Introduction to Explosions and Explosion Safety

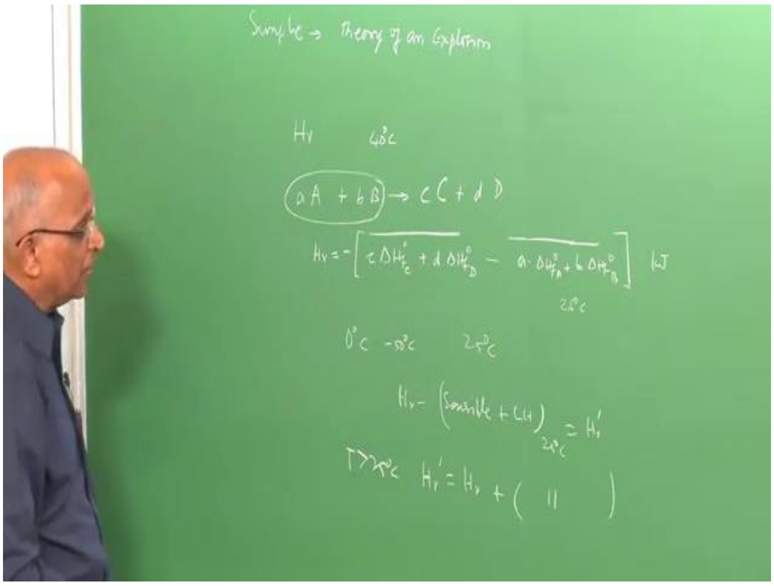
Prof. K. Ramamurthi
Department of Materials Science and Engineering
Indian Institute of Technology, Madras

Lecture - 17

1) Thermal Theory of Explosion: Lumped Mass Assumption, Heat Release
2) And Loss, Ignition Temperature, Critical Conditions, Preheat

Good morning. Now, that we know how to estimate the value of the heat release from a given explosive, and also how to calculate the rate of heat release from the explosive. It is time we think in terms of a simple theory.

(Refer Slide Time: 00:30)



A simple theory, what I mean is something by which we make some assumptions and a simple theory to interpret, let us say a theory of an explosion. We will build up on the theory as we go along, but to recapitulate what we have done so far, you know we calculated the heat of a reaction, and let us be very sure because there are certain things which I still want to add on.

Supposing, we have a chemical reaction between, let us say a fuel A, and let us say oxidizer B. And in this reaction we have a moles of A, that is the fuel a and small b moles of the oxidizer B, and it forms let us say c moles of product of capital C, this is the product, and I have something like d moles of let us say another product D. Then, what did we, tell? Well, the heat of the reaction is equal to minus of the heat of formation of the products.

That means, we have per mole of C, the heat of formation, standard heat of formation, is delta heat of formation at standard conditions into c moles, that is the total for these c moles here, plus I have d moles, I have heat of formation at standard conditions for D over here, this was for C over here, this is for the products over here. And I have minus, the heat of formation of the reactants, which is equal to a into heat of formation under standard conditions for a plus b moles over here into heat of formation under standard conditions for B over here.

Therefore, we got the heat of reaction, and we say well I have a moles. I can refer heat of reaction per mole of fuel or heat of reaction for the total A plus B moles of the mixture, I can calculate this particular value. And this is so much in kilo joules for the reaction. I can also convert it to kilo joules per mole, which we used to interpret the rate of a reaction.

Now, 1 thing you would have noted, that I am talking of the products at standard condition. We are also talking of the reactants at the standard conditions mind you, 25 degrees and 1 atmosphere pressure, if it is a gas, if it a liquid or a solid at 25 degrees centigrade alone.

Now, the question comes well, the reactant could be at a different condition, may be in a very cold climate. Well, the reacting could be at 0 degree centigrade or could be at even minus 50 degree centigrade under different conditions. Well, the reactants need not be the, need not always be a gas like at 25 degrees, it could also be a liquid like you could have a liquid hydrogen reacting with liquid oxygen.

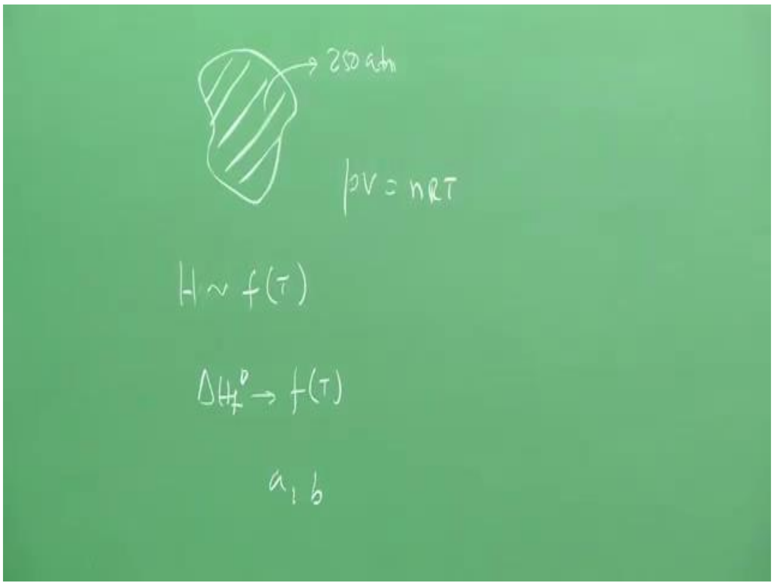
Therefore, how do we get, may be if the reactants are not at the standard condition like, what is specified here, how do you interpret, or how do you calculate the heat of a reaction? Well, you know it is possible to say well, this particular heat of reaction is when the reactants are at the standard condition.

Therefore, if I can supply some heat, may be if the reactants are at temperature much lower than the standard condition, I supply some heat may be to bring that is I have sensible heat, to bring the reactants to let us say 25 degree centigrade. And in case I have something like liquid methane whereas, methane is taken as gas. I also supply the latent heat to at the boiling point and then bring it to 25 degrees. That means, I supply the sensible heat and latent heat to bring the reactants to 25 degrees centigrade, then I can use this.

Therefore, what really happens is well, part of the heat of reaction, minus the sensible heat, and the latent heat to bring it to standard condition, plus let us say latent heat to bring it to standard condition now, becomes the heat of the reaction. I think therefore, this is 1 way I can still do the problem if it at a temperature lower than the standard well, I subtracted, if it is higher than this, let us say it is at 40 degree centigrade, a very warm climate or 50 degree centigrade. What happens is, some excess heat more than what is available, at standard condition is existing.

And therefore, in this case what happens is when, the temperature is greater than 25 degree centigrade that is standard condition. The heat of reaction is equal to the heat under the standard condition plus I have the value of the sensible heat over and above 25 degree centigrade. And if it is something which still corresponds to something else like some other state, may be I have to take care of the latent heat which is associated. Therefore, in this way I can associate, I can calculate the energy liberated from a reaction at any condition what so ever. Therefore, we have talked of temperature, we talked of atmospheric pressure, but I may again ask myself another question…

(Refer Slide Time: 05:45)

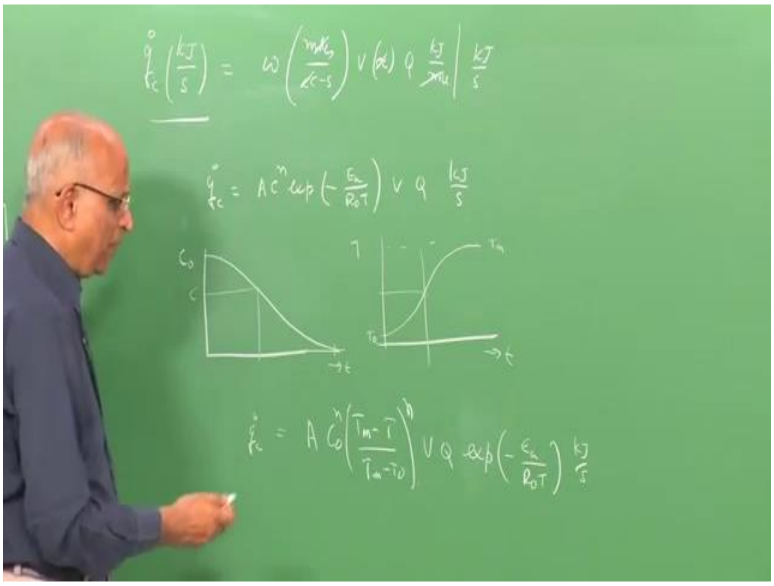


What if the pressure, we say it is calculated under the, under atmospheric pressure which is standard and the pressure at which we do is 1 atmospheric pressure. What if I have an explosive mixture which is contained in a gas, and the initial pressure of the reactant is, let us say 250 atmosphere. How do I calculate the value?

Well, if at 250 atmospheres may be I have to be a little careful because, my equation or state may not be ideal, but in case the equation of state is ideal, I am talking of 10 atmospheres or 5 atmospheres or so. I tell myself well, as per the as per thermo dynamics, the heat of a the enthalpy is only a function of temperature for an ideal gas therefore, pressure will not really influence it. And therefore, the heat of formation what we are calculating is only a function of temperature and therefore, pressure will not affect your calculations.

But we must also remember, when I increase the pressure I am talking of pv is equal to nRT and therefore, the moles are directly proportional to the pressure. Anyway the moles a b what I am talking over here a moles of A and b moles of B are anyway taken care of. And therefore, I can continue to use this same expressions for calculating at different pressures. Therefore, we can calculate the energy liberated from an explosive under different conditions of pressure may be different conditions of temperature and this is how we proceed. With this background of heat release you know when we talked of the rate of chemical reaction in the last class what did we tell?

(Refer Slide Time: 07:27)



Well, I tell that may be the heat release from chemical reaction, we call it as q chemical reaction dot, and what is the unit? You have kilo joules per second and what was it equal to? The rate of the chemical reaction and what was the rate of a chemical reactions in moles per c c into second into the volume, let us say in c c, it becomes mole per second that is this.

If I multiply by the heat release Q in so much, kilo joule per mole we got the heat release in kilo joules per second. What happen mole and mole got cancelled, c c got cancelled, I have kilo joules per second, it is the rate of heat release. We also had the expression for omega and we said well omega is a combination of the reaction rate constant and the arrhenius law. And we were able to write q c dot as equal to A into the concentration. We just said any general concentration we said well, if it is a first order or a simple reaction it is just c.

If it is product of fuel and oxidizer it could be c squared A C n into exponential of minus activation energy, divided by the universal gas constant into temperature well, activation energy we said was large, it has units of joules per mole, this is joules per mole kelvin is the universal gas constant this is kelvin. Into I have V into Q. we said well this is the amount of heat liberated in kilo joules per second.

See, we also wanted to get some idea on how the heat release varies with time. We told ourselves well, if I have initial concentration c naught of the reactants, I just consider 1 let us say c a or something initial concentration in c 0. And by the time let us say with respect to time, when the reaction gets completed well, it the concentration of the reactant becomes 0 because only products are there.

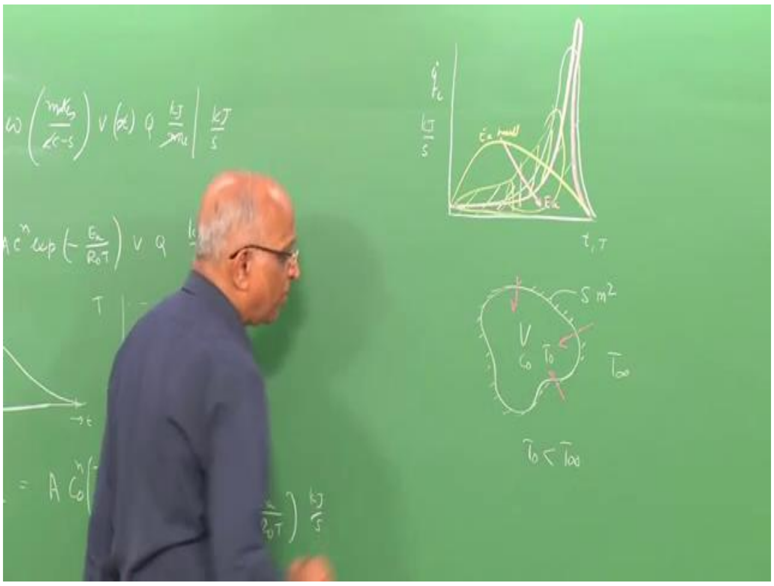
Therefore, may be c naught gets consumed in this particular way with respect to time. That means, when the reaction is completed I have all products and you have c naught going to 0. Well, if I were to look at temperature well, the temperature initially was ambient with respect to time, and what happened, we have plotting temperature with respect to time, initially let us say 25 degree centigrade is the temperature.

Finally, well everything is burnt I get the maximum temperature and therefore, we said well the rate of a reaction goes like this, this is the way the temperature varies. And we were able to put c the concentration, at anytime that means, when the temperature is T, I tell myself when the temperature is T well, the concentration could be c. We put c in terms of maximum temperature and the initial temperature T nought.

And we got an expression well, let us put that down because, that will help us to be very clear about what we were doing, we got A into the concentration, initial concentration to the power n, we also got the expression T maximum. That is maximum value over here, minus the temperature at any point in time into T m minus T naught to the power n again. And I carry the other expressions through namely V and Q so much kilo joules per second.

We learnt how to plot this and we interpreted how the energy will release, and we said well, in this what is missing? I said c is given by this, V and Q well, I have to take this into account. Therefore, I still have the exponential term, and this is what really makes the system interesting because, let us now, take a look at it R naught into T over here, so much kilo joules per second. And we said you know normally, whenever we talk in terms of explosives and chemical reactions in explosives, the value of activation energy is large. And when the activation of energy of chemical reaction is large…

(Refer Slide Time: 11:26)



What did we tell ourselves? well, if I plot q dot c now, as a function of time or equivalently. Since, as time increases the temperature increases or equivalently as a function of temperature either 1 on the x axis, what is going to happen?

Well, I have something like a reaction starts here, goes to the maximum comes back over here and this is where we say well, this is the total the area under this curve with respect to time is a total heat of the reaction. Well, the q dot in terms of k j per second is like this. That means, for some time when the temperature is low, the reaction rate is slow and then, all of a sudden it shoots up your maximum, and once the concentration is essentially completed well, the reaction rate comes down and it comes down to 0 at the final state.

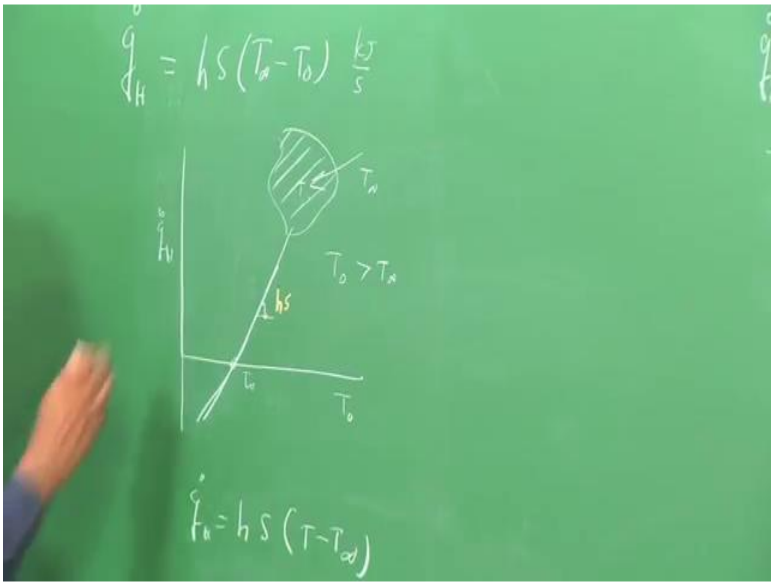
Now, if I put different values of exponential that is Ea, that is the activation energy, what is it I get? If my activation energy increases then, the effect of this particular term is to push it still lower, maybe it comes down over here and it peaks over here and then, it comes down over here. In other words, the effect of increasing the activation energy is to decrease the effective time of chemical reaction, that is the duration of the effective heat release comes down, and this is what happens when the activation energy is small is large.

If I have the activation energy to be very small, what happens? Well, the energy could be release something like this. Because, the moment because, it has to overcome a very small barrier the activation energy is small, and this is let us say Ea small. With this background, see we are only interested in large values, I am not interested in the yellow line for which like we say, phosphorus immediately burns. I am not interested, I am interested in explosive. Therefore, we will address the situation for Ea to be large that means, we will be concentrating may be in this particular zone for which Ea is a large number.

Therefore, let us now, get going let us now, say well I have an explosive, I have certain volume of explosive over here some volume. Well, it contains let us say some moles of the substance and whose initial concentration is let us say C nought. Well, the ambient that means, I have a boundary, the boundary could be a physical boundary or let us say some boundary over here. Let s say that the area of the boundary is S meter square. the volume is let us say V c c or V meter square, this is the initial concentration. Let the ambient temperature be T ambient. Let the initial temperature of this explosive be T nought.

Now, we tell ourselves, if let us say, T naught is less than the T ambient, what should happen? If T naught is less than T ambient well, the temperature that is the heat will flow in this direction because here the temperature is higher, here the temperature is lower, the heat will flow and heat up the explosive. That means, and how do you estimate the heat transfer? Let us put down an expression.

(Refer Slide time: 14:52)



We tell that the heat transfer, and let us put the same thing the rate of heat transfe we say q dot H is equal to, it is depends on the temperature difference. We have T ambient minus T naught, and what drives it is the heat transfer coefficient into surface area? We say so much kilo joules per second is the heat transfer over here.

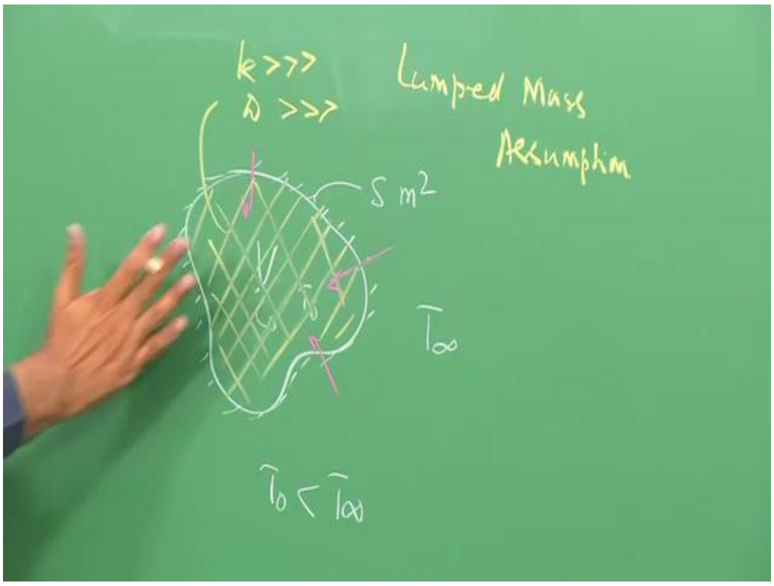
Therefore, if I were to plot this particular figure, what is it I get? Well, I have the temperature here, I have the ambient temperature is T ambient over here. And what is going to happen well, the ambient temperature is higher. And therefore, if I were to plot q dot H over here, I have well the temperature is lower may be the line is somewhere over here.

That means, heat is flowing this is my volume of the explosive, heat is flowing from ambient to a lower temperature here. And when heat flows over here, this temperature rises. Let us say if this temperature T naught by chance happens to be higher than T ambient, what is going to happen? Well, I am plotting now, with respect to T naught over here, that is T naught over here, this is the value of ambient, if T naught is there well, I have a positive heat transfer.

And therefore, I say well, q dot H is equal to heat transfer coefficient into surface area into T minus T ambient where, T could be the temperature at any instant of time. May be the temperature keeps increasing, and where it is temperature keeps increasing, the heat transfer increases. Just like we had the figure of, due to chemical reactions, the temperature is increasing, as the temperature increases in this particular volume, the heat transfer increases.

And therefore, the heat transfer is given by this particular curve over here, which we see is linear from this particular relation. And the slope here, the slope is given by you say q dot therefore, the slope is given by the product of H into S, is the slope of this particular line. Therefore, let us now, examine this in the context of the heat release. In the heat transfer I am sorry, it should have been in the context of heat transfer. And in the context of heat release, let us examine these two and try to build up a simple theory for being able to interpret the explosions. Therefore, let us get started with this you know we have to make some more assumptions to be able to keep going.

(Refer Slide Time: 17:23)

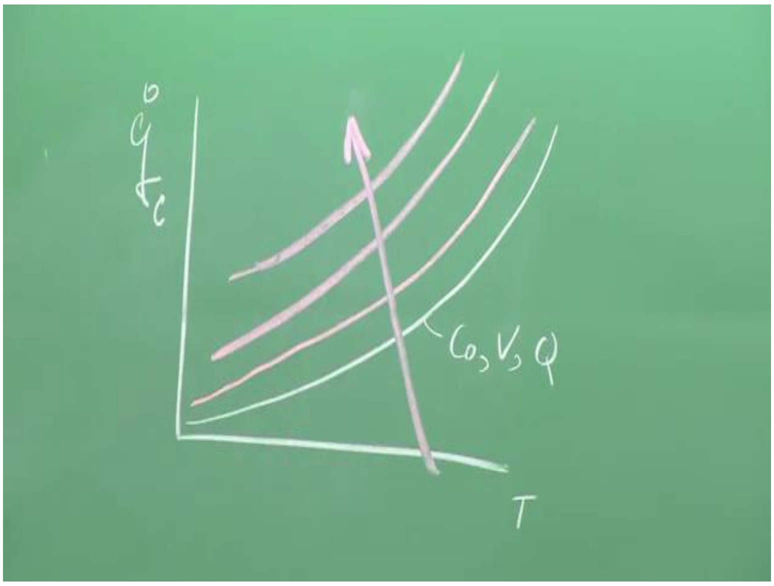


You know one thing we can assume to begin with, maybe we have to relax it as time goes along. Let us say, within this volume of explosive what we are considering. Let us assume, that the thermal conductivity of this particular material of explosive, whether it is a gas, whether it is a solid, whether it is a liquid, the thermal conductivity is very-very large.

Such that, all points have the same temperature. Let us also assume that the diffusivity is so large, that the concentration at all, at all places is the same. That means, we are assuming a point here, and a point here has identical temperature, identical concentration. Or rather a particular point in this particular volume is representative of the total volume. And this assumption of infinitely large thermal conductivity, and infinitely large diffusivity says well, I can represent the entire volume through one particular property and such an assumption is known as lump mass system or lump mass assumption.

That means, we tell ourselves whatever we do, if there is a change in temperature well, it affects throughout the volume. It is not that the temperature gets affected here, the temperature is not getting affected here. We also say the concentration is changing throughout the volume at any time T well, it is a uniform property. With this assumption I can tell myself if I were to plot the value…

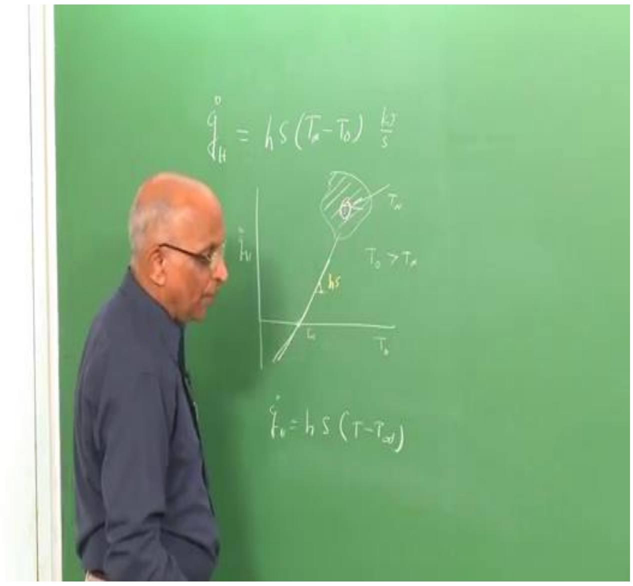
(Refer Slide Time: 18:51)



Let us plot the value of heat release then, look at it with respect to heat release due to combustion. The way we say well, chemical reactions are taking place. Let us take a look at the initial phase of it wherein, the curve went like this. Let us plot it with respect to temperature over here, which we have done just now. We tell ourselves the value, that with this curve, depends on, if I look at this particular expression well, it is going to depend on the initial concentration. Well, it is going to depend on the volume, it is also going to depend on the value of the heat release per mole.

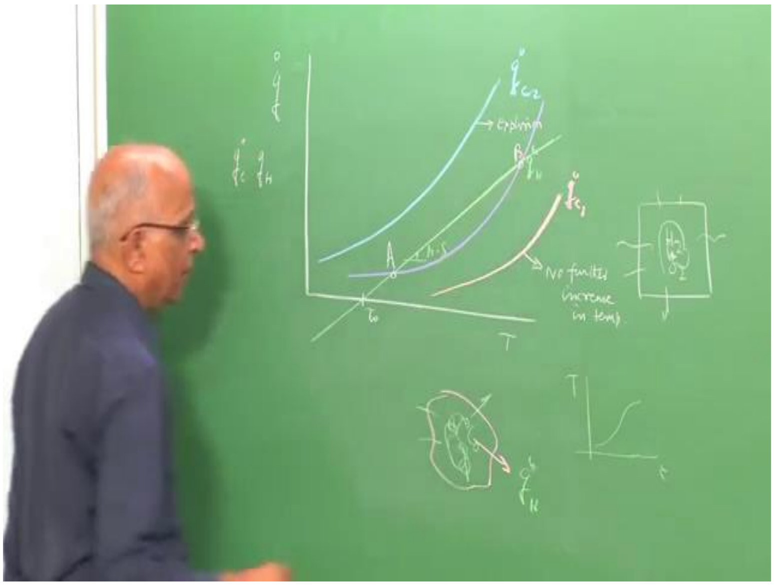
Therefore, this for a given value of C naught for a given value of V and for a given value of Q well, this is the curve. If I increase either C naught V nougt or Q, what is going to happen? Well, the curve will go up. I can have a series of curves. And all these the increases is in as you increase C naught, as you increase V naught, or as you increase Q naught. Either of them the curve will keep going up and this is how the characteristics of the heat release will take place. Now, this is how the heat release takes place in a reaction.

(Refer Slide Time: 20:09)



This is how the heat transfer takes place. And let us consider the case wherein, the temperature here is greater than the ambient, and let us put both of them together and try to see whether we can interpret it or make some sense of it in some way.

(Refer Slide Time: 20:58)



Well, now I tell well, I make a plot of, let us say q as a function of temperature. Let us say q dot, and this q dot could either be q C dot and q H, that is the heat transfer, I want to say this.

Let us for the, for the present assume that the ambient is at a temperature T ambient. And therefore, I tell myself well I can plot the heat transfer relation, that is q H as function of temperature to be given by this particular line over here. This particular line tells me the value of q dot H. For a given value and this slope is equal to, we said is equal to the heat transfer coefficient into the surface area that is h into s over here.

Now, I could have different values of heat release, I want to put it in the same curve. I could have, if my concentration that is a initial concentration or the value of capital Q is such that, I could get a value of q H over here, q dot C over here the heat release from chemical reactions.

I could also think in terms of a heat release, which is such that I get a curve over here, q dot C that is, may be I increase the value of concentration, I say this is equal to 2 this is equal to 1 over here. And what are these two curves with respect to this? May be for a particular value of the surface area for a given volume, may be by changing the initial concentration or the exothermicity Q kilo joule per mole, I can get my heat release to be here or here.

What does it mean if the heat release is here, and my heat transfer is over here? Heat transfer as we told in, this is the volume, heat is getting transferred out, we said the heat transfer is equal to q dot H over here. And what do we find, that the heat loss from this particular volume which is V over here, concentration is let us say C naught and the exothermicity is Q, is higher than the value of energy release due to the chemical reactions which are taking place.

And therefore, what is going to happen? Since, over the range of temperatures of interest, the energy release by chemical reactions is less than the heat which is transferred out. That means, the loss is more whereas, the heat which is getting generated is less and therefore, what is going to happen? The temperature is going to fall further and therefore, what is going to happen?

This particular volume which contains the gas, can never really progress in temperature. That means, the temperature can never really increase temperature with respect to time can never really increase, and it just keeps falling and therefore, this particular volume of the explosive cannot really explode.

This corresponds to the condition which we talked of, you will recall, we said supposing I have an explosive gas mixture like hydrogen and oxygen mixed together, if the heat transfer from this is such that the rate of reactions at low temperature is so small. That means, so small compared to the larger value of heat transfer well, this volume is always stable it never reacts. And therefore, we say this corresponds to the case wherein, no further increase in temperature is possible.

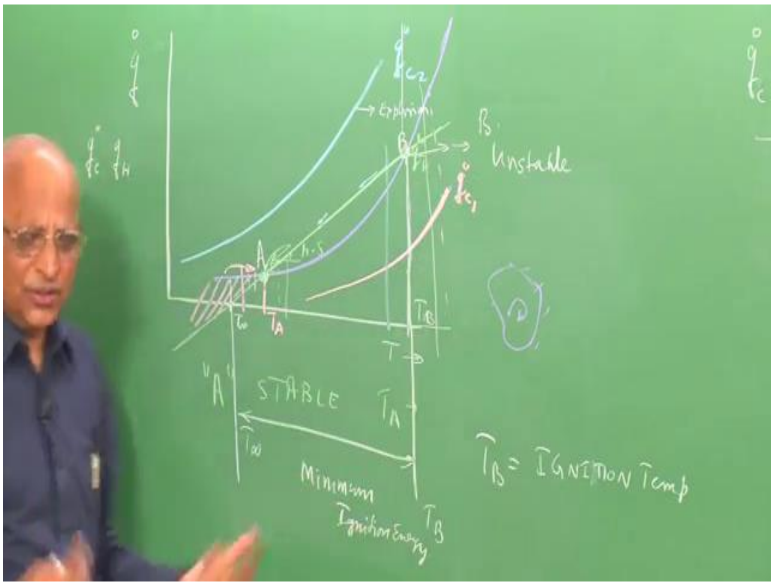
Let us take a look at this, supposeing the initial concentration is such that. Now, what is happening, the heat release is always greater than the heat loss. And therefore, the temperature of this particular volume in which heat is getting generated is excessive of the heat loss, that is q h taking place. Therefore, the temperature keeps on increasing, when temperature increases, heat loss, the heat generation rate is further increase.

And therefore, it goes into the cycle of heat generation being always greater than this and therefore, it just explodes that means, this corresponds to an explosion. Because, the heat generation is progressively increasing, and is always greater than the heat loss. Now, under critical conditions, under some conditions, I can also think in terms of, let us put it in a slightly different color. Under different conditions I can always think well, I can think in terms of a concentration of heat release such that, I can get a curve like this. And in this curve, we see well, I have the heat loss curve which is q h, which is by heat transfer. I have a critical value of may be v or q such that, now it intersects this curve at 2 point, let us say A and at some particular point B.

Therefore, we say well, 1 case is well, no possibility of an increase in temperature. Well, the heat generation rate is so high, higher than the heat loss rate that it just goes into a cycle of reactions and explodes because the heat release is excessive. This volume keeps on increasing temperature and such that, there is an, there is an intensified chemical reaction.

But in general, I can say well it is also possible for given values of heat release, that it can, it can cut the heat transfer curve at 2 points, may be curve point A and point B. Let us examine, what is, what are these 2 points like, do they represent something which is meaningful by which I can interpret this, in some way I can interpret this points.

(Refer Slide Time: 26:06)



Let us start with point A, you know at point A, we find is I have a zone to the left of this point this is, this particular zone over here, may be over here in this particular zone. You know in this particular zone if I take any point that means, I am talking of a point I have a temperature T A over here corresponding to point A over here. And in this zone well, if I take any temperature over here, I find that the heat release is greater than the heat loss that is the heat transfer out of the volume.

And therefore, the temperature will build up and therefore, at the next point it will come over here. I find still the heat generation by chemical reaction is higher than heat loss therefore, the temperature comes up and it will react this particular point. Therefore, we say to the left of point A, if by chance I have the mixture at these temperatures well, the point always goes in this direction and reaches point A.

How about to the right side of point A? If I look at the ride side of point A, what is it I get? Well, over here on the right side, if I say well I choose a temperature over here, the temperature T is higher than T A well, the heat loss is higher than the heat generation rate and therefore, what is going to happen? The temperature will fall, it comes over here well, it is still higher, it comes over here.

And therefore, even on the right hand side, the heat loss rate pushes the point over here therefore, in this region to the right as long as this point does not exceed this particular point. What happens is the point gets pushed over here and the point is always reached over here.

Therefore, it is a stable point. What do you mean by stable? Any perturbation, any change about this point always leads it back to this particular point, and we say well, the point A is stable. And when I say point A is stable, we say well at temperature T A is such that the explosive, the given volume cannot explode.

Because it is always going to be at the same temperature, and this is what really happen. If I consider a mixture of gases in a given volume, such as hydrogen and oxygen at room temperature, whatever you do, it does not really change its initial temperature. It cannot go to higher and higher temperatures and therefore, we say well, it is a stable temperature.

Let us similarly, go back and see what happens at the point B over here. Let us again say well, this is my temperature here, this is my temperature axis over here, this is point T B over here. You know, let us again go back to the left of point B, and what is going to happen to the left of point B? Well, I take a point over here, if I take a point over here I find heat loss is greater than the heat gain which is shown by the purple line.

And therefore, it comes over here it comes back to A over here. Therefore any point to the left of point balways comes back to the table point. But if I were to take a point to the right of point B, what is going to happen? To the right of point B well, the heat release rate that is Q dot c over here is higher than the heat transfer rate shown by the green line over here. And therefore, I will get a higher temperature therefore, the temperature goes up, I have more chemical reactions.

And therefore, what is going to happen the temperature over here, will keep on on shifting to the right and therefore, I have more and more heat release as is shown by the violet line over here. And ultimately the given volume increases in temperature, as temperature increases more heat is generated or the reaction rate is faster and ultimately the volume explodes.

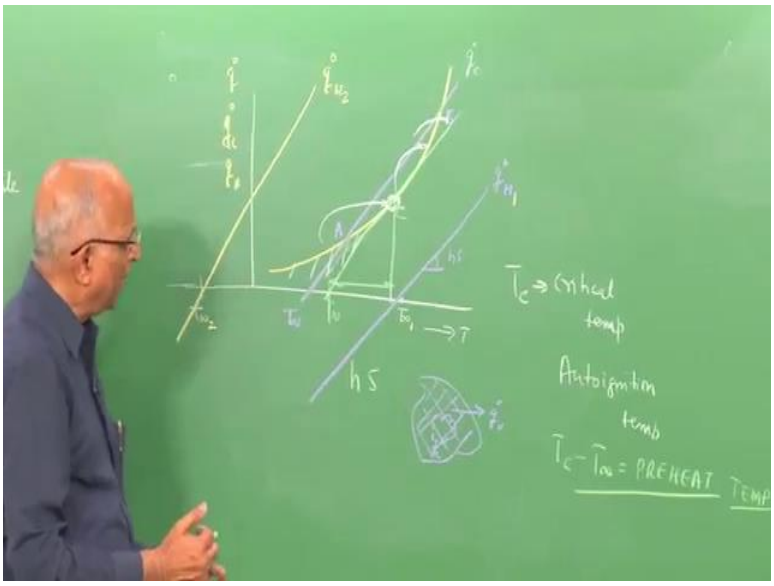
And therefore, we say well, point B will correspond to what we technically call as the ignition point or the ignition temperature. Let me write it down here therefore, T B is a point at which, if I can increase the temperature of this lump volume beyond point B. Well, the substance ignition keeps on reacting and it generated higher temperature and higher rate of chemical reaction, and we got, we got T B as the ignition temperature.

Therefore, to be able to ignite any mixture, what is it I have to do? I am, I am at the ambient temperature, let us say T ambient, I have to increase the temperature to the level T B. That means, I have to supply some energy from ambient, from the ambient condition to T B, and the amount of energy supplied over here is what we call as the minimum ignition energy, or simply we can say so much is the ignition energy.

Therefore, now we say well, the simple thing of relating in a, in a given volume which, in which all the properties are lump. We tell ourselves is able to tell us what do we mean by ignition? We know, we have to go back beyond point B which is the, which we can say just like we say, it is a stable point, we say B is unstable point. And the unstable point corresponds to ignition because anything to the right causes the chemical reactions to go faster. And therefore, we say I have to supply a minimum ignition energy of, to increase my temperature to a level beyond T B and therefore, this is my ignition energy.

Therefore, on this curve of different heat release versus the given value of heat loss, we are able to see this point, namely point A which is stable, point B which is unstable or the ignition condition. Let us go one more, one step further and see whether we can interpret it in a slightly different way because we said well, in the given volume I could have something like, let us say different values of heat release corresponding to different values of concentration.

(Refer Slide Time: 32:08)



But similarly, I can also talk in terms of let us say, I have a given volume and let us say, this given volume has a given value of let us say, q c dot that is the heat release value, so much kilo joules per second, which is given by a particular curve over here. This is the value of q c, I want to put on this same curve. Well, I say instead of plotting just q c over here, I plot q dot in general and therefore, now I plot the value of q h.

Now, I could have an ambient temperature which is very high let us say, this is my temperature axis, this is my q dot axis. Well, I say I have my ambient temperature to be a high value T ambient is high. And for a given value of the heat transfer coefficient, for a given value of surface area well, my heat loss curve could be let us say, the heat loss curve is over here. This is my slope, the slope is equal to proportional to hs over here, this is my value of q dot l or q dot heat transfer, q dot loss from the given volume, this is my value of q dot c over here.

If by chance let us say well, I say no, no, no, my ambient temperature is very low let us say, my ambient temperature is over here, it is let us say, minus. It is 0 degree say minus 20 degrees. And therefore, what is it I get? For different values of temperature, my slope is the same therefore, I get other curve which is over here.

In other words, this is my second curve here which I say is q dot h, this is say is q dot h 1, this is q dot h 2. And therefore, I tell myself, if my heat loss is of this value well, my heat generation curve is always much above my heat loss curve and therefore, the substance will go into further reactions that means there will be an explosion. But if my ambient temperature is so low that, my heat transfer is very much higher than my heat generation rate, well the explosion cannot take place. I could also think just like I thought over here of point A and B, I could have ambient temperature T ambient over here, which gives me point A which is stable, point B which is unstable.

Therefore, we are able to relate the conditions under which an explosion would occur, may be relating from a given volume, what is the rate at which heat is getting transferred out, and what is the rate at which heat is getting built up into the in a, in a given volume? This is we say, the energy rate of energy release within the volume and this is the rate at which the energy is getting dissipated away from the volume.

Therefore, we talk of the ignition temperature unstable point, we talk in terms of stable point. Well, this is all about the theory of a simple theory, but let us not forget that whenever we talk of this, we are talking in terms of a lump mass system. That is the temperature and concentration at any point within the volume, within the volume remains the same. That means, a point temperature, a point in concentration is representative of the whole volume.

Now, let us see whether I can interpret something more in this. What if my heat transfer line is somewhat tangential to this? Let us, let us take a look at this, we tell ourselves well, I am, I am interested in a condition, wherein my q c could be tangent to this particular curve. That means it does not intersect at 2 points and what is happening is well, I have a curve like this, it is tangent at a point let us say, C over here. Or coming back to this particular curve, I tell myself, can I have a curve on in heat release? Let me put that curve in white color chalk.

Can I have a curve in heat release, such that it is tangent over here at the point C? What is this condition of tangency which I am talking of? That means, I do not get a stable point at all, well I also, I am not getting the unstable or ignition temperature, what is this particular point over here? Let us try to interpret this.

Well, to the left of C well, the heat generation is always higher than the heat loss given by the green line and therefore, what is going to happen is any point is going to come back over here. Therefore, it is something like a stable point. But to the right of this particular point. the heat generation is always greater than the heat loss and therefore, the point shifts over hear, temperature increases and you have an explosion.

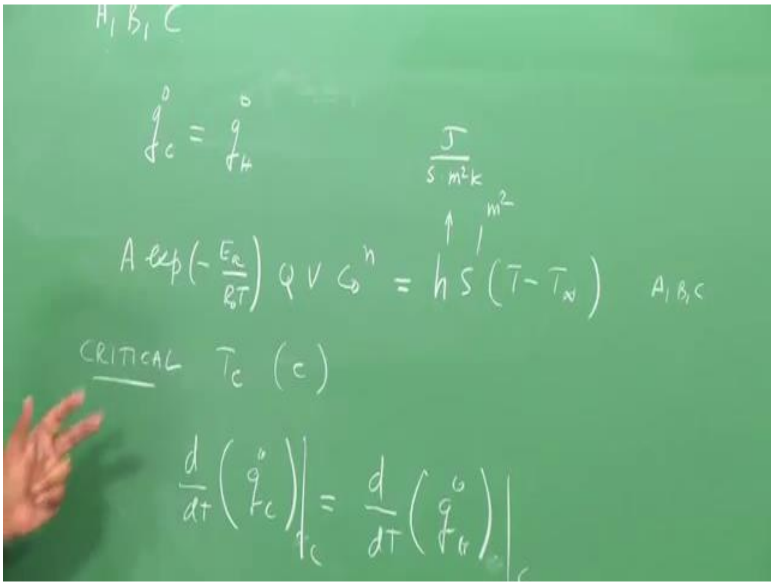
That means, this particular point is something like an unstable point, but it is the minimum temperature at which may be a some ignition is possible, and this particular point c that is T c is known as the critical temperature. People also call it as the auto ignition temperature that means, if I can increase the temperature to a value T c well, the substance automatically goes into this thing. And what is the difference between auto ignition temperature and ignition temperature?

Well, the ignition temperature is higher because I have to supply energy such that, I go to this whereas, in this case that is the minimum value of energy required to auto ignite particular mixture. Therefore, may be I would like to find out what is the value of the auto ignition temperature? And if I say well, this is the point over here which corresponds to T ambient. The temperature increase from T ambient to T c is what we have to heat the mixture, and this temperate increase T c minus T ambient is what we call as the pre heat.

Well, these are the temperatures which we, these are the few temperatures we must remember. I could have a stable temperature A, I could have an unstable temperature B, I could have the auto ignition or the critical temperature T c. The difference between T c and t ambient corresponding to the same heat loss line is what we call as the pre heat temperature.

Right, having done these few things namely, we are able to interpret something, let us try to see whether I can get an expression for T c. And for that you know, let us put down what is the expression at A, what is the expression at B, and whether I can really derive an expression for T c and get the value of T c minus T ambient, and this is what I do in the next five minutes. Therefore let us, let us do this exercise.

(Refer Slide Time: 38:58)



We tell ourselves, may be at point A, at point B, at point C, what is, what is the commonality at A, B and C or we have at A, B and C over here. Well, in these cases, both the heat generation rate q c dot is equal to q h dot point 1. And therefore, what is it I get? We said q c, we have the expression available, we have A into exponential minus Ea by R naught T into, we get the value of q, we have the value of v. That means, A exponential minus Ea, we forgot the value of initial concentration to the power n. This is the heat release by chemical reactions.

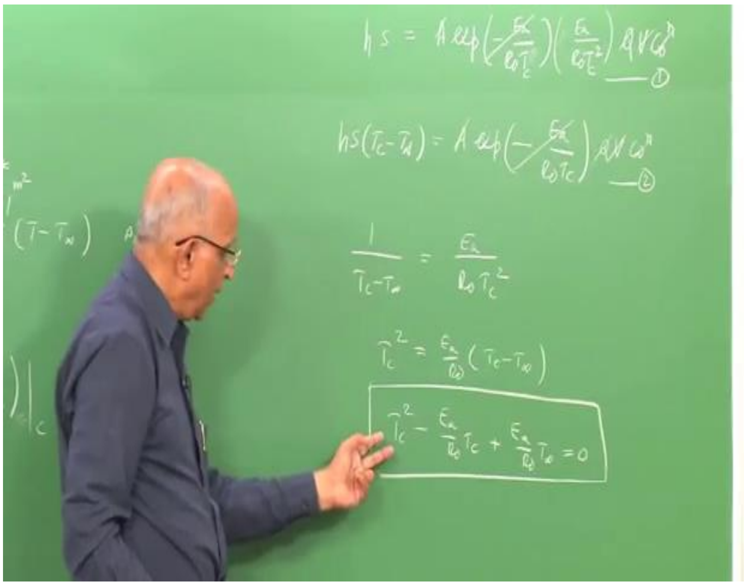
And what is the value of heat which is getting lost from the system, which is equal to heat transfer coefficient into the surface area. Heat transfer coefficient is equal to, may be watts or joules per second meter square degree kelvin or degree centigrade. This is metersquare over here into I get T temperature of the volume, minus the ambient temperature over here. This is true for point A, B and C at which the equality is mention, is obtained.

Now, for the particular case of critical temperature, can I think in terms of any additional condition? See, this is true at point A, B, C, what is so specific to q, specific to the condition at point C, may be at point C over here? What is it I observe? I observe that, the heat transfer line, or the heat loss line is tangential to the heat generating line that means, I have my x axis is temperature.

And therefore, I can tell myself d by dt of the value of heat release rate q c over here, is equal to d by dt of the value of the heat loss rate. And therefore, I can say, at the critical condition of corresponding to T c or the point C as it were, what is it I get? d by dt of q dot c at the condition, at the point, let us say C is equal to d by dt of q dot h at the point C. That means let us say, at the point C, may be at the point C over here.

And therefore, what all I have to do is, may be yes I can differentiate this with respect to temperature, I can differentiate it with respect to temperature, and what is the expression I ge? Let us, let us write out the expression. Well I start with the right hand side, if I differentiate this term, I get hs into, h is the heat transfer coefficient constant surface area is constant, d by dt is 1 over here, well ambient temperature is a constant. This is this is the value of d by dt of q dot h at the point C. and similarly, if I were to differentiate this…

(Refer Slide Time: 42:05)



I get a into exponential of minus Ea by R naught into T square because R naught T, as it is, this is within this particular term. And now, I have to differentiate this expression, it is equal to minus of Ea by R naught into T square. This is the value, but minus Ea came over here, 1 over T is minus 1 over T square therefore, this is positive over here. And what are the other terms I get? Well, I have q into v into C naught to the power n. And this is at the condition T is equal to T c or I get T c, T c over here at the pointy C.

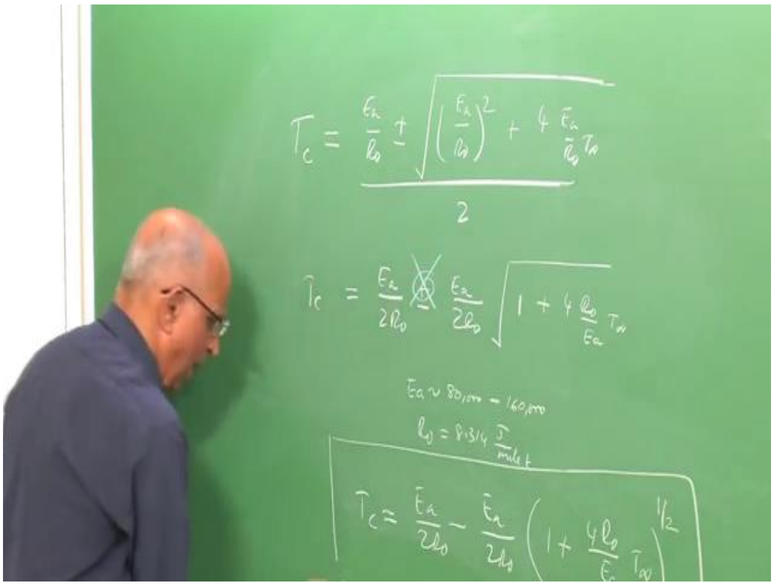
Similarly, I have this expression at point C therefore, it should be T c, at the point T c it should be T c, at the point it should be T c. And therefore, if I were to write the equation for heat being that is the heat transfer being same as the heat generation term, I have into T c that means, T becomes T c minus T ambient is equal to A into exponential of minus Ea by R naught into T c into, I get the value of q, I get this expression q v into C naught n.

Well, this becomes my gradient equation 1, this becomes my equality in the heat release rate. And now, see I am interested in the value of the critical temperature T c. If I were to divide 1 by the other, let us say I take equation 1 divided by equation 2, what is it I get? On the left hand side I get 1 over T c minus T ambient. And similarly, I take equation 1 and divide it by this equation, I get the value as equal to well, A and A gets cancelled, the same exponential term will get cancelled, well the q v c naught n gets cancelledn and what I get is, I have the value of Ea by R naught into T c square.

Or rather this equation, if I were to simplify tells me well, I have T c square, I bring it on the, on this side and now I take T c square is equal to Ea by R naught into, I get T c minus T ambient. Or rather what is it I get? I get T c square minus Ea by R naught into T c. Now, I bring this also on the, on the left hand side, I get Ea by R naught into T ambient is equal to 0.

This is becomes my final equation. I am interested in T c, I find well T ambient is fixed because for a given ambient I am doing this problem, and what is it I get? I find, I have an equation in T c which is a quadratic equation, I want to solve for T c and let us solve this, and let us see what number we get.

(Refer Slide Time: 45:27)



Therefore, I solve this quadratic equation in T c, and what is it I obtain? I get T c equal to minus middle number that is Ea by R naught into plus or minus under root of middle number squared Ea by R naught square then, I find it is minus 4 into the first into the last number, I get 4 into the first number is 1, the last number is Ea by R naught into T ambient is the last number, divided by 2 into the first number.

Or rather, this gives me the value as Ea activation energy divided by 2 R naught plus minus, let me take Ea by 2 R naught out side again, Ea by 2 R naught, again outside into I have the under root over here. And since, I have taken this outside, I have 1 plus now, I have taken this outside therefore, I should get 4 into I get R naught divided by Ea into T ambient over here, and this becomes my value of T c.

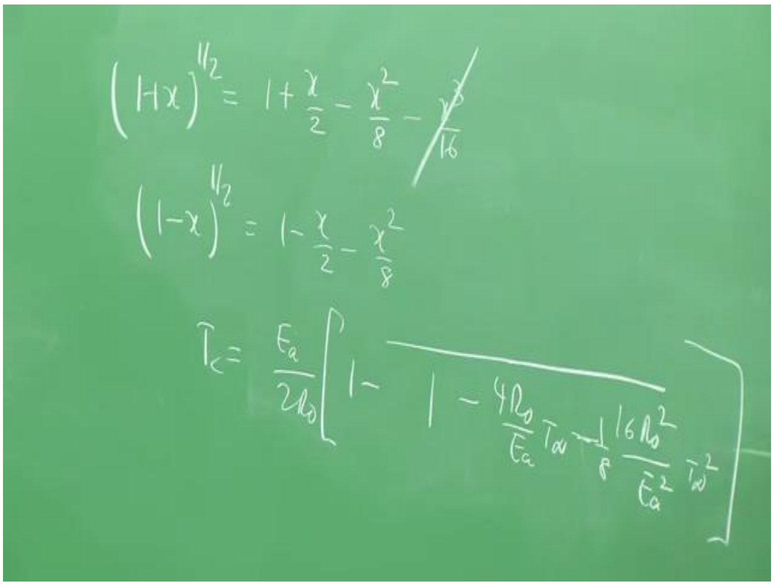
Now, I find yes being quadratic I get 2 roots, let us examine the roots of this equation we 1 thing we must not forget, the activation energy we said is extremely large, and we also said well, the activation energy varies between, let us say 80000 joules per mole to something like 160000 or higher joules per mole. Whereas, the value of R naught universal gas constant is something like 8.314 joules per mole Kelvin.

Therefore, we find well, Ea is extremely extremely large number compared to R naught and therefore, if I have the plus sign over here, what is going to happen? I add 2 large numbers I work, I come back with numbers T c of the order of something like 50000, 100000 kelvin, which is fictitious. And therefore, I tell myself well the number positive sign is not possible.

And therefore, on these physical grounds such that I cannot have such high temperatures which are of no meaning to me therefore, I tell well, the value of T c I can write as equal to E a by 2 R naught minus I have Ea by 2 R naught, into I have 1 plus 4 R naught by Ea into the value of T ambient to the power half. Now, I want to discuss this further, what happens. I want you know, I still have this under root sign, it is not that easy to solve this and interpret this.

Therefore, let us, let us try to find out, what will be the value of this under root term over here? Let us see the magnitudes first, before we can first simplify it. We tell ourselves well, let me assume that 4 R naught T ambient, that is T ambient divided by the value of Ea.

(Refer Slide Time: 48:48)



$$(1+x)^{1/2} = 1 + \frac{x}{2} - \frac{x^2}{8} - \cancel{\frac{x^3}{16}}$$

$$(1-x)^{1/2} = 1 - \frac{x}{2} - \frac{x^2}{8}$$

$$T_c = \frac{E_a}{2R_0}\left[1 - \sqrt{1 - \frac{4R_0}{E_a}T_\infty - \frac{1}{8}\frac{16R_0^2}{E_a^2}T_\infty^2}\right]$$

Let us say is equal to x or x is equal to 4 R naught divided by Ea into T ambient. Well, we are again telling well, Ea is a large number R naught is a small number therefore, we recognize that x is a small number. If x is a small number, I can, I can expand 1 plus x as a binomial expression for half, and what is it I get? I get 1 plus x if I can write an expression. Well I think, we have to be careful about this particular sign, have I done it correctly?

I have, you had T c square plus Ea by R naught, we have middle number squared minus 4 into the first number and therefore, the this number, this particular expression should have been minus over here. Because we are talking of middle number squared minus 4 into the first into the last number, we have minus 4 into the first into the last number therefore, we have minus sign over here.

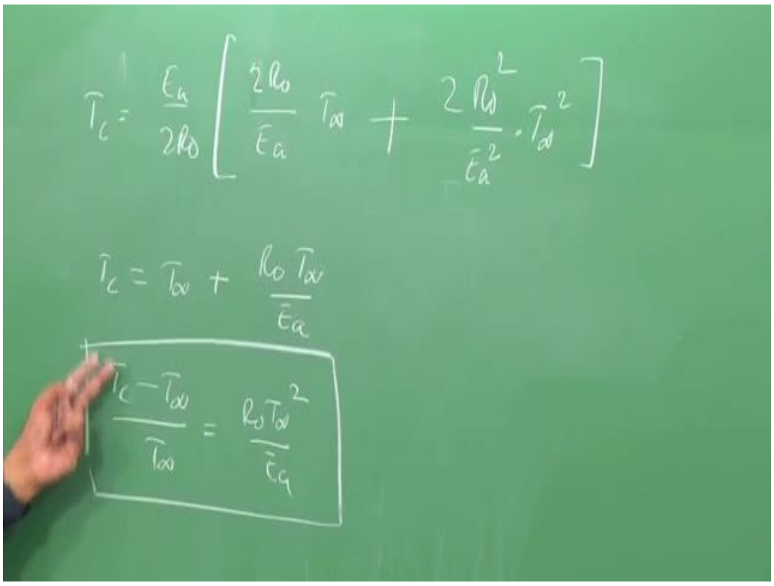
And therefore, I am looking at the value of 1 minus x to the power half, and we know well 1 plus x, I can write as if x is small to the power half, I can write as equal to 1 plus x by 2, and now I say 1 minus half. Therefore, I get minus x squared by 8 plus I have the value of 1, let me get this expression straight. I can write the value of for x being small as 1 plus x to the power half, as equal to 1 plus x by 2 minus x squared by 8, minus x cube by 16.

Or rather, I am interested in x small therefore, I can as well forget about the higher order terms. And I can get the value of 1 minus x to the power half, I substitute this, I get the value as 1 minus x by 2. And x squared then, still gives me the negative value, I get minus x squared by 8, and I substitute the value here. And ultimately, what is it I get? I get the value of T c as equal to the value Ea by 2 R naught into, I get 1 minus, I get 1 minus x.

Therefore, I get 1 minus 1 plus, I get 1 minus the value of 1 minus 1 then, I get over here the value minus x by 2, x is equal to 4 R nought by the value of Ea into T ambient, minus I get the value as 4, that is 16 R naught square by Ea square, into T ambient square. I square these things and divided by 8. And therefore, I have to just simplify it, and immediately you know what is it I have written here 1 minus, I have 1 minus therefore, I have repeated this twice.

Therefore, I have 1 minus 1 into this within this particular bracket. And if I simplify this particular expression, what is it I get? Let just write the expression, and we could discuss it in the next next lecture, what is it I get?

(Refer Slide Time: 52:47)



$$T_c = \frac{E_a}{2R_0}\left[\frac{2R_0}{E_a} T_\infty + \frac{2R_0^2}{E_a^2} \cdot T_\infty^2\right]$$

$$T_c = T_\infty + \frac{R_0 T_\infty}{E_a}$$

$$\boxed{\frac{T_c - T_\infty}{T_\infty} = \frac{R_0 T_\infty^2}{E_a}}$$

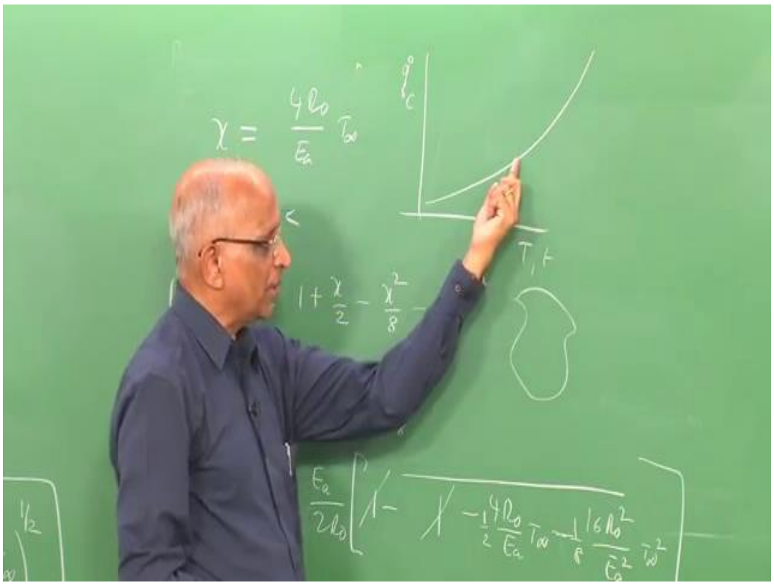
I get T c as equal to Ea by 2 R naught into 1 and 1 gets cancel now I have minus and minus becomes plus, I have 4 R naught, divided by Ea into I have T ambient and mind you, here I should have had x by 2 another 2 over here.

And therefore, what is it I have x by 2 and here I have 8 therefore, 2 and 2 gets over here plus that means, 2 R out over here. And I have 8 two za 16, 2 R naught squared by Ea squared into T ambient square, minus and minus becomes plus over herem this is the expression. And let us take out the multiply this by this number, I get T c is equal to t ambient plus, I get the value as R naught into T ambient by Ea. Or rather, what is it I get? I get T c minus T ambient divided by T ambient is equal to R naught into T ambient square divided by Ea. This is the final expression what I get.

In other words, I have been able to get the value of the critical temperature in terms of the ambient temperature, and in terms of the activation energy and the value of the universal gas constant. And we get an expression something like this. We now know what is the pre heat temperature, and we will continue to discuss this further in the next class.

Therefore, to sum up in today's class, we started by again looking at the value of the energy released in a particular volume, we said well, if the conditions of this initial volume is not at the standard condition, but it is at different condition, at different pressure, we know how to calculate the value of heat release. We again looked at the heat release curves, that is the rate of heat release curves.

(Refer Slide Time: 55:04)



And we found well, the heat release curve goes that means, if I plot heat release as a function of temperature or as a function of time well, it goes like this may be especially for large values of heat release. That means, heat release is localized in a small volume, initially it takes off slow.

And if I were to look at the initial distribution or for the initial conditions till the maximum value is reached. I tell myself heat release goes exponentially like this, into this I put the heat loss that means, I go to a system and say a system also loses heat just the same way as it gains heat. I was able to define a stable point and unstable point, that is an ignition temperature and and auto ignition temperature, that is a critical condition and we got the expression for the critical temperature. We will continue to discuss this in the next lecture.

Thank you.