Introduction to Explosions and Explosion Safety

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Lecture No.- 18

1) Thermal Theory: Characteristic Heat Release
2) And Heat Release
3) And Heat Transfer Times
4) Spurt in Heat Release
5) Auto-ignition Temperature
6) Damkohler number of an Explosion
7) Non-Dimensional Explosion parameter

Good morning. In the last lecture we considered based on the heat loss from a particular volume of the explosive and the heat which is getting generated within the explosive. We were able to define something like an ignition temperature.

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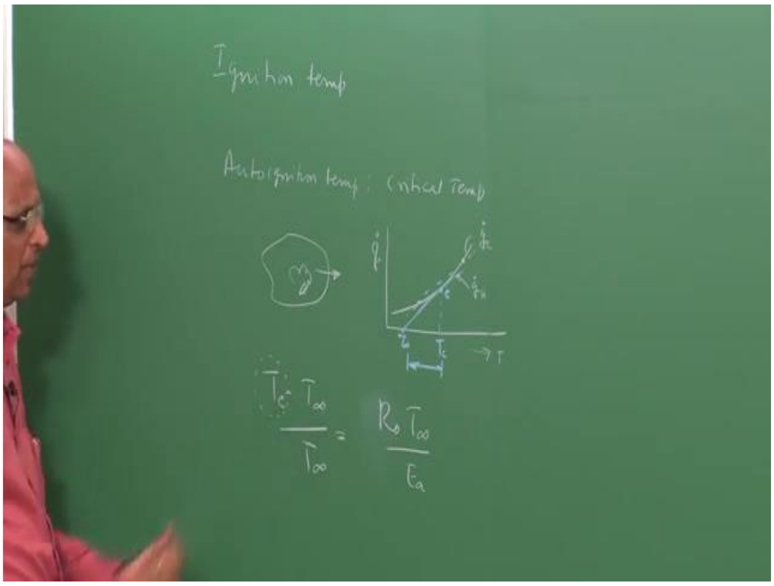

We defined something which we called as an auto ignition temperature, which we also termed it as the critical temperature. You know these things were based on, you have a certain volume of the explosive, some heat is lost from the explosive. We determine the heat loss, we also determine the heat which is generated within. And based on these things, we had on the plot of heat, rate of heat whether it is generated, well it is generated, whether it is lost under some conditions. We could have a stable point and ignition temperature over here, and when the heat loss curve happen to be tangent to this, we call this as point c, or this temperature as critical temperature.

Mind you, the x axis was the temperature, the y axis was heat release, the y curve here was heat generated q c dot, and this curve was the heat which is lost to the surroundings rate of heat loss. Now, we have, we have got an expression for T c and the expression was. We had the auto ignition temperature or critical temperature, minus the ambient temperature divided by the ambient temperature was equal to, we had the expression, activation energy divided. I am sorry it should have been the activation energy came in the denominator. We had the universal gas constant into the ambient temperature divided by the activation energy over here.

Therefore, you know today we will try to get some more physics of this auto ignition temperature or critical temperature. We also said T c minus T ambient, like for instance had the heat release curve been extrapolated. We would have got the ambient temperature at which the, if the temperature of the explosive was the same as ambient temperature, we said well this is the value of the ambient temperature and initially could the explosive could be at ambient temperature. The heat required to go from t ambient to this, we called it as preheat or the temperature T c minus t ambient we called as pre heat temperature

Therefore, we will also try to take a look at the pre heat temperature, and how the auto ignition temperature varies. Let us first take a look at the preheat temperature namely the temperature of pre heat namely T c minus t ambient.

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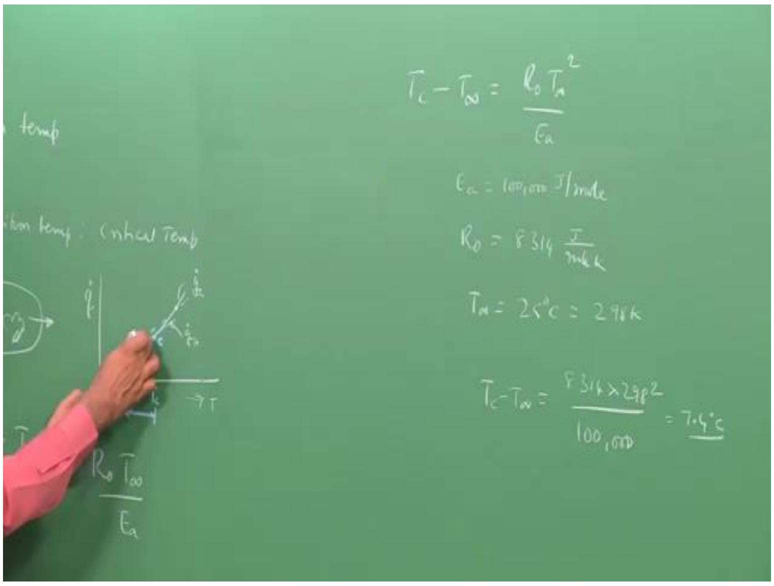

I can now write it as equal to R naught into t ambient square I just take the t ambient on top and I put it as activation energy over here. I am interested in determining the magnitude of this, let us do for a specific case. We always say that the activation energy of an explosive is quite high, let us take a value of Ea equal to 100000 joules per mole. Anyway the value of the universal gas constant R naught is equal to 8.314 joule per mole Kelvin. And we now take the ambient temperature as equal to, let us say 25 degree centigrade, which is equal to 25 plus 273 which is equal to 298 Kelvin.

You know, first of all before doing that, we should also check whether this equation is homogeneous that means, it has same dimensional left hand side. Left hand side is a unit of temperature well, Ea is joules per mole, R naught is joules per mole Kelvin, this is one over temperature well right hand side also temperature. Therefore, this equation has the same dimensions. Let us now plug it, plug it in. The value of T c minus T ambient therefore, works out to be 8.314 multiplied by T, that is 298 square, divided by the value of activation energy, we said it is equal to 100000 joules per mole.

And when I calculate this value, it comes out to be something like 7.4 that means, the change in temperature between the auto ignition to the ambient is something like 7.4 degree centigrade. Well, this is a small number that means, the pre heating required, the heating required to go from here to here is a small number and that is a cause for concern.

That means, if I have an explosive gas mixture such as here, and if I allow some pre heating to take place by a small amount well, it could go into an explosion, or it could automatically spontaneously auto ignite. Therefore, but you know this is something which poses some problems, and if we go back to the examples which we took, like for instance let me site one or two examples. You know if you go and see the example of let us say, the Texas city disaster.

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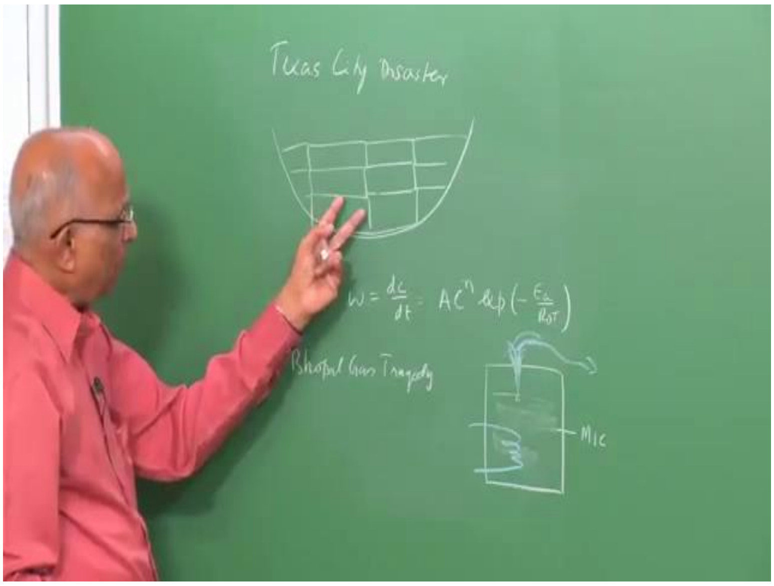

And what was in this particular accidental explosion? We had lot of this ammonium nitrate, things being piled, the cartons of ammonium nitrate being stacked one on top of the other. And it was something like 7700 tons, this is all within the hull of a ship, and you know the hull of the ship is insulated, it does not allow heat to leak through and therefore, it is in an, in an environment in which it is not losing much heat.

And if by chance, you know any chemical reaction at anytime, like we say omega is equal to dc by dt, like dc by dt, that is rate of change of concentration with respect to time. We had written it as AC to the power n into exponential of minus Ea by R 0 T. At any temperature, there is some incipient chemical reaction taking place. And if by chance some small temperature increase happens well, it could just explode or it just could cumulatively react. And so such a high temperature takes place, that a thermal explosion can take place, and this is what happened in the Texas city disaster

Well, in the, in the example of the Bhopal gas tragedy, if you take. What happened? You know, we told in terms of tank containing methyl isocyanide being stored. And we also told may be because of the conditions have like a faulty valve which was there and not properly hooded somewhat leaked in and some chemical reactions started.

But mind you, if the system was alright, what we should have had? We should have had a refrigeration coil, which would still keep the methyl isocyanide cool. And somehow it was not working and that is how we got the reaction to take place, temperature built up, the higher temperature caused the rate of reaction to go up. And this cumulative type of a reaction which keeps on increasing with increase in temperature is what caused a lot, caused the leakage, or a high pressure. And the leakage of methyl isocyanide, the isocyanide liquid and vapor got leaked and that is what affected the people.

Therefore, you find that yes we have to keep the pre heat to a low temperature, and may be or what is the procedure is maybe you should increase the heat loss from the system.

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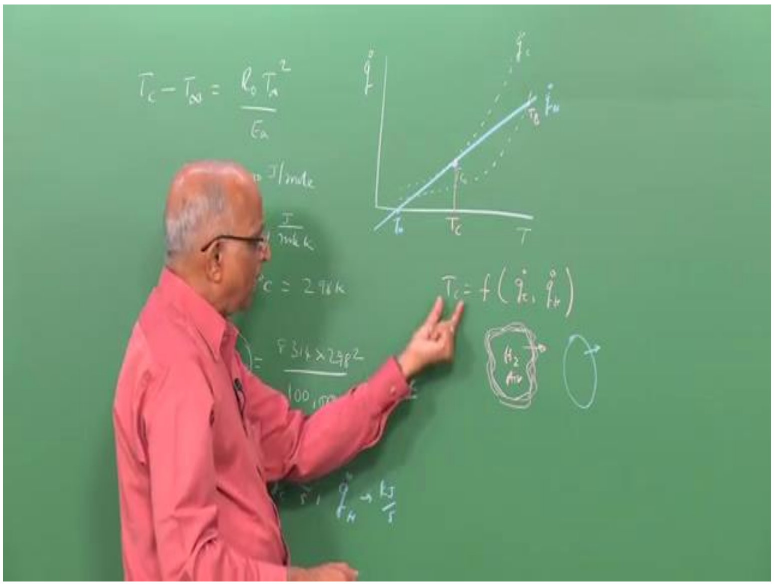

Therefore, now we ask ourselves one question you know, see we are telling well the temperature T c, the ignition temperature T b, and also the stable temperature T a, depend on heat generation q dot c so much kilo joules per second. And also the heat loss from the system, namely q h dot which is also in kilo joules per second. It is the competition between these two which gives me my critical temperature that is the auto ignition temperature and the ignition temperature.

But is it really so? You know let us put this figure again because you know we need to be clear about this you know, we talk in terms of generally q dot kilo joules per second, we talk of temperature. We say well the heat loss rate is given by this we call it as q dot h over here, this is the ambient temperature at which well the heat loss from the explosive to the ambient is 0.

Now, the below this temperature well the explosive receives heat from the ambient. For the condition of auto ignition, you have the heat release curve which is show by dotted line over here, something like q dot c, and this is my point t c. If I had, something like an ignition temperature I am looking at, maybe I would be looking at something like this over here, this dotted line this is my ignition temperature t b. But we are let us focus first on the auto ignition temperature, that is the critical temperature, T c over here.

Now, this T c is when the heat release that is q dot c is same as q h, and we also said the two conditions are it is equal, and the line is tangent to this particular curve q c. That means, auto ignition temperature really depends on, let us say T c should be a function of q c dot, and also the heat loss to the surroundings.

Therefore, the auto ignition temperature if I take, if I supposing I want to measure the auto ignition temperature of let us say hydrogen with oxygen or hydrogen with air. Therefore, you know if I want to do this well, if I have a casing in which this particular explosive is contained is something made of ashes, and this is the structure in which the gas is contained over here. And in one case, it is made of stainless steel which allows some amount of leakage of hydrogen.

In the other case, I have it made out of some, out of some material and in some other geometry such that, it does not allow the heat to go through. Well the auto ignition temperature in these two cases will be different, it is a system problem because it decides on the heat generated and how the casing allows the heat to get transferred. Therefore, it is a system problem therefore, but you know if I look at the literature, I get values of auto ignition temperature which is given. Let us take a look at some values which are given in literature.

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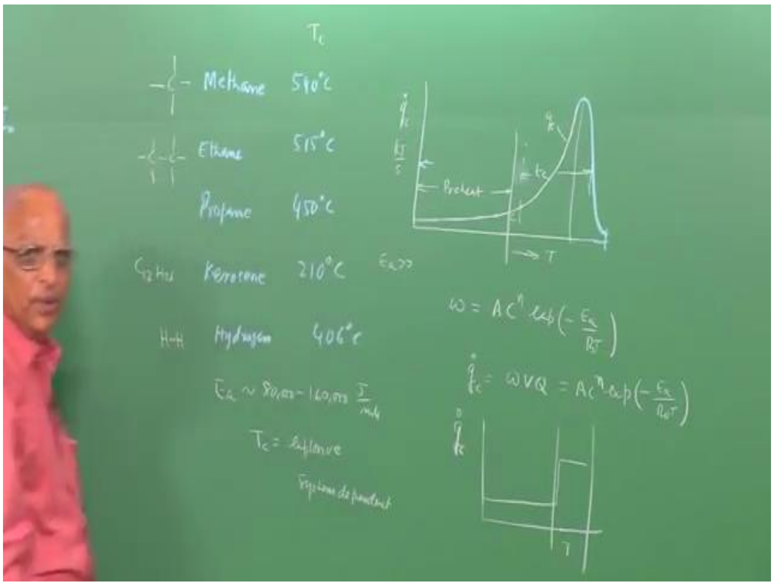

You know we find that yes we can have for methane, the auto ignition temperature is given as 540 degree centigrade. If I go to ethane, methane is CH 4, this is C 2 H 6, the value is 515 degree centigrade. Let us put some three or four down and discuss why, how they are able to specify this?

In the first place if it is a system level problem depending on the type of system well, the auto ignition temperature should change. Propane is 450 degree centigrade, if I take kerosene now I go to a large molecular mass substance kerosene, again in the same alkane structure, it is equal to 210 degree centigrade. And I take the last one may be hydrogen, the auto ignition temperature is given in the literature as something like 406 degree centigrade.

How is it that the auto ignition temperature is given as a property of the fuel? Mind you, this is mixed with air, air, air, we are not talking of anything about heat loss or the system under which the auto ignition temperature is measured. Is it really right, are there some reasons? Well, the reason is, whenever we talk of these substances, we talk of all explosives as we keep telling are, substances which have large values of activation energy, that is the value of activation energy Ea, we said is typically between 80000 to something like 160000 joule per mole. When the activation energy is high what is the implication?

Let us see the implication, if I were to make a plot versus temperature over here, and let us say I have q dot c over here, what is going to happen? Well at the ambient temperature low temperature the value, let us put down the value of omega, omega is equal to the rate of a reaction is equal to A concentration n exponential minus Ea by RT.

If I look therefore, at q c dot, q dot c the rate at which heat is getting generated, which I want to plot over here kg per second well, it is equal to omega into that is so much moles per c c second into volume moles per c c into the heat which is generated per mole. And therefore, q c dot is equal to AC n into exponential of minus mind you, it is universal gas constant R naught minus Ea by R naught T over here.

And we found that, for large values of activation energy, it goes slowly initially with time and temperature that is both can be represented on this axis because as time increases, temperature also increases. Therefore, as a function of temperature, if I were to plot this well, initially the temperature increases rather slowly because of large value of this. And after sometime well, it goes off exponentially when the value of Ea becomes sizeable, corresponding to R naught T becomes sizeable with Ea well, it goes off.

And therefore, what is happening is you have a period in which there is hardly any temperature increase, and after sometime which corresponds to the critical value or the auto ignition value, and that is where it takes off and this is what we said preheat. That is during the preheat process, what really happens is, there is small perceptible increase in the temperature, and that causes the reaction to proceed further faster, and after the pre heat stage is over well, the reaction goes fast.

And this is why, what happens is the actual heat is liberated in this particular phase and mind you, we did this total problem also, we said it reaches a maximum. When there is still some concentration left and therefore, thereafter it drops down like this, and this is when the total temperature total reaction is over and the maximum temperature is reached. After this, there is hardly any change in temperature.

And therefore, what is it we find well, you have a period in which heat is getting released after a certain amount of pre heat. And during preheat, some chemical reactions occurs it is something like an induction time, a time during which the reactions occur and make sure that the quantities of the change which are required to make the reaction go faster ready. And once that is ready well, it goes into this. Or rather I can, I can now re plot this reaction as saying well, my q c dot as a function of temperature is almost something like in a, in some phase. The temperature is not changing at all I will go through it tomorrow, or in the next lecture.

And then after sometime well, I have a step increase and this corresponds to the rapidly increasing phase. Therefore, this is the duration of chemical reaction. And since the chemical reaction occurs over a much shorter period well, this is the chemical reaction time. Since, the chemical reaction time takes place well, you know this is the period may be I will just therefore, say this is the period from here to something like, this is the chemical reaction period.

Since, this is much shorter than this, what is happening? During this short period of time, there is not much time for heat to get rejected and therefore, the heat transfer really does not play a role because this is occurring very fast and therefore, the question of heat transfer does not really affect my T c when the value of activation energy is large. And for these substances, we do find well the activation energy is large and therefore, these explosives that means, methane with air, ethane with air, propane kerosene vapor with air, and hydrogen with air, are things which have a large value of activation energy.

So, also the condensed explosives liquid explosives which we talk of and therefore, we say well under these conditions T c that is the, that is the auto ignition temperature is sort of a function of the explosive only. That is the chemistry of the explosive alone, and does not, and is not a system dependent parameter by system dependent parameter I mean under all conditions of experiments. The heat loss from the system, or the type of wall of the system does not really affect my auto ignition temperature.

Therefore, this is what we learn about auto ignition temperature and therefore, it is still possible to decide the auto ignition temperature as a function of the chemistry of the explosive. What we find from this table is, methane has a simple structure, as the structure becomes more and more complicated or more and more involved, the auto ignition temperature drops. Until for kerosene it is dodecane that means, I am talking of C 12 into H 26. Well, the auto ignition temperature has decreased, we find as the structure becomes more complex it ignites little bit easier.

But it also depends on the structure of the substance like for instance, H being a structure H 2 over here has a much higher value than many of these alkanes over here. Like this you know, in literature you have values of auto ignition temperature, and they are not a function of the containment, or the structure, or the system they are in, just because it so happens that the activation energy is a large number.

Well, this is all about the auto ignition temperature, the ignition temperatures, the same thing holds good. But since we talked of the time for, time of the chemical reaction, can I put this down in terms of chemical? Can I get an expression for the time for chemical reaction?

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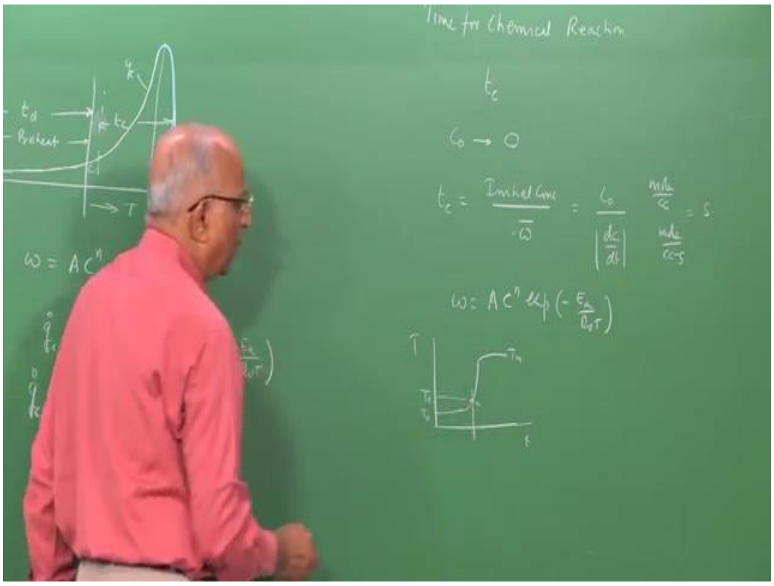

Can I get a value like, let us say T c, can I derive an expression T c, and discuss further? See, because you know when we talk of pre heat, which corresponds to the induction time, let us call the induction time as t d.

Whenever we talk of a large value of activation energy well, I have long induction time followed by a small value of chemical reaction time, let us first get an expression for T c and then, we will later on take a look at the induction time. If we take the time for a chemical reaction well, I can tell myself you know, chemical reaction liberates heat, and why does it liberate heat? The initial concentration from C naught it falls to a value 0 at the end of the reaction.

Therefore, I can tell myself well, the time for a chemical reaction, after all I am interested in time that means, I have initial concentration, divided by the mean value of the rate of reaction, let us say omega mean value. Rather I can put this down as equal to C naught which is the initial concentration, divided by dc by dt. Let us not look at the sign, we just say well the value of dc by dt, C naught has units of mole per cc, this has units of mole per cc second.

And therefore, the unit of initial concentration divided by the mean reaction rate, comes out to be second, and that is the chemical reaction time. Can I get a value for this? If I were to get a value for this, I must also say well my omega which we just discussed, We said is equal to AC n exponential of minus Ea by R 0 T well, the temperature is continuously changing, and what is the change in temperature we see?

Well, you know to begin with well, with respect to time, the temperature starts at T 0, it starts slowly, after some time when the pre heat is over it jumps up and then, well the temperature steadies out and you reach a maximum value. You know therefore, we find that till that time, the critical condition is reached that means, the temperature is T c. There is hardly any reaction, and chemical reaction is starts here at a high value. Therefore, when I refer to the mean value, maybe I should be taking off in terms of the T c value.

And therefore I can write the value of the chemical reaction time, or the T c as equal to C naught divided by I say A into concentration n, into exponential of the value of minus Ea by R 0 into T c, and this gives me my mean chemical reaction time. Well, we talk of time for chemical reaction, you know we must also remember, yes while evaluating the auto ignition temperature well, we find that the chemical reaction are not important as long as the activation energies are large.

But, in an ordinary situation well, the balance between the chemical time and the heat loss time, or we must consider the heat loss also, can I have something like a time or characteristic time for heat loss?

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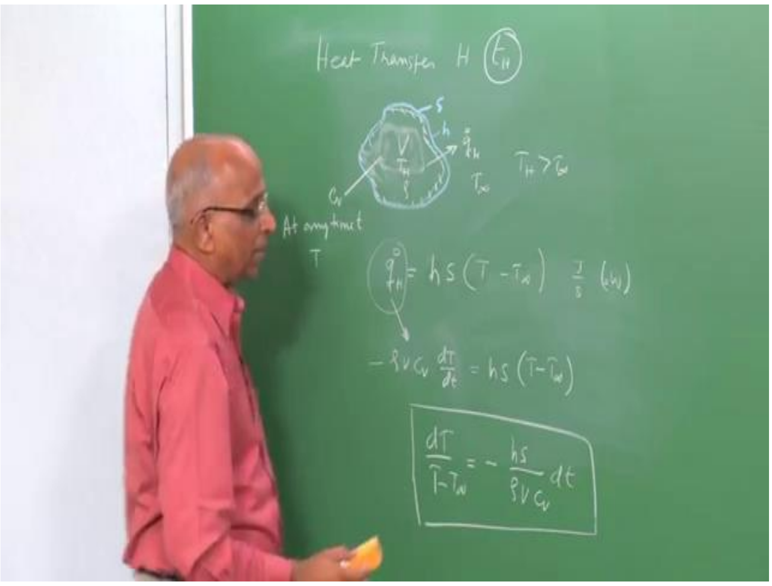

Let us, let us take a look at this, the question I am telling is see we talked in terms of heat generation. We say well, heat generation initially is very low and thereafter it picks up. And we are talking of a heat generation time which is, which is characterized by the heat time for chimerical reaction T c. Supposing, we are talking of heat loss, can o also have a characteristic time associated with heat loss, or let us say heat transfer? What is the time associated with heat transfer? Let us say, I am, I have heat H therefore, I say, what is my characteristic heat transfer time? Can I define, can I determine it?

To be able to do that, let us take a look yes, I have a volume of explosive, let us say volume, we are again locked in this particular assumption of this volume containing the explosive gas mixture. We say well, it is a lump mass system, the properties are uniformly same throughout this particular volume over here.

Let that temperature initially be, let us say hot, I am just not looking at chemical reactions, I am interested in heat transfer. I say let the temperature initially be t h over here, let the volume be v meter cube dot v over here, let the substance be of density rho is uniform throughout. And this lump mass, let us say is rejecting a certain amount of heat q dot h to the surroundings that means, it is losing some heat.

To be able to lose heat well, the ambient temperature T ambient must be lower than t h that means, t h is greater than T ambient. Can I get an expression for q h? Yes, we have been doing this, and what did we do? We had the boundary, at the boundary we said let the surface area of the boundary be S over here. Let the heat transfer coefficient at the surface be small h so much watts per meter square Kelvin.

And therefore, what is the rate at which heat is getting lost from the surroundings, to the surroundings? q dot h is equal to the area into the heat transfer coefficient or I should rather put heat transfer coefficient, into the surface area, into we say t h minus t ambient is the total heat which is getting lost. Therefore, at any point, let us say the initial temperature is t h, let us assume at any time T that means, at T is equal to 0, the temperature is t h, at any time T, let that temperature of this lump volume be T, why is that?

Because it is losing heat, the temperature is falling therefore, we say well, the heat loss when the temperature T within the body is T, the ambient temperature is T ambient. Because the ambient temperature remains same because it is something like a reservoir, its temperature does not change is equal to so much, so much joules per second, which is equal to watts over here, so much watts.

See I am interesting in a time element, I am interested in how the temperature inside this body is changing, and based on the change just like we had a heat release curve I was able to define something like a chemical reaction time. I want to determine a heat transfer time how do I do this? If I look at the value of the heat which is lost, why is it is losing heat? I have a certain mass over here, a thermal mass whose temperature is changing. And therefore, if I look at this well, the mass of this particular volume is equal to rho v is the mass. If the specific heat of this is the constant volume let this specific heat be Cv so much so much joules per kilo gram Kelvin.

Therefore, I say well rho vCv is the thermal mass over here mind you, the thermal mass in terms of mass into specific heat, and what is the rate at which the temperature is changing? Well, it changes by let us say a small volume dt delta T in a small time, small time, delta T over here, which if the, if the time elements are small, I can call it as dT by dt that is, d capital T by small t. Well, it is losing heat, this is negative therefore, I have minus rho we Cv dt and this must be the value of q h.

Therefore q h can write it as again equal to hs into t minus T ambient, this is the rate at which it is losing heat. And therefore, now I can write this expression as dt by t minus T ambient is equal to minus, I bring the minus over on this side, I have minus hs over rho v into Cv. This is the thermal mass of this particular system, and h is the heat transfer coefficient at the surface, s is the surface area through which heat is getting transferred outside, I have dt by this.

Now, I want to find out what is the net value or net change in temperature corresponding to this well, I had dT by dt here therefore, I should have had dt over here. Well, this is my expression in the differential form. Well, to be able to calculate the time required for the heat to be transferred that means, let us find out the time taken let us put that down.

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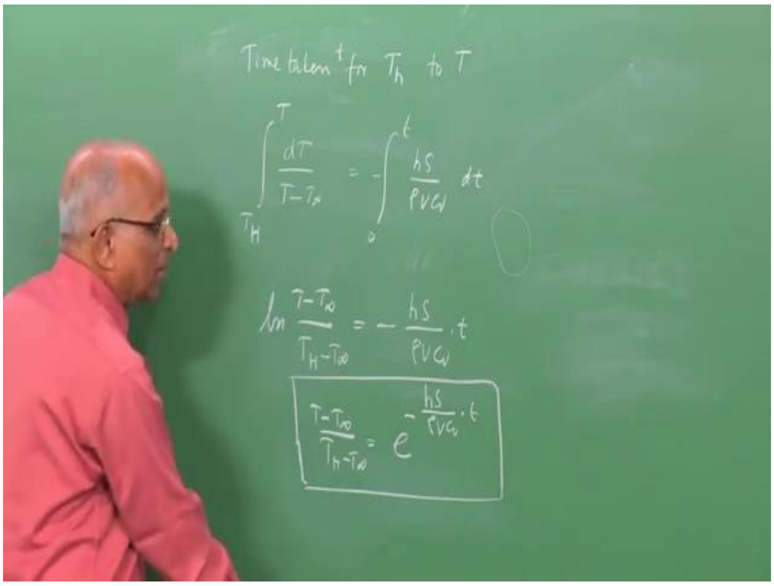

We are interested in finding out the time taken for the heat which is getting generated hat is, let us say time taken for the temperature to drop from a value T h to T that mans, time T which is taken, or let us say T taken for temperature to draw from T h to T.

Therefore, I just integrate this expression from, let us say dT by T minus T ambient. I integrate from the initial value h from the hot value to any temperature T h. let us say T capital H is the initial value, and what does it correspond to? It is equal to the time taken on the right hand side is equal to minus hs divided by rho vCv into dt over here. When I, when I integrate this expression that means, I go from the high temperature to the low temperature, and it is losing heat, I go from 0 to T over here.

And therefore, what is it I get? I get well, this is lawn form therefore, I get lawn of T minus T ambient that means, T that is lawn of T by T infinity, the limits of integration are from T h to T. Therefore, lawn T minus T infinity divided by T h minus T infinity is equal to minus that mans, ambient temperature over here minus hs divided by rho vCv into the time over here.

Or rather, if I were to put it in explicitly in terms of this, I can write T minus T ambient divided by T h minus T ambient, take exponential on both sides, I get e to the power minus hs divided by rho vCv into time over here. Let us try to plot it, let us try to discuss it, what is my characteristic heat transfer time?

Well, this is what we say is the Newton’s law for cooling anybody which is hot, when it is radiating out, it follows this particular law as exponential to the power minus hs by rho vCv T where rho v is the mass, this is the specific heat into the time. Well, let us try to plot this out and see whether we can, we can infer something on the characteristic heat transfer time. We plot that value let us see, you know the initial temperature was let us say hot temperature.

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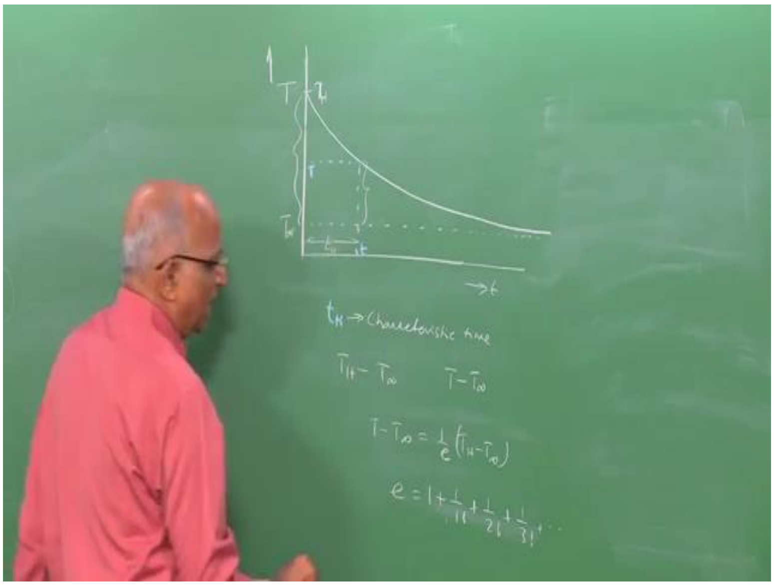

This is my temperature axis, the initial value is T h over here well the ambient temperature is T ambient. What is this, what does this expression tell us? At any time T, the temperature is t minus T ambient, and if I want the final temperature to be equal to ambient temperature, I get 0 here, or that will happen only after infinite time.

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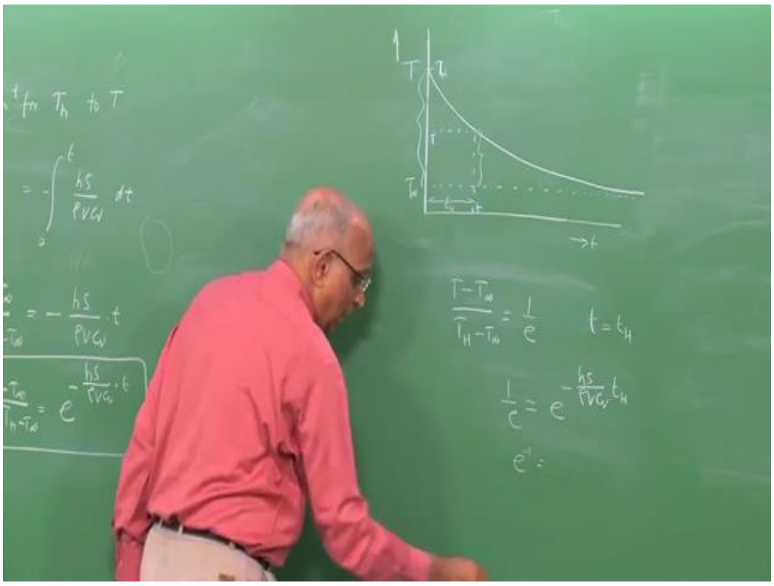

Or rather, if the, I can get the final expression reach the final value, this is the time axis over here, rather I start over here and it keeps on going, and it takes infinite time to reach the ambient value.

At any intermediate value T at which I am interested in. At any value T well the temperature is T over here. But then you know according to this it is a gradually decreasing value, and it never really reaches the ambient value, it takes infinite time, it is almost impossible to have something like a characteristic heat transfer time. You now there is no point in telling well, the heat transfer takes infinite time by which I cannot really make much sense out of it

But one thing we also see, in this particular expression we see. Since, it is exponential, the major changes takes place in the initial phase, and after some time well, the changes are very small. If that is so, can I, can I still use this figure and write? Well, can I write a characteristic heat transfer time?

You know, mind you, I am not able to clearly pursue a heat transfer time from this particular curve, but since the major changes are occurring in the initial phase. Well, I say the initial value, or initial or, initial value of the heat in the body compared to the ambient, it is T h minus T a ambient. At any time, we say it is equal to T minus T ambient, we tell ourselves well, it is gradually falling fast initially. Therefore, if I say T minus T ambient is equal to 1 over e, 1 over exponential of let us say T h minus T, T h minus T ambient.

That means, since its exponential, what is happening? See exponential curve, if I say the value of e, what is e, is the Neparian value, that is we say log to the power e, that is the Neparian base e, and e is equal to, we say 1 over 1 plus, 1 factorial plus 1 over 2 factorial plus 1 over 3 factorial and so on. What does e say, see it is something like it takes care of the cumulative effects and therefore, if you take the cumulative effects and you say well, based on the initial value which is this.

Well, I say when the value is 1 over e of this well, this could be my characteristic heat transfer time. Because beyond it the values are changing rather slowly therefore, I tell myself well, I define the heat transfer time as the time required for the value to fall to 1 over e of the original value. And therefore, I tell well in this particular expression now I can put this value down.

I say well, it is an exponential decrease and therefore, I write when T minus T ambient divided by T h minus T ambient is equal to 1 over e value. Then, I say well, my characteristic time is equal to the heat transfer time and therefore, let us workout the time based on this particular expression.

Therefore, now I say T minus T ambient divided by T h minus T ambient is 1 over e therefore, I say 1 over e is equal to, on the right hand side here, I have e to the power minus hs by rho vCv T. That means heat to the power minus hs divided by rho v into Cv this becomes my characteristic heat transfer time because I am, I presume that this is the time during which the maximum heat transfer takes place, afterwards its going slowly.

And therefore, on this left hand side, I have e to the power minus 1 is equal to e to the power minus therefore, minus 1 is equal to this value, let us put it down and see what we get.

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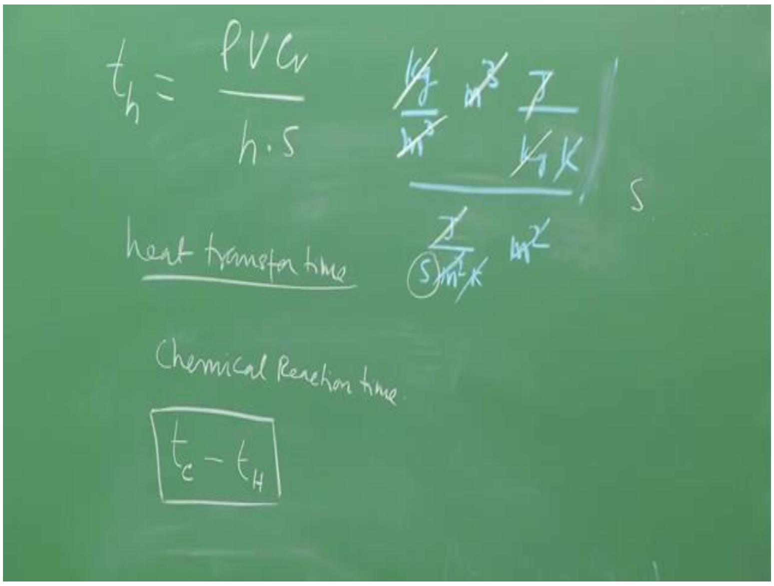

Therefore now we will, we will, get a value, say minus 1 is equal to minus hs divided by rho vCv into t h over here that is the characteristic heat transfer time, minus and minus gets cancelled and I get t h is equal to rho vCv divided by h into s over here.

Let us ensure that the dimensions are alright, rho has units of kilo gram per meter cube, volume is so much meter cube, specific heat unit is joule per kilo gram Kelvin divided by…What is it we get? The unit of h let us just put it down over here, the unit of h is joule per second watts per meter square Kelvin, and s is meter square the surface area.

Therefore, what is it I get? Meter squared. meter square gets cancelled. Kelvin and Kelvin is gets cancelled over here. Kilo gram. kilo gram gets canceled meter squared gets cancelled joule gets cancelled. We are left with time and this is second. Therefore t h in seconds is the ratio of the thermal mass of the system rho vCv divided by the product of the heat transfer coefficient into the surface area through which it is rejecting heat. Therefore, now we are able to get a characteristic heat transfer time.

And let us see whether I can make some sense out of all this, whether I can relate. The characteristic heat transfer time with the characteristic chemical reaction time. Rather I am looking at an expression between T c and t h over here, is it possible?

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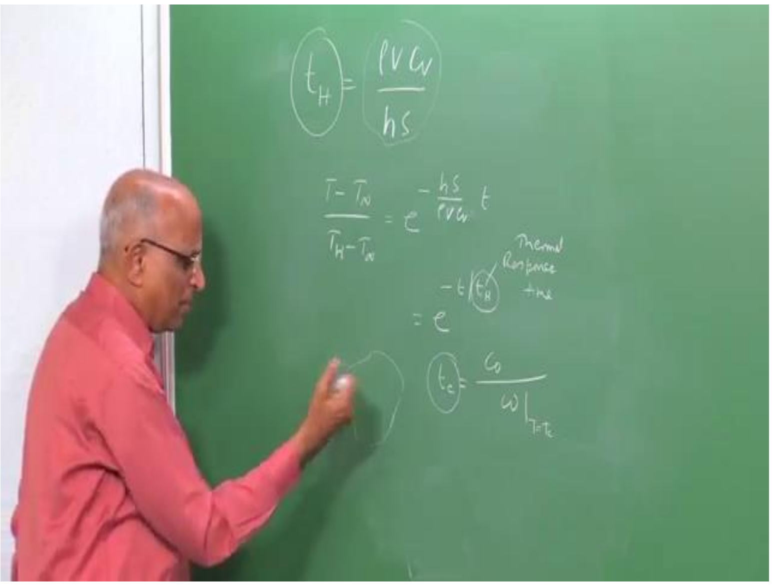

Before doing that let us, let us let us discuss what is the role of these times, whether they may have something to do in the case of an explosion. And therefore, let me broaden the discussions at this point in time, we tell ourselves well, I have been able to calculate the heat transfer time let us let us let us put it down I say well t h is equal to rho vCv divided by hs. You know many people also call the heat transfer time in terms of may be the thermal response of a system. Why is it? If Itake a look at the expression, I have T minus T ambient divided by T h minus T ambient.

That is the initial value is T h over here, we had it equal to e to the power minus hs divided by rho cVv into something like rho, Rho Cv into v. Or rather I should have put it as rho vCv into the time over here. If now I were to put this characteristic time over here, I get is equal to e to the power T over the characteristic heat transfer time, and this is sometimes known as the response time of your particular body.

We say well, the body is hot, it takes a time T h to respond, and we get e to the power minus T by T h is the, is the dimensional ratio of the excess heat compared to the ambient into the denominator divided by the excess heat at any particular time over here. Therefore, this also talk in terms of the thermal response time. Whereas when we talked of the chemical reaction time, what did we tell? Yes chemical reaction time is the initial concentration divided by the rate of chemical reactions at, when the temperature T is equal to the critical temperature over here.

Now, I want to examine whether there is some relation between T h and T c for which we wanted to discuss a little bit more and see whether, there is some relation. Let me consider the following cases, let me consider the following.

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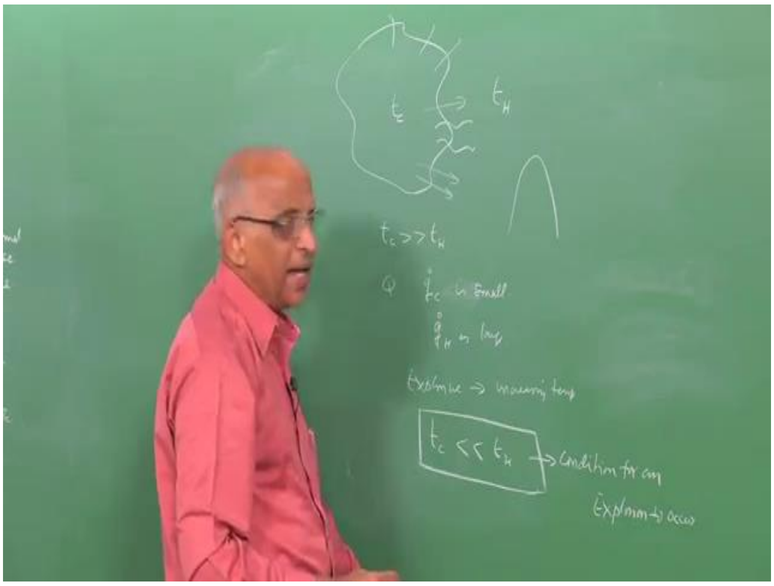

Let us say I have a substance over here, an explosive substance an energetic substance well, the substance in the given medium or in the particular system in which it is contained, has a characteristic heat transfer time T h. If the characteristic chemical reaction time of the substance is T c. And if we say well T c is very much greater than T h, what is the implication? In other words, all what we are saying is well, T c is larger than this therefore, if I say some heat is getting generated then, I say well the heat is getting generated over a large time.

That means the value of q dot c is going to be very much less that means, the time for heat generation is large therefore, the rate of heat generation is small q dot small. But, since the heat transfer time is now much smaller than the chemical reaction time, the rate at which heat is getting lost that means, q dot h is large.

That means, the before some significant amount of heat that mans, heat is getting generated, heat is also getting lost. Since, the time of the chemical reaction T c is large, even before some heat is getting generated since, the time of this heat transfer is much smaller than T c. Well, it gets dissipated into the medium, and the explosive can never equally sort of go into this cycle of increasing temperatures and have chemical reactions which generate more and more products. And therefore, it explodes the explosive cannot really explode.

While, if the chemical reaction time is smaller than the heat transfer time well, what happen? During the short time itself, the chemical reactions takes place, heat gets generated therefore, q c is very large. Whereas, since the heat transfer time in this case is large you know, what is happening? It is not able to transfer out the heat which is getting generated, and that was the condition we observed. You know when we have a spike in the reactions, the heat, the rate is so fast, and whatever be the time the time is quite large compared to this.

And therefore, the amount of heat which is conducted away or which is sent away is much smaller. And therefore, heat begins to accumulate here because of the heat accumulation, the temperature further increases and it goes into a cycle, and all of a sudden you have a spurt in the energy release. And therefore, this condition of T c being very much less than T h will be a condition for an explosion to occur. I think I should repeat, this is a slightly different language what have, we said so far. An explosion occurs when the activation energy is large. In other words, all what we are saying is an explosion takes place,

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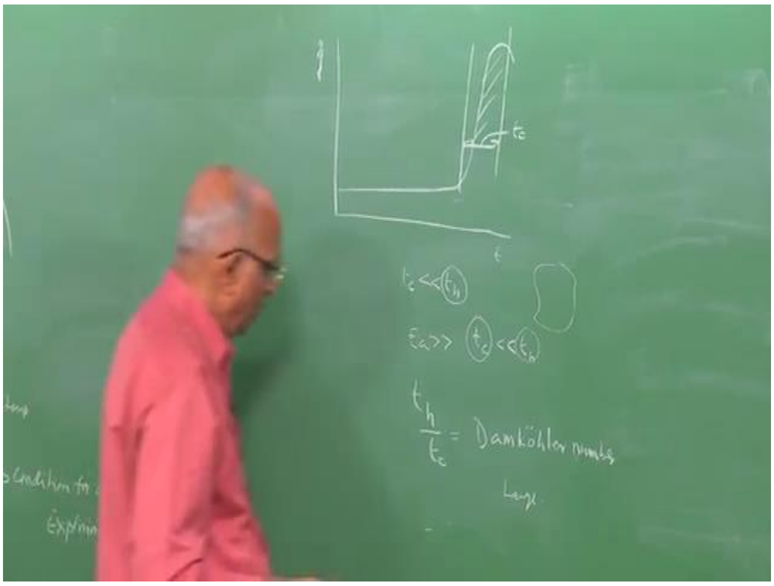

When the rate of heat release is such that, we say q dot as function of time is such that, initially nothing really much happens. All of a sudden there is a spurt in the rate of a reaction, lot of heat is generated and you have an explosion taking place here

That means, the energy release takes place over a very small time. But along with this, we also now see, if I were to now say well, my chemical reaction time is such that I enclose it in a system, in which my heat transfer time is much larger that means, T c is less than this. The heat from heat transfer is such that, it takes longer time for the heat to get transferred out. Therefore, there is accumulation of heat during this short time. Well, the system which is their, keeps on increasing in temperature and it sort of explodes, that is one. Second is well therefore, we say the activation energy being large, indirectly gives us the condition the T c is very much greater than T h.

Therefore, let us, let us work on this let us, see what is the relation we get between T h and T c. And it is a, and it comes out that we will be able to catalog an explosive based on this particular ratio. And this ratio T h by T c we said well, heat transfer time must be larger than the chemical reaction time is told the ratio T h by T c is known as Damkohler number. And for an explosion to occur, the value of the Damkohler number must be large. That means, the characteristic heat loss time must be very much greater than the chemical reaction time. Let us try to use this let us, try to see whether we can get the expression for the type of explosive, which will undergo an explosion.

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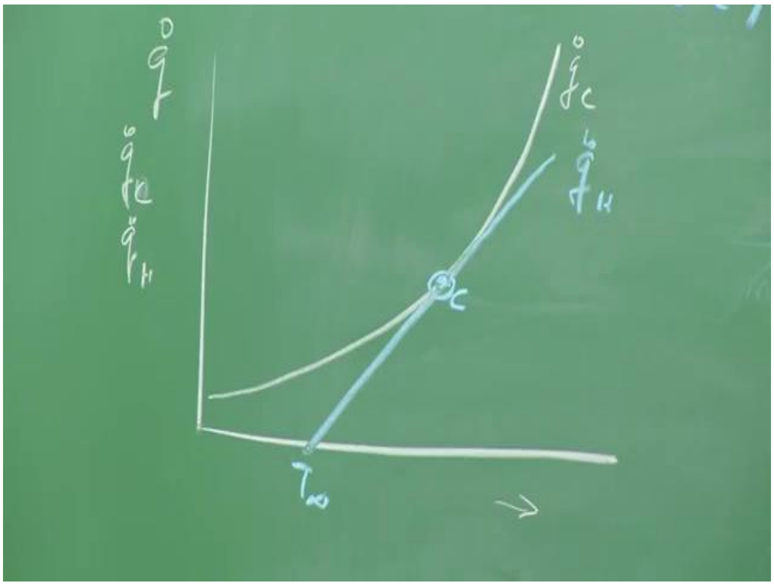

Based on these two times since, we have determined these two times, it should be possible for us to put it together. Let us say I am interested in the ratio of T h by T c. Well, I say, well I have just now calculated the value of T h and, what was it? It was equal to rho v into Cv divided by hs, so many seconds. What was the value of T c?

Well, T c also I know, it is the initial concentration C naught divided by the reaction rate, and at what temperature do we say? Well, we take it at the critical temperature that means, AC n that is omega AC n into exponential of minus Ea by R naught into T c. I want to get the expression for this. Can I simplify this in some way? Can I, can I get? You know now, you know it is quite difficult to solve this, I have an exponential term, I have T c here, I have all these properties over here.

You know, can I solve it, and get the expression for T h by T c based on which I make some recommendations. Therefore, let us try to solve it you know we also recognize when we talked in terms of the energy loss and energy gain. That means we had q dot over here, which could have been q h and let us say, q c, q dot c and q dot h, as a function of temperature. What did we say?

Well, the q c curve was something like this, q dot c curve. And the q h curve was a straight line, this was the point c, we had this is T ambient over here, and how did we determine T c? The value at T c, and or the value for the condition c? We say that, the magnitude of q c dot is equal to the magnitude of q h dot point one. Second is, the q h curve is tangent to the q c curve at point c.

Therefore let us, let us look at the tangency condition and see whether I can simplify this expression. We will go to the other side of the board and try to solve this.

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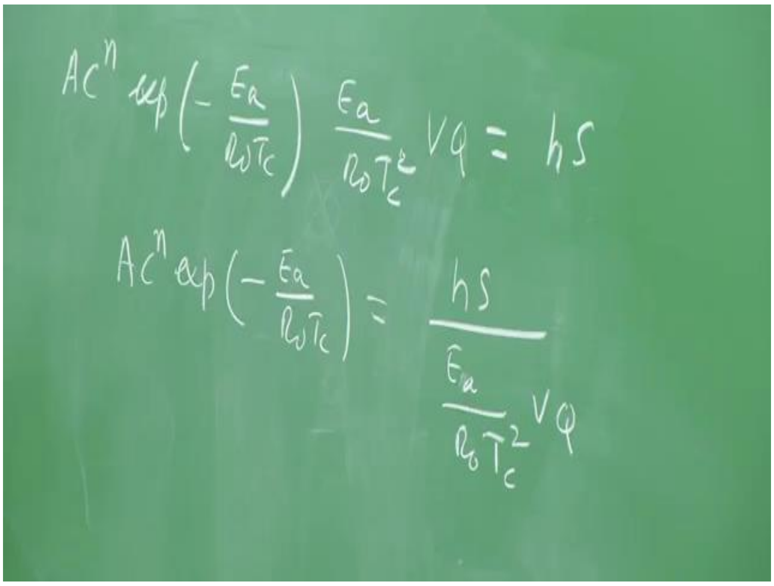

$$AC^n \exp\left(-\frac{E_a}{R_0 T_c}\right) \frac{E_a}{R_0 T_c^2} Vq = hS$$

$$AC^n \exp\left(-\frac{E_a}{R_0 T_c}\right) = \frac{hS}{\frac{E_a}{R_0 T_c^2} Vq}$$

Well, we have the expression d by dT, that is the tangent because the x axis is time axis AC n exponential minus Ea by R 0 T. That is we are looking at tangency condition at T is equal to T c. We also found that it, this is per, this is equal to so much moles per c c second.

Therefore, I had to multiply it by v to get moles per second. I would also to multiply it by q to be able to convert that means, I had so much joules per mole that was the value of v over here. Therefore, we had AC n exponential minus Ea by R 02 into v into q. And this was equal to the value being tangent over here, the heat loss was equal to hs into T minus T ambient. Let us change the bracket to a curly bracket over here, this was the condition. Let us, let us solve for this, what is it we get?

This is under T is equal to T c therefore, I can write it as AC n into exponential minus Ea by R 0 T c, at T equal to T c, differentiate this, I get e 0 minus and minus e 0 by R 0 T. This becomes minus T square therefore, minus and minus gets cancel over here e 0 R T square into v into q is equal to, this differentiated gave us hs because T ambient is a constant. And therefore, I had the expression, AC n exponential of minus Ea by R naught T c is equal to, I get is equal to hs divided by E 0. I am sorry, it should have been activation energy Ea divided by R naught into well, I am evaluating it under condition T c square over here.

That means this should have been T c because I am, I am evaluating it at the critical condition T is equal to T c into v q. Well, this gives me the expression for AC n exponential minus Ea by R T c which is in the denominator over here. Therefore I can write this expression as let us, let us use this part of the board to write the final expression.

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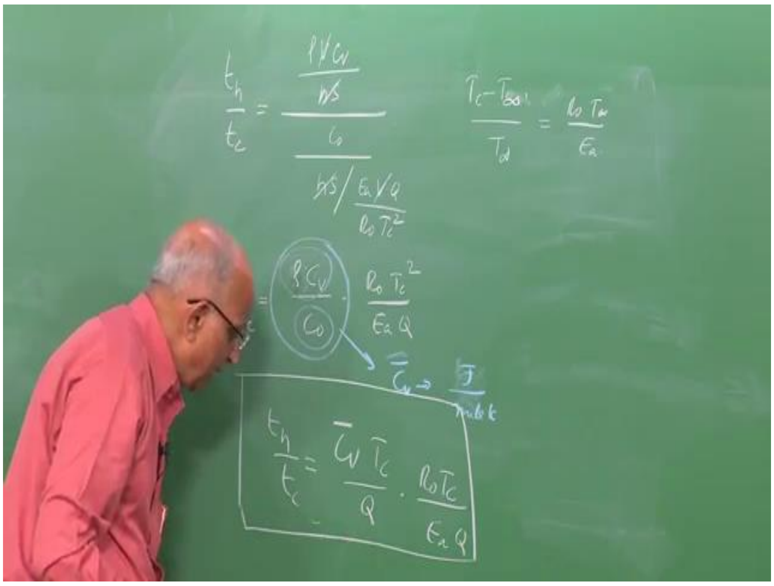

I get the value of T h by T c as equal to rho vCv divided by hs divided by now, I get C nougat divided by the value what I get here, again hs divided by Ea activation energy into v into q divided by R nought into T c square. I want to simplify this and therefore, I note well hs should have go on the numerator, and this and this gets cancelled. I also get well the volume and volume get cancelled because this comes in the denominator, this goes in the numerator.

Therefore, I get T h by T c as equal to rho v divided by rho v has already got cancelled rho v gets cancelled with v over here, I get rho Cv divided by C 0,. Rho Cv by C 0 into the value of R naught into T c squared divided by Ea into q. Let us check this T h by T c is equal to rho Cv divided by C naught into R naught into T c squared goes on top into activation energy into the heat release per mole.

Let us see whether I can simplify some of these things. You know if I talk in terms of the thermal mass, and if I talk in terms of the initial concentration well, I am talking in terms of may be kilo gram per meter cube. I am talking in terms of Cv so much joules per kilo gram kelvin. I am also taking in terms of moles here let us say, moles so much centimeter cube or meter cube. I am talking in terms of moles per meter cube.

Therefore, you know this expression tells me something like kilo gram and kilo gram gets cancelled over here. I am talking meter cube, meter cube gets cancelled. This is something like joules per mole into Kelvin that means, we are talking of specific heat per mole, and we can say this is equal to Cv bar wherein, we are talking in terms of so much kilo joules or joules per mole Kelvin, which is equal to the specific heat in per mole.

And therefore, I can write this as equal to Cv dash, which is instead of taking in terms of joules per kilo gram, I am considering joules over mole Kelvin. And therefore, I get the value as T h by T c is equal to the specific heat into let us say, T c. I bring one T c here divided by q over here. And then I am left with R naught, T c by Ea that is activation energy into q. Well, this becomes my expression for T h by T c.

Let us try to see, whether I can make some sense out of it? Can I put it in some other form? Can I use this which I have studied already to be able to interpret it. First of all, I would like to say well, you know we have already learned that, T c minus T ambient, which is their pre heat value, is a small number. And we said T c by minus T ambient divided by T ambient.

That means, I should have put it as T ambient over here, T ambient over here is equal to R naught T ambient divided by, we had Ea activation energy over here, which was a large number, and this was very small. And therefore, we say when the activation energy is very large well, T c is almost equal to T ambient. And therefore, I can simplify this expression, and write it because we are interested in trends, we are not working out a numeral.

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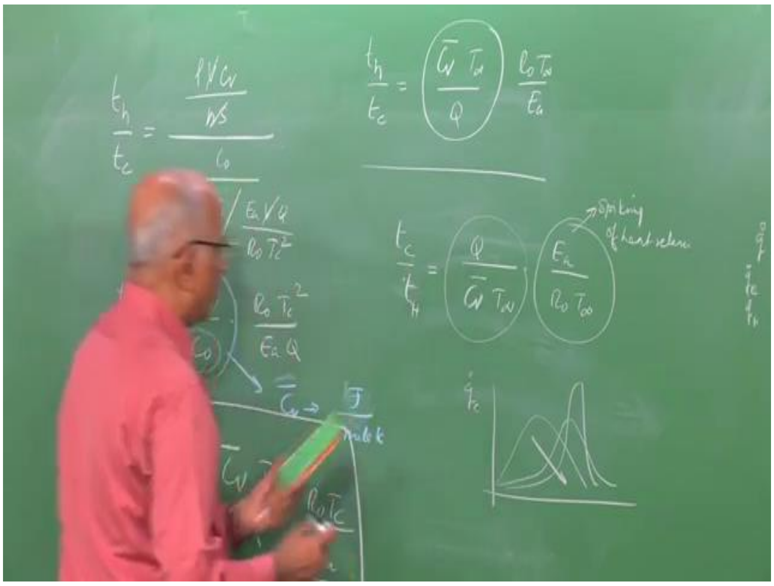

And therefore, I can tell well, the value of T h by T c is equal to, I have the specific heat in joules per mole Kelvin into T ambient divided by the value of q so much joules per mole, what is getting generated. I have R naught into T ambient divided by Ea, is what we are getting. See here I have taken q twice you know, I should have taken q once may be since, I took q over here, it should have just been over here Ea.

Therefore, I have taken q here and here which was not correct, q is only over here. Therefore, this is the final expression what I get, and what does this tell me? Well, here you are looking at, if I look at the value of q by Cv into T infinity. We are talking about the heat generated whereas, we are talking about the initial heat which is available to you. Here we are looking at the activation energy effects.

Therefore, let us since, we are looking at this divided by this, let us put it in terms of T c by T h, we say is equal to q divided by Cv into T infinity, divided, multiplied by Ea divided by R naught into T infinity. Therefore, you know you see, that this is a dimension a list number, joules per mole, joules per mole. We are talking of the energy release per mole, divided by the initial energy which is a non-dimensional number, which tells me what is the magnitude, how much heat is getting generated?

If I take a look at Ea by R naught infinity, all what it tell me is, what is the spiking which results? We told ourselves as Ea increases well, if Ea is large I have, let us, let us put that down. This is basic to our discussions therefore, we say if I, if I were to look at the progress of the chemical heat generation. Well, when Ea is small, I have this, when Ea is large well it goes like this, when Ea is still large, it goes like this.

Therefore, as activation energy goes, the spiking or the rate of heat generations spikes up therefore, this is a spiking non dimensional term for heat release spiking of heat release. Whereas, this tells me how much heat is getting generated. We also see if the value of the ambient temperature is high then, what is happening? The ambient temperature is high, the amount of heat which, or the amount of spiking what we have cannot be very large because temperature goes up and the spiking comes down.

And therefore, we can quantify the value of the, of the chemical reaction time divided by the heat transfer time, by these two non-dimensional parameters. And mind you, we come to the end of our discussions with this, we told that what we want in an explosion is the time for the chemical reactions must be very much smaller than T h or rather we get the value of T c by t h.

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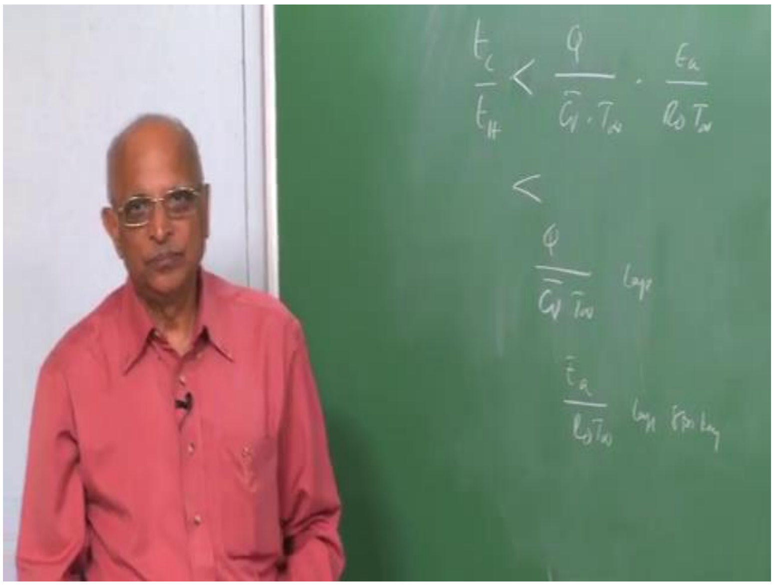

As equal to, let us, let us put that down q divided by Cv into T infinity multiplied by Ea divided by R naught into T infinity. Therefore, if the chemical reaction time has to be much shorter than T h because then only an explosion could occur, we say well this is the number. Well, this number must be a large number because if this is a large number I can get T c by T h to be very much less. I want this to be the condition well. And for this number to be large well, I find q by Cv into T infinity could be large that means, the amount of heat generation must be larger. We also said Ea by R naught into T infinity must be large for spiking to take place.

And therefore, for a chemical explosion to take place, you should have large activation energy giving rise to a huge spiking, and we must also have as much energy as possible to result in a large heat release. Well, this is about the theory for explosion based on chemical reaction time and the heat transfer time. And therefore, what is the conclusion?

The conclusion is well, I should have large vales of activation energy which gives spiking under large heat release, but if my ambient temperature is smaller, I am better off because I can get better spiking and more heat release when the, more heat release non dimensional term when my T ambient is smaller. In the next class, what we do is? We follow this up, we will take a look at the formation of chain carriers during the induction time, and we will interpret one or two explosions.

Well, thank you.