Fundamentals Of Combustion (Part 1) Dr. D. P. Mishra Department of Aerospace Engineering Indian Institute of Technology, Kanpur

Lecture – 22 Collision theory (Contd.)

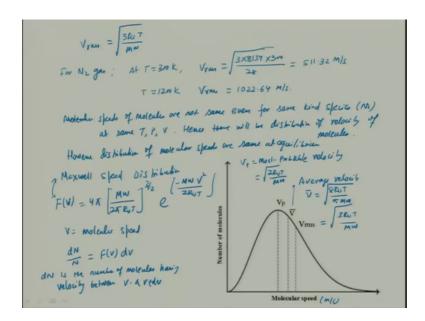
Let us start this lecture with a thought process

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Lecture 22 Belief of being a divine person is the ignition switch for realizingg your potential lying dormant in your mind. D. P. Mishra

Belief of being divine person is the ignition switch for realizing your potential lying dormant in your mind. So, coming back to that like what I was telling that in the last lecture we derived very simple way the root mean square velocity of the molecule, right considering the kinetic theory of gases and now, in that case we did not really consider the how the distribution of particle will be will be doing today. But before taking of that I want to you know continue from the last that we had derived relationship between for the V rms, right.

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If you recall that V rms is equal to 3 R u T divided by molecular weight root over, right. Yes or no? So, now if you look at we will take an example just to have a feel what will be the velocity. I had asked this question in the last lecture, right what will be the order of velocity?

Let us consider simple molecule right for nitrogen gas, right and for that we need to find out right let consider the 300 Kelvin right. At 300 Kelvin what will be V rms right this will be 3 into R u; R u is your universal gas constant. So, I can use 8134 into temperature 300 divided by molecular weight for the nitrogen is 28, ok. So, if we use your calculator and find out that value will be 511.32 meter per second.

If you look at the molecule nitrogen molecule is moving it a very high velocity, right even higher than the speed of sound is not it? Such a high velocity it is moving and of course, this is a very simple (Refer Time: 02:41) theory and of course, if you take concededly it will different than it may be layer, but that will be that order it would not change, order of magnitude will not change, ok. It would not be 50 meter per second now if I increase this temperature to something let us say 1200 Kelvin what will be V rms, what it will be? Just multiply by 2, right and that will come 1022.64 meter per second because a everything is same here just you know increase in temperature by 4 times. So, square root of 4 is 2 therefore, it will be 2, that is all.

Now, if you look at the temperature is higher the velocity will becoming much higher that is a reason why you know at high temperature some reactions may occur at low temperature reaction will be very very reaction will be occur, but very very minimal because the collision would not be there the it would not be moving at high velocity, right. So, now, till now what we have done we have consider the particles of course, number of particles per unit volume like number densities and other things, but in this case what we have assume, the velocity will be isotropic you know like that kind of things we have assumed, right and it will be that all particle will be moving with the some velocity, yes or no? But, is it possible it is not possible, right.

So, why it is not possible for example, let us say only nitrogen gas is there container, but is it possible each particle will moving with the same velocity?

Student: No.

No. Even in the same direction no why because when there is a series of mole collision is taking place, right, in a even in proper orientation that lead to a higher velocity. Let us say there is a head on collision what will happen head on means two molecule are coming and colliding head to head, right. We do head on collision in our interaction with the people, then there will be a quarrel that might be some problem you know like [FL] right, exchange of word will get into the physical right. So, head on collision, head on collision means both will be coming to stand steel that might be 0 velocity, right or may be small velocity.

So, therefore, there will be wide range of velocities each molecule will be having even though it is at low temperature it is at the with the same molecule let us say for nitrogen right the means molecular speed are not same, right or I can write down speeds of molecule again speeds of molecules are not same even for same kind of species or molecules, right let us say nitrogen at same temperature, pressure and same volume everything same. However, there will be a distribution, right.

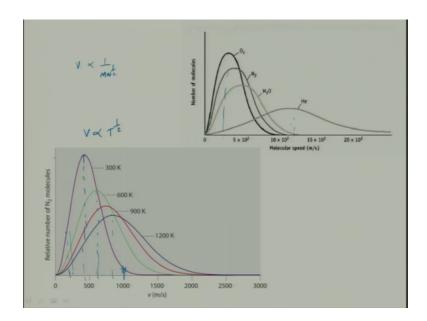
Hence, there will be distribution of velocity of molecules right and if you look at statistical way right one can see keep in, but however, keep in that that molecular speed at equilibrium is distribution is steady, right. Distribution would not vary, distribution vary then there will be problem is not it? That means, the molecular speed at equilibrium right distribution of molecular speed at equilibrium is same. However, distribution of molecular speeds are same at equilibrium. Of course, we are considering equilibrium case and other things.

So, and these distribution is basically given by the Maxwell right and that is known as I will be not getting into detail, but I will just mentioning that the Maxwell speed distribution that will be this is F right V; V is the velocity 4 pi molecular weight 2 pi R u T e molecular weight V square divided by 2 r u t is equal to V square, keep in mind that this V is the molecular speed.

Now, when you plot that thing right so, that will be basically number density right that will be dN by N this is change in the molecules, right what you call number density by the number density, that means, volume-volume cancel it out, right will be equal to what is that F V into dV and this is what is this dN? dN is the number of molecules having velocity between V and V and V plus dV that basically dV in between the what is that like in between right.

So, now, if you plot this thing will be number of molecules vertical these things like and molecular speed this will be meter per second right you can say and you will see that this is having V p. What is this V p? V p is the most probable velocity. V p is the most probable velocity and from this you can really calculate V p will be equal to 2 R u T and m w and this is V is basically average velocity, right V thus will be 8 R u T pi m w and V rms already we have derived this root mean square velocity is equal to 3 R u T by m w. Keep in mind that R u is your universal gas constant and T of course, the temperature and m w is the molecular weight, right.

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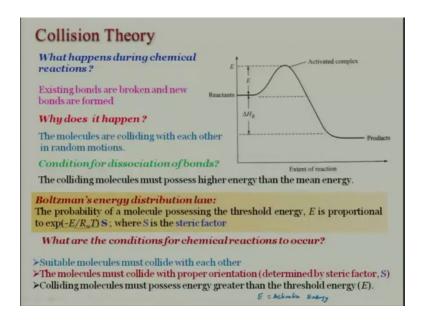


Let us say this thing relative number of nitrogen molecules we have considered at three different temperature, that means, if I will consider that 300 Kelvin, right of one temperature, we will find the velocity is here in this range if you look at is something in this range it will be something may be 400 50 kind of temperature is coming at that you know it is having higher what number density right, but at the lower temperature it will be low and then at the temperature you know sorry the velocity of the molecules will be lower at the you know less number of molecules sorry less number of molecule will be occurring in this lower temperature and also lower velocity range right velocity range and if you go to higher velocity range the number of particles will be very low, right.

Let us say this temperature the number of particle will be very very low, right, are you getting, but as it is temperature increases if you look at the number density for particular temperature it became you know higher here right again velocity will be higher, let us say something 600 meter per second as the temperature increases, right. What happen the probable velocity is also increasing right big velocity values then these will thing range if you look at more number of particles are coming and that is true also if you consider other diagram that we have seen na that V is basically whether it is a average velocity or probable velocity or the r m s velocity is proportional to 1 over the molecular rate half now this corresponding whatever discussing area, it is T half power 2 right the molecular weight means basically mass.

So, oxygen the molecular rate is what we call higher right. So, the you will get the molecular speed is very low and number density here it is higher where number of particles more number of particles will be having lower velocity. Of course, there will be certain high range of the certain molecules will be having higher molecular speed, but those are numbers are very less. Similarly, nitrogen and then water and helium; helium is a very lighter gas therefore; it is particles you know probable of the more number of particles will be having higher velocity, right.

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Now, let us look at what is happening in the collision theory because this we have talked about kinetic theory of gases. Now, if you re call what happens really during the chemical reactions is very simple I have emphasize several times, that is, there will be formation of new bonds and breaking of old bonds, right. Of course, you know it does happen, right in our interaction, is not it? You may keep in memory, but something will be there.

So, if it is happening question arise is why does it happen because there will be collision, there will be interaction between the molecules right, molecules will be colliding each other in a random motions right and even if they are colliding each other like is it like a there will be some reaction taking place it will be taking place need not to be there is a you know the certain molecules will be have certain higher energy right such that it can

lead to right breaking of bonds during collision and it should be properly collide it should be collided properly you know orientation at proper orientation it should be collide, right.

So, that means, you know you will have to look at that condition for dissociation of bonds that as I told the colliding molecule must possess higher energy than the mean energy, right. For example, you know I am talking it will be having some effect in your mind right provided you know a person is having little higher label. So, similar way there will be not that all interaction will lead to the reaction or all collision need be reaction there will be depend on what is the energy level you are having right. Leaders are those who are having higher energy level higher better ideas and other things, right similar manner.

So, that is what you call like you know if you look at reactants will be there, but here it need not to be, but there will be some higher you know what you call energy level that we call it as a activation energy right and this is of course, will be getting to a higher energy level and then the reaction will be occurring then after that energy level come back. So, therefore, get into the product and keep in mind that this is the activated complex will be discussing little bit about activated complex little later on.

And, whenever this collision is taking place then we need to look at the what is the probability of a molecule possessing certain amount of threshold of energy that we call it basically activation energy right and this probability is proportional to exponential E R u T and this E is your activation energy if you look at this kind of term we saw in the what you call velo speed distribution Maxwell speed distribution right and also multiplied by the S. S is your steric factor that will tell you whether it has proper oriented or it is collided at proper orientation or not with proper orientation or not, right.

So, just to summarize what are the condition of chemical reactions to occur if you look at the suitable molecules must collide with each other right suitable molecules should collide with each other, right and molecules must collide with proper orientation and that will be a basically quantified by a steric factor and colliding molecule must possess energy greater than the threshold energy and E we call it as a activation energy this E is basically known as e is the activation energy. Of course, this is about what we call in collision theory what we are going to do is basically look at how we can relate this thing to the reaction rate, right that is the basic idea ok.

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$$\frac{d(a)}{dt} = \begin{bmatrix} NS & g'(bllifius) & frontility of species of s$$

So, having same this thing let us say there is a reaction by molecular reaction we are considering, let us consider A is reacting with B going to C plus D and if you look at I want to find out basically what is that d C a by dt right. So, if you look at from the collision point of view what I will have to look at? I will have to find out is equal to right of course, this will be a minus because it is destroyed right is consumed. Therefore, it will be a minus I can say this is number of collisions taking place right per unit volume per unit time that means, ok.

And then I will have to say that then what is the probability of successful collision during reaction or for a reaction to take place that is probability of successful collisions for a reaction to happen right into the what you call number of moles of a species right a you can say kilo mole of species a right by the number of molecules number of a molecules makes sense, right.

But, if you look at this first term what is that this is basically collision frequency per what per volume see if I say this is Z let us say A right or A by this will be volume if I say all the A molecule are taking place of course, it do not occur right, but let us consider that or I can consider B right AB, A between B colliding right per this is basically collision frequency.

Frequency means number of collisions per unit time, right into V. V is the volume into probability what is that we have already seen that is E by R u T into steric factor S is the

steric factor into what is this term? This is nothing, but your AN. AN is your Avogadro number make sense. Now, I will have to find out this collision frequency because this I can take from what you call Maxwell distribution, right and this I can take now we will have to determine the collision frequency, right.

I think we will stop over here, right. We will be discussing about the collision frequency by considering in a simple collision event, right and later on we will look at basically how will relate to this and the reaction.

Thank you very much.