then react with that you will get a C O; C O is carbon the monoxide which is a fuel ok. We can bound the C O right and get some heat, but that is not that easy so, but; however, we do the express you. So, keep in mind the C is the solid and g is the gas sorry carbon dioxide is gas the carbon is in solid form; that means, this the one kind of reactions. So, therefore, we need to find out what are the kinds of reaction is taking place in a chemical reactions right in a during combustion what are the kinds of chemical reaction taking place we need to also.

Understand also aware; what is happening? We have learned that, what are chemical compositions and adiabatic temperature at equilibrium. We already did with how to handle that right we need to also look at how fast a chemical reaction takes place, and what will be the overall rate at which the reaction will be taking place that might be several reaction which is taking place simultaneously right. And what are the mechanism by which chemical reaction takes place right for example, two moles of hydrogen reacting with one moles of oxygen going to the two moles of water is it really occurring or it is not possible it will be going to series of chemical reactions.

And the end you know some product water will be coming and some other (Refer Time: 05:18) combustion will be there you have already seen in chemical compositions whenever we are determining at the equilibrium, but there we consider arbitrary chemical reactions we did not really look at it what is happening whether it is happening or not right we only looked at s two is you know dissociated to H O 2 is dissociated into O right. We are not bother about whether that is; possible or not, but in mechanism you need to bother about what are the steps will be which will be important at when pressure is 2 atmospheric pressure which will be important at some other thing at particular temperature, what will be you know like which reaction will be important those things we need to.

Bother about and also mechanism right. So, then question arise is we need to also learn about chemical reaction and it is reaction rate, because the rate is very important as I told the heat release rate is very; important to know how much heat being released how much not being it release; and what is the rate? If it is rate of reaction is very high then it may lead to explosion right it may be un-control because what we need in combustion is a control release of heat. If it is un-control it will be explosion ok.

So, explosion has to avoided and also the it is ramification. Beside, this very important point is that chemical kinetics of the chemical reactions is very important to look at the propagation velocity or propagation of flame (Refer Time: 06:58) you might be knowing in a fire any of you from the village, rural areas; you know this tell the house they are using the fire one place fire has occurring it will be spread like a wild fire you know like it will be becoming like very wild like the way today face book is creating problems of you know spreading the rumors. Are you getting? So similarly the fire were just moving you know.

So, and then we need to know. And also whether it will be united or not whether it will be extinction will occurring in that; suppose I want to exiting with a fire and that will be dictated by the chemical reaction and some flame stability heat release rates and several others things are governed by the chemical reactions and it release rates right.

So, therefore, those things we need to predict and also understand for that we need to learn the chemistry of part right chemical reactions we need to learn otherwise we cannot handle it will be like your IC engines research a black box you know like: input and output. They do not what is happening inside you your our about in tern piston.

Engines right; they do some research they are not bother what is happening? They will just major some graphs things right and they do not know. In the some cases we do particularly engineering, but you want look at the understanding are the some phenomenon, then you need to get into the chemistry.

So, beside this another very important point is the today we are phasing the problem of environmental pollution. And we need to control, for that we need to understand the mechanism how to intervene. So, that undesirable pollutant should not be formed. So, that is also another challenge we still need to look at therefore, we need to look at chemical you know reactions and rate. And when you talk about that, we basically look at a science that is the physical chemistry part.

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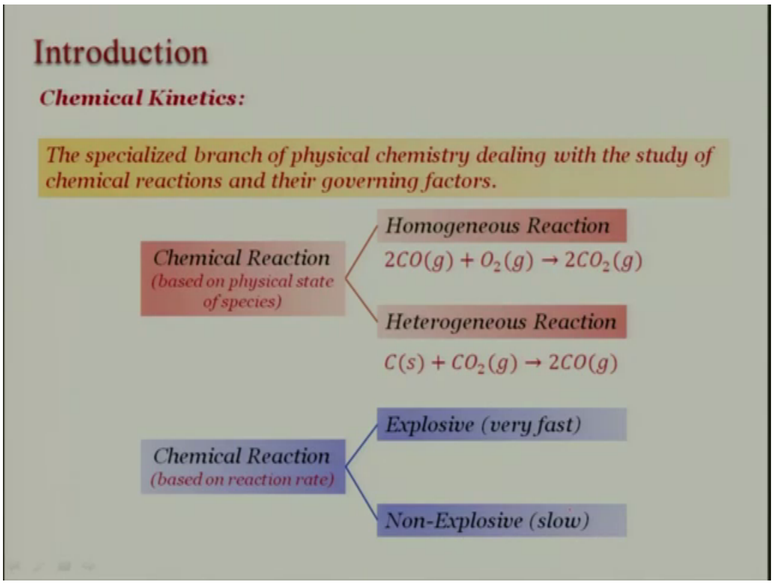

Right, which is very important and that specialized branch of physical chemistry dealing with the study of chemical reactions and their governing factors you know which is known as chemical kinetics. So, what will be dealing with in next few lectures will be basically about the chemical kinetics right. So, for that if you look at the chemical reactions can be broadly divided into two categories: based on the physical state of the species that is; homogeneous reaction and heterogeneous reaction.

Homogeneous reaction means where the state will be same for all the reactant and species in a reactions. For example, two moles of carbon monoxide is reacting with one mole of oxygen going to two moles of carbon dioxide. If you recall this reaction we had seen in the earlier in the just opposite way right. So, all this participating species are in gas space therefore, we call it homogeneous reaction.

And heterogeneous reaction is the one like where one of them will be solid or others will be gas or they will be at a different state different physical state. For example, one mole of carbon which is at a solid state reacting with the carbon dioxide going to the two moles of carbon monoxide gas right this is known as heterogeneous reaction and heterogeneous reaction do occur, but particularly when you are handling the solid fuel and some extent to liquid fuel right, but most of the reactions whatever will be taking place in gas face right.

And as I told the chemical reactions can be broadly again divided into two categories: one is explosive reaction and other is non explosive reaction based on the reaction rate. If it is very fast, then we call it as a explosive or explosion will occur therefore, we call it as explosive like you if you look at most of the explosives use in the war fares and also blasting of mountains right and other places, wherever the blasting required you know you do the terrorist they use explosive ok.

So, those are basically fast reactions which is occurring very very fast and non explosive do not consider it slow I have written slow no it is a moderate right. So, as compare to this explosive this will be slow, but it will be definitely not that slow ok, it will be good enough for this non explosive reaction. And sometimes a you know you will be talking about little later on like deflagrations and detonation basically detonation will be explosive in nature deflagrations will be combustion.

General combustion; what we will be dealing with? So, let us look at now.

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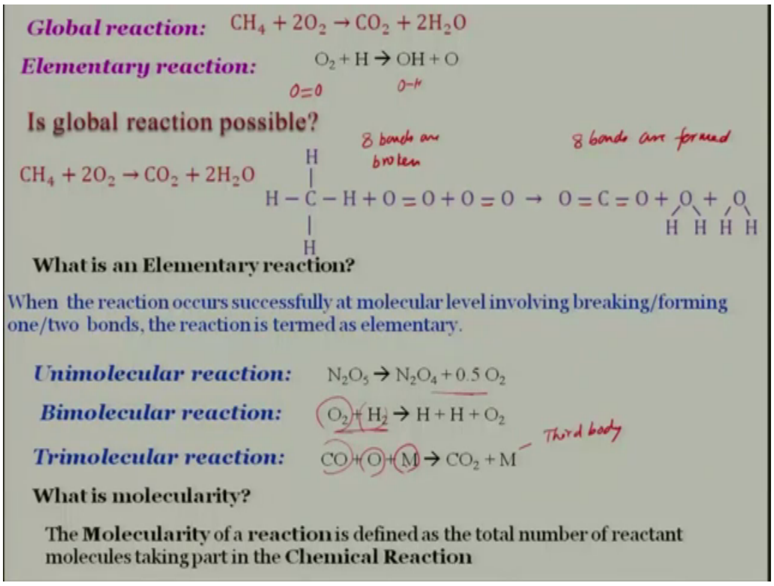

Let us say on mole of methane is reacting with two moles of oxygen going to the one mole of carbon dioxide and two moles of water. Let us consider another reaction oxygen reacting with H going to O H plus O. Now these reactions, if you look at these reactions the first reactions right methane and oxygen, what you call?

We call it as a global reactions and O 2 when reacting with H going to the O H plus O, this we call it as a elementary reaction right. Why you call global reactions? Why you call elementary reactions? We will see. Let us first consider the global reactions. And ask a question whether it is really possible to have this right for that let us consider.

This one like this reaction and methane is having how many bonds this is total four bonds and oxygen will be basically double bond right and carbon dioxide also will be having double bond yes or no; that means, if you look at on the reactant side; during this reaction what is happening; that means, this four bonds in the methane are broken right.

So, also in the oxygen this four bonds are broken; that means, on the reactant sides; how many bonds are broken? 8; Yes or no? And in the carbon in the product side carbon dioxide these are the total four bonds this also 1 2, 1 2 this are total is 4 bonds; that means, 8 bonds are broken if you look at this side is 8 bonds are broken right; reactant side and these are 8 bonds are formed yes or no right; that means, there will be bond total 16 events will be taking.

Place is it really possible? You imagine you know this room is mixed with methane and oxygen right to start with you raise some temperature. So, that it will be already mix with some reaction is taking place right; that means, this 8 bonds are to be broken is it possible; that means, you know molecular will be moving that moving they suite in a simultaneously; how it will break?

You can think of few collisions ok, they will be colliding then it will be having enough energy to that and also it will be collision will be taking place at proper orientation yes; suppose there is coming and going back like you collide you know you meet some people and then forget; do get any exchange of anything no right. Similarly molecular will come and closer kiss each other and go away means touch each other right.

So, therefore, right nothing will happen, they like today we are having friendship hi, bye and fly right. So, there is no friendship as well. So, no interactions; so similarly is not really possible to have 8 bonds are to be broken and 8 bonds are to be formed simultaneously. Is it possible? That is not really possible it is impossible right. So, therefore, it is not really possible to have this reaction taking place in this way; that means, this only a representative of what is happening?.

That we call it as a global reaction; are you getting? but; however, if you take some elementary reaction for example, this like what will happening here if you look at O O will be O and O right O 2; that means, this can be broken and two bonds are broken. If you look at O is coming to the O H. This another bond; that means, and one bond is formed here O H right one bond is formed.

Which is possible, but 8 bonds are formed 8 bonds are broken is impossible ok. Are you getting? So, therefore, this is known as elementary reactions, when the reaction occur successfully at a molecular level involving breaking and forming of one or two bonds, because you know this is a kind of a two molecules are involved that might be tri-molecule that might be 2-3 three bonds are broken right; may be 1 or 2 bonds either breaking or forming.

The reaction is termed as elementary; are you getting my point? That means, elementary reactions are lightly to be formed, but whereas, the global reaction will never formed this is all a what we use for our own convenient. Are you getting? Is that clear to you if you imagine that in molecules are?

Moving and then there are interacting they are colliding you know then you can think this looks to be right fine. So, now, let us consider N 2 O 5 is going to N 2 O 4 and half O 2 of course, this may not be possible, but I am just writing and O 2 plus H 2 going to H plus H plus O 2, basically this is 2 H right; plus O 2. And I can say that there is a C O carbon monoxide is reacting with O with a M; M is any species which is not participating M can be nitrogen ok. And going to C O 2 and nitrogen is an M example is M this is third body is known as basically third body it can be any inert which is not participating in that.

Reaction that is known as third body; Now in this reaction I want to talk about molecularity; that means, what is the molecularity then you must have studied this thing in your plus 2 ok. You might have forgotten by this time, but you must be knowing molecularity is basically how many reactants are participating in the chemical reactions right; that means, molecularity of reaction is defined as the total number of reactant total number of reactant molecules taking part in chemical reaction.

If you look at this equation what it would be molecularity, it will be one or you can say unimolecular reaction yes or no. And the second one is two moleculars are there this is one right and this is another two this is a bimolecular reactions right if you look at this is the three molecules are there this is 1, this is 1, this is 1. So, 3 this is known as trimolecularity you can say molecularity is 3 is that clear right.

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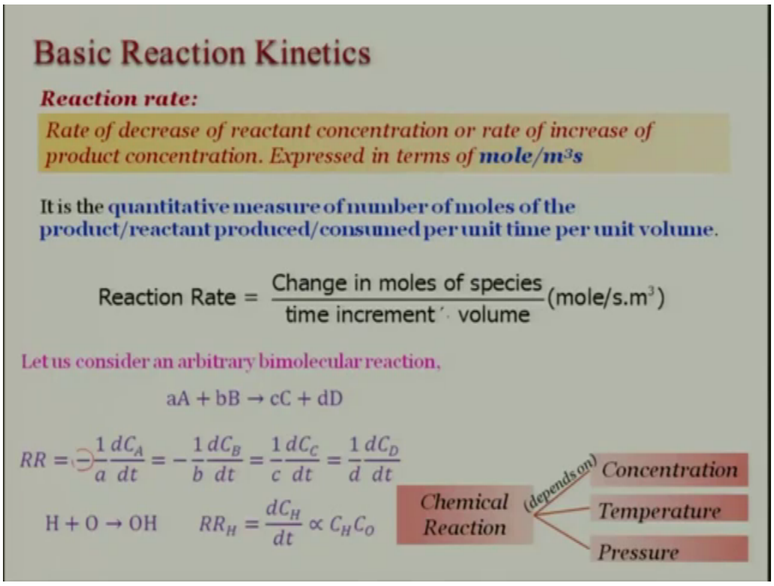

Now, let us look at basic reaction kinetics and when you talk about that we will have to look at reaction rate. What do you mean by this reaction rate? We know that rate of decrease of reactant concentration or rate of increase of product concentration right or vice versa right; is basically and which is express in terms of moles per meter cube second right is the unit what you can use and this you can; in other words it is the quantitative measure of number of moles of product reactant whether it may be produced or it may be consumed per unit time per unit volume that is the meaning basically right and reaction rate.

I can write down change in moles of species divided by time increment per unit volume right per unit volume. And there is mole per meter cube second. Let us consider an arbitrary reaction right a moles of species A going to the b moles of species B going to the product c moles of C and d moles of D right. So, if I want to write down this reaction rate right I can say that 1 over a.

Divided by d C a by d t is equal to minus 1 over b divided by d C B by d t right. How we are writing this? Basically by the law of mass action; we have already studied and this is minus sign indicates what? This is basically the structure of species therefore, it is negative right the in other words it is getting consumed the C a the concentration you know decrease will be negative, because initially it will be some amount then it get consumed this thing and this basically you know for the product C d C by d t 1 over c is equal to 1 over d d C d by d t and this is positive, because it is being produced right and if I consider H plus O right O H, what I will do? I can write down the reaction rate of H is equal to d C h by d t which is proportional to what C H and C O right so; that means, this reaction rate is basically function of concentration right.

Now we know the reaction rate also will be dependent on temperature it will be dependent also on the pressure right, but how it is; So, because here this is showing only the concentration of the participating species.

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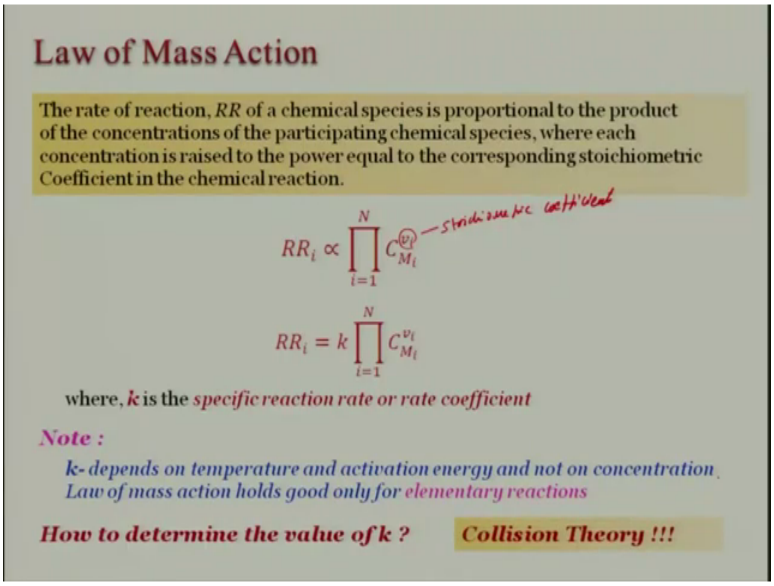

We will see that for that of course, we will have to look at the law off mass action it says the rate of reactions of a chemical species is proportional to the product of concentrations of the participating chemical species where each concentration is raised to the power equal to the corresponding stoichiometric coefficient in a chemical reaction right that we have already seen.

And for that I can write down the reaction rate of i species is proportional product of C M i v i where i is equal to 1 to N number of species whatever you can say that right and that is equal to r i is equal to k into product of all these species and these are stoichiometric coefficient these are stoichiometric coefficients right corresponding to the right and what is this k? K is basically specific reaction rate or the rate coefficient ok.

And k depends on temperature of course, activation energy not on the concentration right and also their coeff[icient] stoichiometric coefficient because keep in mind that this is law of mass action holds good for elementary reaction only. Now, we need to basically determine this k right, is not it how we will do that for that we will have to invoke the collision theory ok. And also right we will have to learn that about in the next lecture that is the and before doing getting into the collision theory we will have to discuss about also the kinetic theory of gases and before that I like to look at how to write these reactions compactly right and with this we will stop over.

Thank you very much.