Energy Release: Examples of Energy Release Calculations, Higher and Lower Calorific

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Lecture - 15
Introduction to Explosions and Explosion Safety

Good morning, you know in the last class we discussed about the energy released from explosives when the explosive composition was such that it was either stoichiometry or it was sort of fuel lean that is fuel lean or let us say the oxygen rich.

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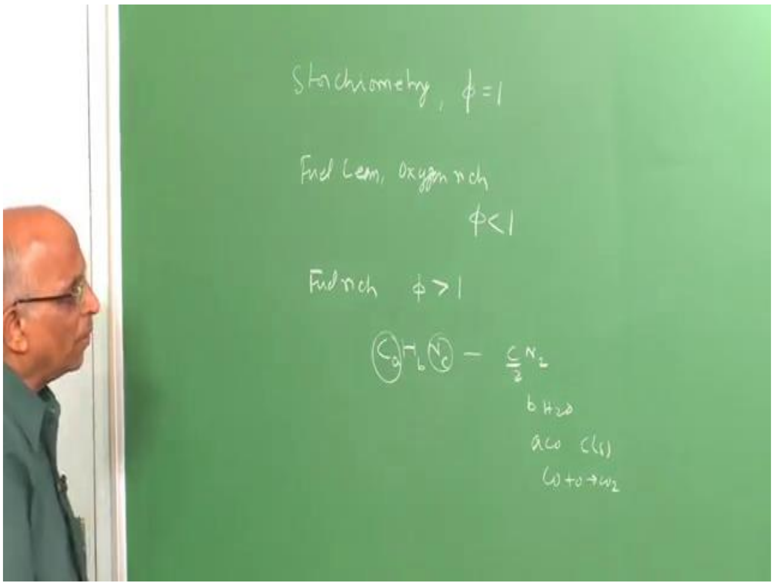

So, when we said something is stoichiometry what we meant is the chemical reactions takes place such that completed products of combustion are found. But, the particular equivalence ratio which we define in the case of air mixture was z equal to 1 equivalence ratio was 1 when they said fuel lean or oxygen rich.

So, we mean there is not, there is, there is excess oxygen which is available more than what is required for the completed products of combustion to be formed. Therefore, completed products of combustion are anyway formed and we are left with oxygen in the products of combustion and when we say it is fuel lean. Well, the stoichiometry the fuel equivalence ratio is equal to less than 1 because equivalence ratio is defined as the actual fuel by air by weight or by mass divided by the fuel by air.

So, for a stoichiometric reaction after doing this to we went into the fuel rich mixture that means fuel rich. So, that means it is starved of oxygen in which case we said in a most of the explosives may be the condensed explosives what we have are generally fuels rich. Therefore, we must learn to how to do this for this, the equivalent ratio if we can put it in terms of some equivalent, equivalence ratio is greater than 1. But, which means there is not sufficient air to burn all the fuel we found it was difficult to do this problem and we, therefore defined a way or an approximate procedure of doing this problem.

So, that approximate method was we said a fuel consists of carbon some hydrogen and may be some nitrogen and what happen. So, let us say the molecule of fuel consists of C a or the mixture consists of C a H b into N C what we said was hydrogen is more reactive than carbon. Now, with the result in this approximate analysis which we find to be quite reasonable for fuel rich compositions what happens is the nitrogen first is available.

Now, in the products as C N 2 at means C by 2 into because I have N C atoms of this it gives me C by 2 into moles in the products. So, after this we look at these two carbon and hydrogen we told well hydrogen is more reactive since hydrogen is more reactive. So, it combines with the oxygen available to give b H 2 O in case sufficient oxygen is available for this particular purpose.

Therefore, I am left with some if I am left with some more oxygen a, of carbon reacts to form a C O provided I can form this. But, else I just get carbon in the solid phase and if oxygen is still left may be some of the carbon monoxide reacts with oxygen to form C O 2. Now, you know let us do an example to determine this and we go back to the same example of the butane air mixture to be able to do this problem.

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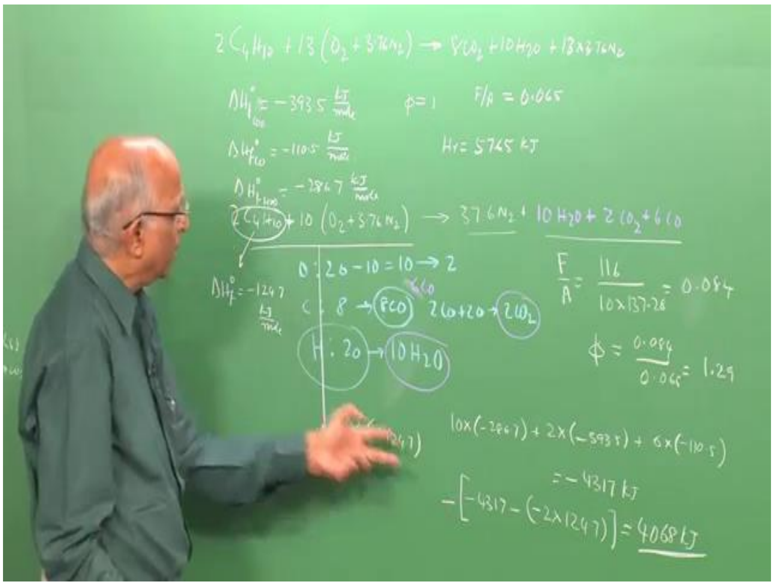

You know we said for a stoichiometric mixture we had C 4 H 10, 2 moles of it plus we had 13 moles of oxygen and each mole of oxygen in air had 3.76 moles of nitrogen along with it. So, for this stoichiometric case I want it completed products of combustion, therefore I had 8 C O 2, I had hydrogen forming 10 H 2 O and I had nitrogen which is now available as 13 into 3.76 of nitrogen in the products.

So, we evaluated the heat content of this particular reaction and we found that in this case 5 is equal to 1 the fuel air mixture in this case. So, that is the mass of fuel divided by air is equal to 2 we had 58 for the molecular mass of it and we had 13 into 32 plus 3.76 into 28 and we had a fuel air mixture. So, the energy release in this in this particular stoichiometric composition was may be the products 8 into heat of formation of this that is per mole.

But, I know the heat of formation 10 into heat of formation of water and this was the products we had so much of the value. So, for the reactants only this was there because these are all elements at the standard state and, therefore we had this and we subtracted this minus this with a negative sign. Now, we had the heat of a reaction which we calculated as equal to 5765 kilo Joules, now we ask this question if the reaction is starved of oxygen.

So, that means instead of having stoichiometric composition of 5 is equal to 1 let me find out in the, if you have I am starving of oxygen. Now, that means I have 2 C 4 H 10 plus instead of having 13, I have 10 of O 2 plus 3.76 of nitrogen this is air over here and, what is it will I get. Now, can I balance this equation, how do I find the products we told well to find the products I first need to assess the temperature and then do some equilibrium. So, find out the chemical equilibrium in which the products can be in equilibrium with each other we can do that using Gibbs' free energy.

But, we said well the problem is the method is a little complex, therefore will do the approximate method. Now, we will observe in this particular case, let me use a colored chalk to determine this, I have oxygen which is available is 20 atoms of oxygen. So, we know the nitrogen is going to come back to me in the products, therefore let us put the products down I have 37.6 nitrogen which is anyway it is, it is assumed to be inert. Therefore, it is going to be come as it is in the products, now I have oxygen atoms which is 20, now I have carbon atoms which is 8, I have hydrogen atoms which is 20.

Therefore, you know you have 10 O 2 plus 3.76 I have 2, therefore 20 of this, therefore if I have to form if hydrogen is more reactive. Well, the oxygen atoms first come and react with the hydrogen over here and, therefore I can form 10 H 2 O, let me do this. So, if I form 10 H 2 O I have consumed 10 atom of oxygen while forming water and, therefore the oxygen atoms I am left is minus 10 which is equal to 10 atoms are still left. So, out of these 10 atoms which are left I have eight carbon atoms well if I have had to form C O 2, I need 16.

But, I have only 10, therefore what happens is the 8 carbon atoms combine with 8 of the oxygen atoms to form 8 C O and still what I am left with is 10 minus 8, 2 atoms of oxygen are still left. Now, these 2 atoms of oxygen of the 8 C O which is found I take 2 C O and react it with 2 oxygen atoms to form two C O 2.

Therefore, what are the products which I am able to form I am able to form 10 H 2 O and then I am also able to form 2 C O 2. So, out of 8, 2 have come over here that means I am left with 2, 8 minus 2 that is 6 C O and, therefore the products of combustion. So, if I have to write I will write it as 36 that is the nitrogen as it is plus 10 H 2 O plus I have 2 C O 2 plus I have 6 C O.

Now, see in this phase we are able to balance the reaction and we find that if I calculate the energy content or the heat of this reaction as I said. Well, it works out to be quite logical and quite near to the experimental values and the reason for that is the temperatures. So, whenever we talk in terms of fuel rich reactions are not very high, so that the dissociation and other things which govern the products are really not present. But, these approximate methods work well for this reaction let us put down what is the stoichiometry, what is the.

So, what is the fuel by air content by mass for this particular reaction if I have to find out what is the fuel by air? Well, fuel we said it is 48 plus 10, 58 into 2 that is 116 grams air is equal to 10 into 32 plus 3.76 into 28 that is some something like 137.28. So, this fuel air ratio come comes out to be 0.084, 0.084 compared to 0.05 the fuel air ratio, for this fuel rich mixture is 0.084 and the stoichiometric coefficient. Now, comes out to be the actual is for this case is 0.084 divided by 0.065, for this stoichiometric case and the equivalence ratio of this mixture is 1.29.

Therefore, this fuel rich mixture has a equivalence ratio of 1.29 and the fuel air mixture is 0.084, I want to determine what is the heat release in this reaction and to be able to get the heat release. So, I have to calculate the heat of formation of the products has to look at heat of formation of the reactants and the decrease in the heat of formation is what gives the energy release in this particular reaction. Therefore, let us do that we know that the heat of formation of C O 2 we had taken it earlier and that was equal to minus 393.5 kilo Joule per mole.

So, the heat of formation of carbon monoxide we had told that is equal to minus 100 and 10.5 kilo Joule per mole. Well, these are all available in the form of tables the heat of formation of water at the standard condition is equal to minus 286.7 and the heat of formation of butane we said was equal to H f dot was equal to minus 124.7.

Therefore, if now I want to calculate the total heat of formation of the products what is it I do well nitrogen is 0 being an element naturally occurring element I have to calculate these. So, the heat of formation of these three things and let us do it we have 10 H 2 O let me put it here 10 into minus you have for water. So, the value is 286.7 plus I have 2 into minus we have for C O 2 minus 393.5 plus I have for 6 into I have minus 100 and 10.5.

So, this is the net heat of formation of the products and this comes out to be minus I have minus, minus, minus over here. So, this comes out to be minus 4317 kilo Joules for the products when I look at the reactant side over here. Well, oxygen is 0, nitrogen is 0, I have only this and the heat of formation here is minus 124 and, therefore the heat of formation of the reactants is 2 into minus 124.7. Therefore, the net heat of the reaction is equal to minus of what is for products minus 4317 minus the value of minus 2 into 124.7 which if I calculate comes out to be equal to 4068.

Now, we will observe that in the earlier case of a stoichiometric reaction we had for an equivalence ratio 5 is equal to 1 stoichiometry, it was 5765 when it is fuel rich. Well, the energy release is slower at 4068 and this is how we calculate the energetic of the reaction supposing we are interested per unit mass. But, I am interested in the mass of this plus mass of this, I divide it by the mass of the reactants I get the energy release per unit mass.

So, if I am interested in a particular volume I say how many total V moles are contained in the volume this is for the moles which are contained in this reaction I multiply by the total moles in the volume. Here, I get the energy release and this is how we do it you know we must do one more problem relating to fuel rich composites such that we are absolutely clear how to determine the products. So, having determined the products how to calculate the energetic of the reaction, therefore I will go to the next step of this I still consider the last case where in let me assume that it is terribly fuel rich I have 2 C 4 H 10 plus I have only 5, let us say of oxygen plus 3.76 nitrogen.

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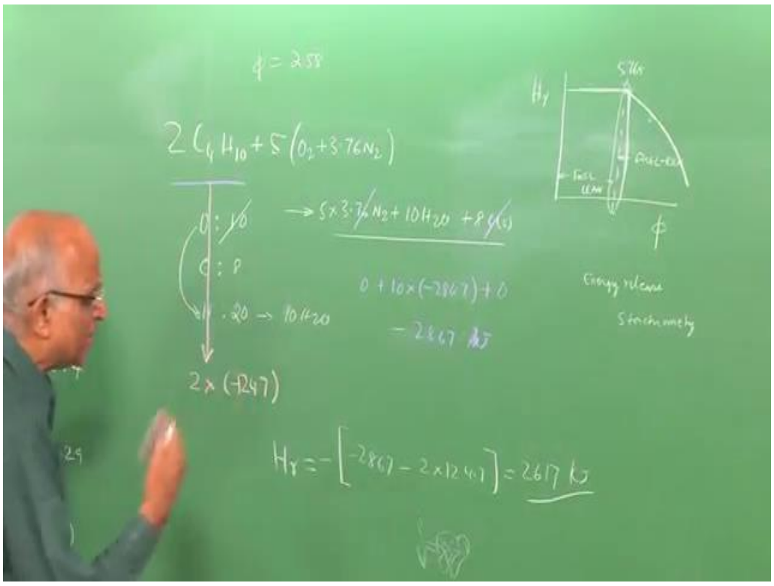

I want to first determine what is the fuel by air ratio well it is quite simple. Now, we are used to this we say fuel by air mass of fuel divided mass of air mass of fuel is equal to 2 moles of this per mole of this I have 58 over here have. Now, have 5 into the mass of air 32 plus 3.76 into this we said is equal to one 37.28 which gives me a number which is twice this value which is equal to I get the value as 2.585.

Now, the equivalence ration, this mixture is equal to, I am sorry this should have been 0.168 and the equivalence ratio is 0.168 divided by 0.065 which was the fuel air ratio for a stoichiometric case and this comes out to be equal to 2.585. Now, at this phi is greater than 1 it is fuel rich you have excess fuel, how do I determine the products let us do that first.

Well, I do the same thing I have oxygen amount of oxygen I have 10 atoms carbon, I have 8 atoms, I have hydrogen which is 10 atoms. Now, what happens in the products if I have to write the equation for the products let me erase the fuel air mixture and the equivalence ratio which we said is 2.5.

So, we just make a note of it here well phi is equal to 2.58 or, so for this particular reaction I want to write the products which are coming out. So, first I say that nitrogen comes in the products as nitrogen 5.2, 3.76 nitrogen, now I want to find out how much C O 2, how much C O how much 2 O, how much of other things are being formed and to be able to do that. Well, the oxygen first attacks the hydrogen and I have 10 atoms of hydrogen available, I have 10 of no 20, 10 into 220.

So, let us make sure we have done it, yes H is 20, if you have 20 of this and if I have to form water then I have to get let us say 10 H 2 O. Now, it consumes all the 10 oxygen gets consumed there is no oxygen left to burn to form carbon monoxide and still no additional oxygen to make it carbon monoxide into carbon dioxide. Therefore, I get 10 H 2 O and what is left I get all the 8 carbon as carbon in the solid that means a suit. Therefore, the products of combustion for this reaction are 5 into 3.76 nitrogen plus 10 water plus 8 of carbon and if I have to evaluate what is the heat which is generated.

Well, I need to evaluate what is the heat of formation of the products let us put it down, well nitrogen is 0. So, I have 10 into the value heat of formation of water is equal to minus 286.7 plus carbon is naturally occurring element this is naturally occurring element this is 0. Therefore, the energy the heat of formation of the products is just 286.7 kilo Joules, why so much heat of formation is kilo Joule per mole I have 10 moles. So, this is the heat of formation and what is the heat of formation of the reactants over here if I have had to write the heat of formation of the reactants.

So, I get 2 into as in the earlier case minus 124.7 which is the 124.7 kilo Joules per mole is the heat of formation of butane. Therefore, the energy of this reaction is equal to 2 you have minus, this is minus, therefore minus of minus 2867 because we are looking for a decrease in the net heat of formation. Here, minus I have this over here 2 into 124.7 which work out to be equal to 2617 kilo joules in this particular reaction.

Therefore, compared to when the equivalence ratio was let us say earlier we had equivalence ratio 1.29 the energy release in the reaction was 40, 68 when the equivalence ratio has gone up to 2.58. Well, the energy has still come down and this is what we see, you know in practice we see when we have this cotton waste or something which is dipped in oil. So, you have this cotton waste which is dipped in oil in a workshop and we light it you know the amount of air available for burning is limited.

So, that we get a thick smoke that is mainly suit and this is what happens when we have very fuel rich mixtures. Therefore, the conclusion which we were to draw from these type of discussions is may be if, now we have to plot the heat of the reaction versus let us say the stoichiometric or equivalence ratio. Well, for the stoichiometric value for which equivalence ratio is 1 the energy release we form that is the heat of the reaction was equal to 5765. But, if it is going to be less than one for which it is, it is, it has sufficient amount of air that means fuel lean air rich mixture.

So, that means we say this is fuel lean I always get completed products of combustion and the heat of reaction remains steady. But, the moment I go to equivalence ratio is greater than 1 that means I look at fuel rich compositions. So, what is going to happen as it increases I find, yes when I had something like 1.29 the heat was something like 4060 when the value was around 2.6 it was around 2617. Therefore, it keeps coming more down over here, therefore the fuel rich compositions give products whose net heat of formation are smaller.

So, that means smaller in the negative sense that means completed products of combustion are still not formed and the net energy released in the reaction tends to low. Therefore, the heat liberated in a reaction is something like this horizontal up to 5 or equivalence ratio 1 and, therefore droops backwards. Therefore, this gives us an indication that if I am interested in enhancing the energy released in a chemical reaction.

So, if I want more energy release and in an explosion it is better that I operate around these stoichiometric values because we also told when I operate the mixture in fuel lean conditions. Now, what happens is the mass of the reactants go up because I have more oxygen which is again coming back as oxygen over here. Therefore, per unit mass or per unit volume it drips over here and, therefore it is desirable to operate the composition around stoichiometry to get more heat release or more energy of this.

Well, this is how you compute the energy from a chemical reaction for fuel rich may be for oxidizer rich and this is how we go about it is quite interesting to do these problems. So, and may be if some time permits towards the end of the class I will do one more simple problem, but to be able to quantify it you know see we must also take some examples. Now, and then you know let us take the example of an incident which happened let us say in Oklahoma in the Murray building you know here.

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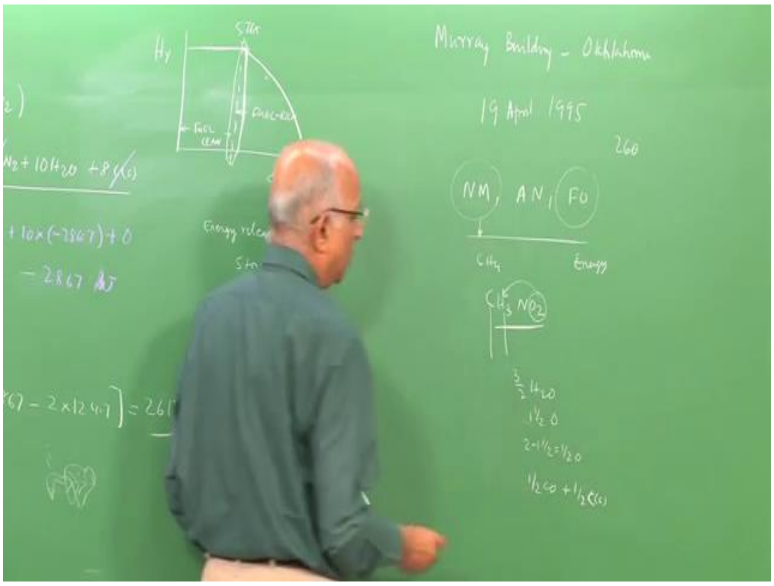

You had a terrorist strike at the Murray federal building in Oklahoma you know what happened in this case I think it happened on 19th April 1995. So, you know some disgruntled people what they did was they had they Parkedah a truck having some explosive in it these explosives were as essentially nitro methane. But, it also had some ammonium nitrate it also had some fuel oil you know when you mix ammonium nitrate and fuel oil together. Well, ammonium nitrate we said earlier had was oxidizer rich may be we will do a problem relating the heat released in ammonium nitrate shortly.

Now, fuel oil is something like carbon and hydrogen together you know it could be large chain which is thick or something these two put together contains fuel and oxidizer it is explosive, nitro methane is again an explosive. So, it was used as a solvent earlier you know when we say methane nitro methane we talk in terms of C H 4 is methane.

Therefore, when I have C H 3 and one of the H I replace by N O 2, well we say nitro methane over here when I look at nitro methane may be as a substance which contains hydrogen and carbon and oxygen. Well, it could be an explosive because well carbon is a fuel, hydrogen is a fuel, oxygen 2 O something which can oxidize and, therefore it becomes an explosive.

So, I find well in this case may be the O 2 first comes and reacts with this 3 H to form 3 by 2 H 2 O and then I am left with half I am left with you have 3 by 2 H 2 O. Therefore, I have used 1 and half of the O over here and, therefore what is it I am having, I am having 2 minus 1 and half that is half oxygen atom. So, this half oxygen atom cannot really oxidize the carbon over here the total into C O 2 I just get half of C O and the balance half is coming as solid.

So, this is how we do for a fuel rich substance, therefore nitro methane is fuel rich well fuel oil is totally fuel rich does not contain any oxygen at all. Therefore, what did these people do you know they knew that this is fuel rich and this is also fuel rich and if I can add lot of ammonium nitrate to this. Well, I can shift the energy release from a fuel rich substance to something like a stoichiometry by putting more and more ammonium nitrate and they were able to release lot of energy in the explosion. But, the energy release was so intense or so high that it resulted in this explosion resulted in something like 168 people dying on the spot.

But, may be some 680 people being killed and something like 260 buildings around this Murray building which was something like 16 storey building was damaged and something like 260 buildings in and around it were shattered. Therefore, you know when we use or when people use stoichiometry compositions or near stoichiometry compositions the energy release is higher. So, that is why may be people keep adding substances like ammonium nitrate 2 or some other or some other oxidizer rich substances to explosives to make it even give a higher yield of energy.

But, having said that let us go to the example of, let us say the energy released in the case of ammonium nitrate itself let us, let us do that problem. Then we do one more composition and with that I am sure we would have understood how to determine the energy release in an explosion let us take the example.

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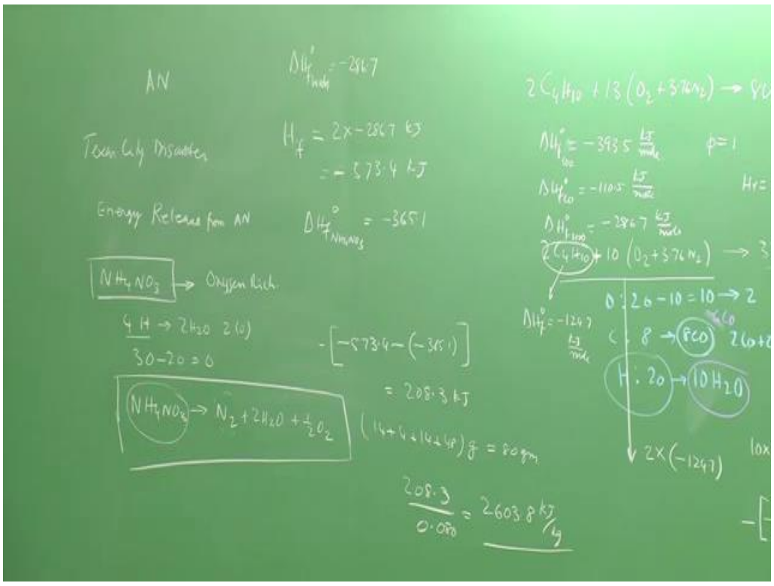

Well, you know ammonium nitrate we have been keeping talking of even earlier we said that Texas City disaster in 1947 what is it we said 7700 tones of ammonium nitrate were contained in the hull of a ship. So, what happened the chemical reactions got started, it started smoking a little bit and later on the chemical reaction progressed to an extent that all the ammonium nitrate sort of blasted or exploded and the explosion was extremely severe.

So, let us find out what is the energy release from let us say energy release from ammonium nitrate we said that the ammonium nitrate was of fertilizer grade we called it as f g a m with a coating of wax. So, let us forget about the coating, let us just take a look at the energy release in ammonium nitrate. Well, you have N H 4 N O 3 is the formula for ammonium nitrate, well I want to find out what are the products of this composition to be able to find out products of composition.

So, first thing what we have to do is determine whether this particular substance and this substance have fuel hydrogen has oxygen over here. Therefore, it is an explosive we have to first determine whether it is oxygen rich or is it fuel rich let us find out. Well, I have 4 of hydrogen, I have 3 of oxygen, 3 atoms of oxygen to burn 4 of hydrogen that means I can form 2 H 2 O, I require 2 of oxygen.

Therefore, I have 3 of oxygen minus 2 of oxygen, I am still left with an oxygen and, therefore we tell this composition is oxygen rich or rather fuel lean. Now, if it is oxygen rich I can readily write my chemical balance equation or the chemical reaction equation I can write N H 4 N O 3 is equal to. Well, the nitrogen comes back in the products N and N, N 2 plus I have 2 H 2 O from I have from the 2 atoms over here I am left with 1 atom and that gives me half O 2, O over here.

So, let us see if it is balanced I have 3 atoms of oxygen 2 plus 1, 3 I have 4, 2, 2 are 4 nitrogen, well this becomes my chemical, my equation and I am able. So, I now know what are the products formed and to be able to find out how much heat is released in this reaction I know the heat of formation of water we said we have been telling this. Now, let us write it out heat of formation of water is equal to minus 286.7, therefore on the right hand side I have nitrogen which is an element does not have any heat of formation.

But, because I assume the products to be at standard state this to be at standard state difference between them or the drop I, the heat of formation of the product is compared to this. So, what is the energetic, therefore I say this is 0, this is 0. Therefore, heat of formation of the products is equal to 2 into minus 286.7, so much kilo Joules which is equal to let us multiply 14 carry 1, 13, 16, 17, 573 so much kilo joules with a minus sign. So, I want to get the heat of formation of the reactants for ammonium nitrate the hat of formation of ammonium nitrate N H 4 N O 3 at standard conditions.

So, standard heat of formation is equal to minus 365.1, therefore the energy released in this reaction is equal to minus of heat of formation of products minus 573.4 minus of minus I have only one mole of it. Therefore, I have minus 365.1which is equal to 573 this becomes plus minus and minus this becomes plus 573.4 minus 365.1, and it is equal to 208.3 kilo Joules. So, this is the energy released in this reaction if I take what is the energy release per unit mass that is per kilogram of ammonium nitrate.

So, we find this heat is generated from the mass corresponding to this and what is the mass, one molecular mass and one mole contains. So, let us put this down the molecular mass is equal to N H 4, N H 3, N is 14 plus H 4 is 4 plus I have one more N here 14 plus I have 16, 3 are 48 over here so much grams for 1 mole. So, I add it together the value is something like 14, 18, 18 that is equal to 80 grams.

Therefore, the energy release per kilogram of this is going to be 208.3 divided by 0.080 kilo gram which is equal to 603.8 kilo Joules per kilo gram. Well, this is how we get the energy release per kilo gram in this example we had 7700 tones, therefore 7700 into 1000 kilograms into the energy release. So, you see a huge energy which gets released in this reaction this is how we get for an oxygen oxidizer rich explosive and first we find out whether the explosive is oxidizer rich fuel rich.

Then find out the energy release, therefore this is how we do different problems let us do one last example we will consider again a solid this was the solid substance over here. So, let us consider another last example in which case we take a fuel rich explosive and as I keep telling most of the explosives which are used today are fuel rich. Now, there is a trend in to increase the oxidizer content slightly such that the fuel rich explosive is nearer to stoichiometry and not away from stoichiometry, let us do this example.

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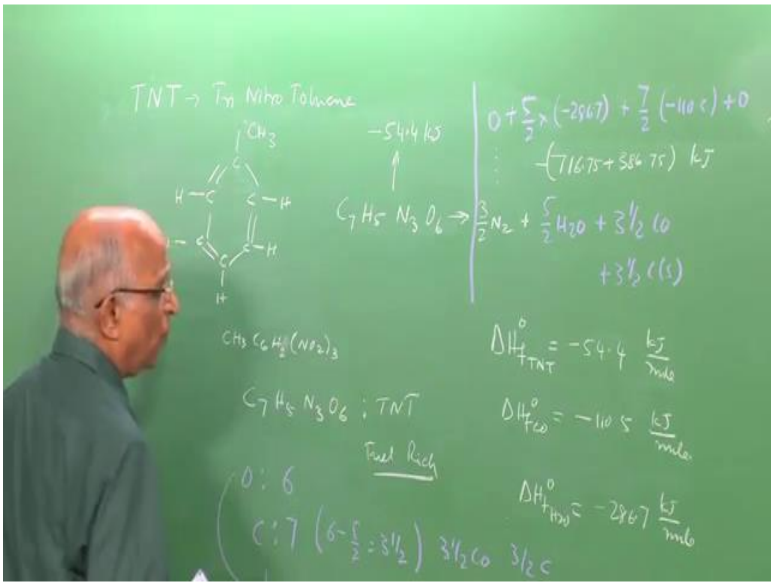

Let us consider one particular explosive which is known as T N T you know when we read the paper very often whenever there is an explosion they say, they say T N T equivalence of this explosion. So, what is this T N T we will study this when we study the condensed phase explosives much later in this course. But, when we state T N T we mean tri nitro toluene T N T that is what it stands for what is this T N T.

Now, you know actually if you, if you have it toluene is something like methyl benzene if you have benzene you know benzene is a chain. So, you know it consists of alternate bonds, this is 1 C over here it consists of alternate double bonds over here you have hydrogen atoms which are attached to the carbon atoms over here. So, hydrogen, hydrogen, hydrogen, hydrogen this is the benzene chain and if you replace one of the hydrogen by methyl. Well, it becomes methyl benzene and you know what is done is you have something like a methyl benzene let us say C H 3.

Now, it becomes C 6 H 5 which is left here C 6 H 6, one is taken over here you remove 3 of the hydrogen over here. So, that means you oxidize it to form toluene that is you have C 6 we had C H 3, C 6 H 5 we have removed 3 we have left with 2. So, it could be O H 3 which is toluene you replace it by N O 2, 3 times, well it becomes tri nitro toluene and this is what I said is an explosive which is a reference explosive. Now, it reacts very fast and generates sufficient amount of energy we want to calculate how much energy is calculated.

Therefore, if I look at the chemical composition I say well C H 3, C 6 H 2 N O 2, 3 times N O, N O 2, 3 times if I were to put it in terms of this. Well, I have C 7, I have H 5, I have N 3, I have O 6, well this is the chemical formula for T N T, I want to find out how much energy is released in this particular substance. So, when it undergoes a chemical reaction and, therefore the first thing which I have to do is find out whether the T N T is oxidizer rich whether it is fuel rich or is it stoichiometry.

Therefore, to do that I tell well oxygen content in the T N T is 6, the carbon content is 7, the hydrogen content is 5, well the nitrogen content will come to me as products of the combustion let us write it out. Therefore, I will write C 7, H 5, N 3, O 6 gives me I just remove because I do not want to carry nitrogen, I say well it will in the products it will come as nitrogen.

Now, I want to find out the other products I do not know whether I have still not found out whether it is oxygen rich or fuel rich I want to do that exercise I tell you know first the oxygen comes and balances this. But, even without it I can find out whether it is oxygen rich or fuel or fuel rich if I were to form may be this 7 carbon atoms into 7 C O 2 I need 7 into 2, I need 14 oxygen atoms.

But, you know and for hydrogen I need 5 by 2 of oxygen atoms, therefore clearly I need 14 plus 2 and half, 16 and half what I have is only 6. Therefore, it is it is a fuel rich composition I do not have sufficient oxygen for getting completely combustion products. Therefore, it is fuel rich composition and for this fuel rich composition I want to determine the products. Therefore, let us, let us put the products down, thus based on these same arguments again let us find out the products of combustion we tell that.

Well, I have o which is 6 atoms carbon which is 7 atoms hydrogen which is 5 hydrogen being reactive, the oxygen atoms first strike the hydrogen and form 5 by 2 H 2 O. Therefore, let us not put it in terms of O 2, we just have 5 by 2 H 2 O, therefore I have 5 by 2 of O is finished over here. Therefore, what is available for carbon, oxygen which is available for oxidation for carbon is 6 minus 5 by 2 which is equal to 3 and half. Now, I have seven carbon atoms I have only 3 and half oxygen atoms, therefore 7 of the 7, only 3 and half form 3 and half C O.

So, that is of the 7 carbon atoms, I form only 3 and half carbon atoms and what is left is 7 minus 3 and half that means I am left with 3 and half again carbon is still left. Therefore, what will be my products of combustion let us put it down let us put in down in a different color we have I have 5 by 2 H 2 O plus. Now, I have 3 and half of carbon monoxide plus 3 and half of carbon in the solid form, well this is how we determine the products of combustion we say when T N T explodes.

Well, I get nitrogen, I get water, I get carbon monoxide, I get carbon as a free substance and once the products of combustion are known. Well, I can find out the heat of formation it is a simple job let us, now put down the values over here let us put down the heat of formation the heat of formation of T N T. So, you know people measure it is available in literature this standard heat of formation of T N T is minus 54.4, we have been.

But, we have already used the heat of formation of carbon monoxide is equal to minus hundred and 10.5 kilo Joule per mole kilo Joule per mole here. So, heat of formation of water which we have been using all along is equal to minus 286.7, therefore what is the net heat of formation of the products. Well, let us write it above the reaction this is my reaction well for nitrogen standard element 0 for water it is 5 by 2 into the value of water is minus 286.7 I have 3 and half C O.

Therefore, I have 7 by 2 into C O per mole it is 110, I have 7 by 2 moles minus 110.5 carbon is again an element well it is 0 over here. Therefore, the net heart of formation of the products is equal to if I were to take it down I have this value as 716.75 plus I have minus over here plus within the bracket I have 386.75.

Now, this is the so much kilo Joules is the heat of formation of the products if I take the value of heat of formation over here well we said it is minus 54.4 kilo Joules because I have only one mole the heat of formation. So, this is minus 54.4 kilo Joule per mole I have one mole it is 54.4 and, therefore the net heat released in this particular reaction if I were to write it on the other side.

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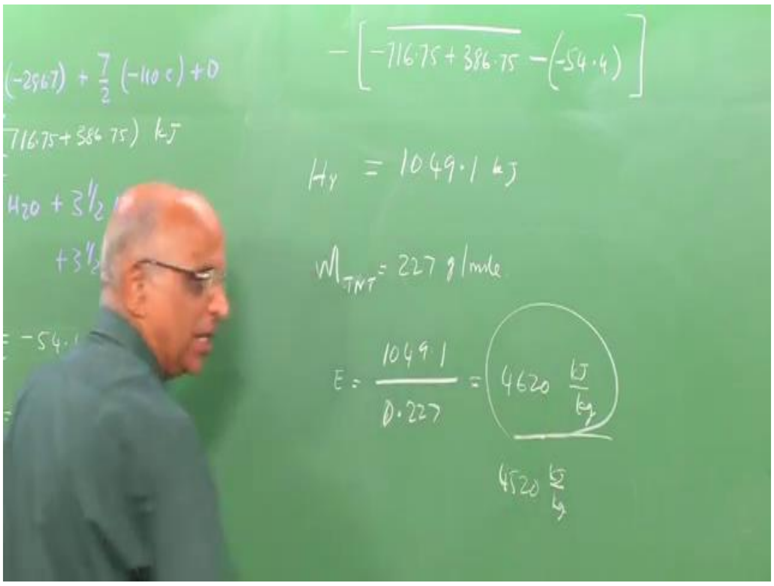

So, it is given by minus of minus 716.75 plus I have 386.75minus the value of minus 54.4 and this becomes plus and this becomes minus. So, the net heat released for this particular reaction comes out to be 1049.1 kilo Joule, this is the net heat of the reaction. Now, I want to find out how much heat is generated by 1 mole of T N T over here and what is the molecular mass of this one mole contains 12, 7s are 84 plus 5, 89 plus 28 into 3 plus 6 into 16 and if I calculate the molecular mass of T N T.

So, the value is 227 grams per mole and, therefore the energy release per kilogram is equal to 1049.1 divided by 0.227 kilogram per mole and this comes out to be equal to 4620 kilo joule per kilogram. Well, this is how we calculate the energy release and mind you know we did the simple calculation and if I do an experiment and measure the energy release during the explosion of T N T. So, you know you get a value around very similar to this around 5420 kilo Joules per kilo grams mind you in this we had a number of assumptions mind.

So, we took water in the products of combustion namely we had H 2 O in the liquid phase may be at high temperature water evaporates we did not consider equilibrium of products at the product temperature. But, still we find well the energy release what we calculate comes out to be very close to what is experimentally measured and this is how we determine the heat of release for different explosives.

So, whether it is oxygen rich, whether it is stoichiometry or whether it is fuel rich having said that since we talked of the different reaction it is also interesting to find out. Now, you know some people use some readymade values of energy release, we call them as calorific value or heat value of explosives and whenever we talk of heat value.

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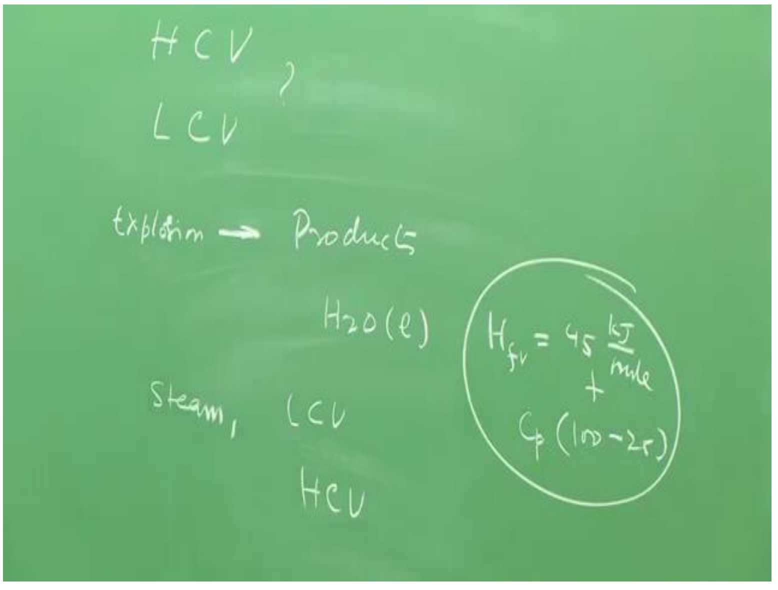

Which is nothing but the heat is calorie calorific value people talk in terms of higher calorific value that is higher and lower calorific value what is this how can a chemical reaction give two values of heat release. Now, it so happens you know whenever we talked of reactions see we had the explosive on one side or the chemical reaction consisting of reactants on one side. So, we had products which are being formed when products are being formed one of the products was essentially water H 2 O.

So, you know what happen is if in the products H 2 O is available in the form of water, well we are getting the total energy out from the products and it gives a higher value of calorific value. But, if this water was to get converted into steam what is happening during conversion it takes some amount of energy from the water that means the latent heat of vaporization. So, let us say for steam is equal to something like 45 kilo Joule per mole plus you know the water also has to be heated because we are forming products at the standard condition of 25 degrees.

Therefore, you also have sensible heat corresponding to C p per mole of water into something like 100 degrees is the boiling temperature and 100 degrees centigrade is the boiling temperature. But, at ambient conditions we are referring it to 25, therefore I have to, I have to supply so much of heat. Therefore, in practice when the water evaporates, I will be talking in terms of lower calorific value because I am using some of the heat generated in the reaction to be able to evaporate the water.

Therefore, what happens is whenever we form water from the water in the products of combustion, if I assume that the water is converted to steam my net heat value is shorter by the amount of sensible heat. So, the latent heat of vaporization of water which I call as lower calorific value, if I presume that in the products the water is available it cools down. But, the energy gets liberated during the condensation of steam that means water is available in the product I have the value higher calorific value.

Well, these are the different terminologies and we can use either higher calorific value or lower calorific value depending on the conditions of the particular explosion. So, what we have one last thing which I want to add during these discussions we have done the energy release. But, you know we must also remember something you know, we talked in terms of heat of formation and we when we talked of heat of formation, we presume that we are talking of constant enthalpy we say…

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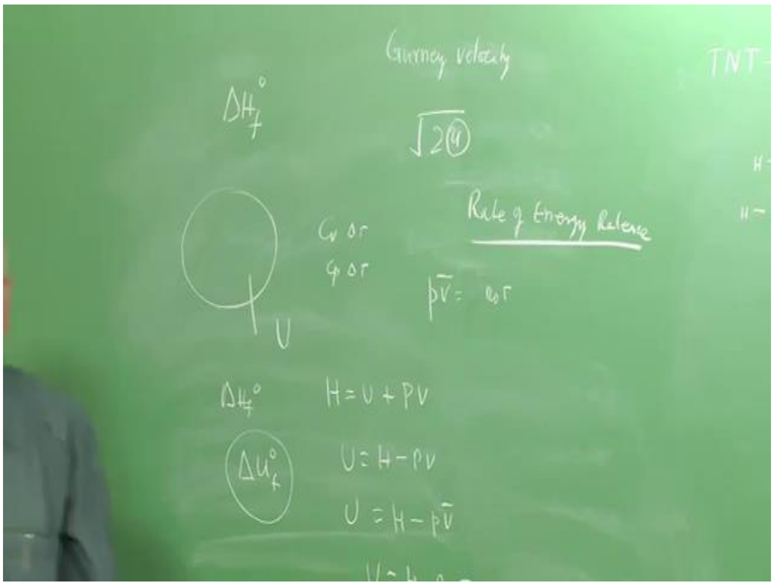

Well, the heat of formation enthalpy of formation at standard condition if I consider let us say a constant volume at constant value, I am exploding something. So, I have a mixture which explodes at constant volume you know you can tell, you know why is it you use enthalpy. Now, enthalpy is constant pressure systems where you are considering a constant volume, therefore if I assume constant volume. So, I must use the internal energy rather I must use constant volume C v into delta T and not C p into delta t.

Therefore, you know it is possible for you to work with internal energy of formation that means instead of using delta H f which is the enthalpy of formation or heat of formation. Now, it is also possible to use the internal energy of formation if we are, if we want a problem to be solved for a constant volume explosion what is, what is the internal energy.

So, we say, well enthalpy is equal to U plus P V and therefore, U is equal to H minus P V and we are talking of enthalpy per mole over here. Therefore, when I write this, I am writing as H heat of formation minus P that is the volume per mole of the substance this is the energy over here. Well, P V is equal to N R 0 T this is per mole, therefore 1 over here, therefore I can write it as H minus R 0 T is the internal energy.

So, tables of internal energy of formation are also available and if we want to do an explosion problem in which we are considering a constant volume explosion. Well, I can use the internal energy of formation instead of the heat of formation in terms of the enthalpies, well this is also one of the cases and you will also recall when we talked of blast waves we talked in terms of the gurney velocity. So, that we said was equal to 2 into U under root here it was essentially what we talked as the internal energy of the explosive which was here U over here.

Therefore, you can use both the internal energy of formation in the same way as we use the heat of formation and do the explosion process. Well, this is all about the, about the energy released in an explosion, we talked in terms of stoichiometry, we talked in terms of oxygen rich substances. But, we talked in terms of fuel rich substances and we have taken a few cases we know how to now determine the energy release in an explosion. But, in an explosion we want the energy release to be spontaneous and, therefore in the next class what we do is we take a look at rate of energy release.

Well, thank you.