Material and Energy Balance Computations
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Lecture –26
Combustion Reactions Balance

Hello everyone, Welcome back once again in the NPTEL online certification course on material and energy balance computations. We were discussing the chemical reactions stoichiometry and some related problems, where we have seen that how to apply balances on the single reaction or multiple reactions in case of several applications by different meteorology like molecular species balance atomic species balance, as well as the extent of reactions.

We have seen their pros and cons which one would be easier, which one is straightforward for a certain cases. Now, after that we have introduced the recycle and the purge stream. The necessity of those we have already discussed and we have solved problems related to recycle the bypass and we introduced purge and its necessity, we have also discussed. Now today, we will take up a new subsection under this chemical reaction stoichiometry or the balances, based on the chemical reaction stoichiometry that is on the combustion reaction.

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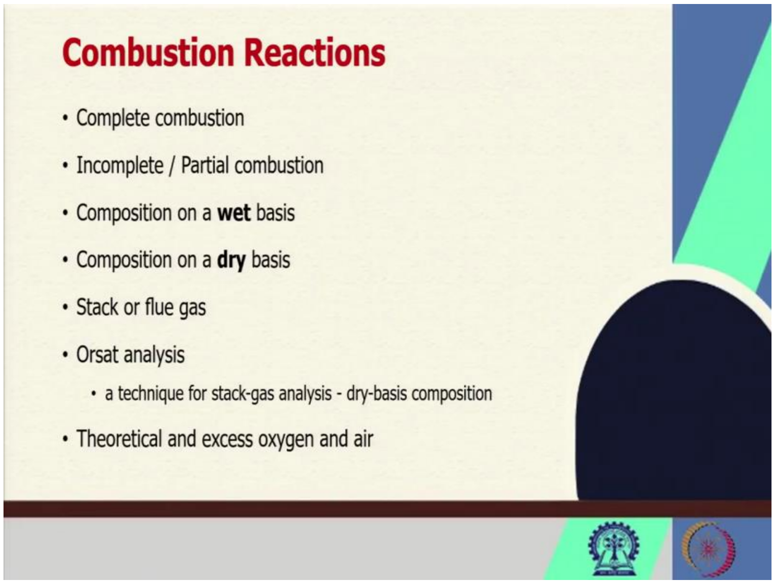

Combustion Reactions

- Complete combustion
- Incomplete / Partial combustion
- Composition on a **wet** basis
- Composition on a **dry** basis
- Stack or flue gas
- Orsat analysis
  - a technique for stack-gas analysis - dry-basis composition
- Theoretical and excess oxygen and air

Now, this combustion reaction the importance is that such reactions or such type of reactions are of huge importance to our regular applications as well as in commercial cases because this combustion is basically rapid reaction of a substance in presence of oxygen. Now, the examples of these combustion reactions are like burning fossil fuels or natural gas, etc. Now, these have immense application in our daily life because we extract energy from those reactions.

Now, these combustion reactions, while this happens it emits or is exerts substantial amount of energy and those energy are then converted to electrical energy or some other means for our applications or daily uses. Now, if you consider fossil fuel burning, it is basically hydrocarbon. Now, in presence of oxygen, quite naturally it creates carbon dioxide, carbon monoxide etc, and also not only that, there are some trace amounts of sulfur and nitrogen.

Now, those also sometimes reacts, particularly nitrogen reacts like a very high temperature around 1800 degrees centigrade, and that is why we have considered nitrogen as inert till now, and in fact most of the cases until unless it is explicitly mentioned that nitrogen is also consumed or reacted. We typically consider nitrogen as inert, but sulphur if it is burned or combusted in presence of oxygen, what happens it creates sulphur dioxide, which is harmful species as well as carbon monoxide, carbon dioxide.

So, if we study such reactions, what happens is that we understand or we can monitor that the amount of these species, these gases mixtures are being generated, so that we can have a control after monitoring these amounts. So, for these, this section would be useful because we will understand how do we apply balances the material balances on such combustion reaction. Now, before we go into the problems let us simplify a couple of jargons that you may find in the problem statement.

One is complete combustion the complete combustion means that when you have carbon after complete combustion, it would generate only carbon dioxide. So, that means if there happens partial combustion or the incomplete combustion that means the carbon mage also generate are also generating carbon monoxide. So, if there is complete combustion, there is no chance of producing carbon monoxide as a by-product or a product, in incomplete or partial combustions, carbon can generate carbon monoxide.

So, similarly, after complete combustion, sulphur would generate sulphur dioxide and etc. when nitrogen is burnt or it is reacted with oxygen there are several species that it can create and we typically call those as NO_x depending on whether this is partial or complete combustion, typically the NO_x is the one of the variations that is, we have a NO_2. Similarly, nitrous oxide and etc can be generated from such reactions, that is why in generic form it is called NO_x and x stands for the various number.

So, if a problem statement says that there is complete combustion and the product streams are not specifically spelled out that is, the product composition has not been mentioned, and then you can safely assume that there is no carbon monoxide in the product stream. But if there is incomplete or partial combustion is mentioned in the problem statement, then you have to be careful and should take carbon monoxide as one of the product when the fossil fuel or hydrocarbon burned or combusted.

Then we have the composition analysis of the product gas. Now, this analysis happens, say whenever you have a hydrocarbon fuel and if it is combusted, the hydrogen component or the atomic hydrogen reacts with oxygen and creates some water and H_2. Now, while analyzing this product stream, what happens that the composition would be having one of the components as moisture or water. Now, that if it is included in the composition analysis, it is called the composition on a wet basis.

That means there are compositions or analysis happens on the dry basis as well because the dry basis is then without any water component added in the analysis. Now, typically, whenever people does in a analysis in a laboratory several equipment's are available in order to find out what is the composition of a mixture as a gaseous mixture. Such analysis provides us the composition on a dry basis, and it specifically mentioned that this is the moisture content, but the other compositions are this, this in certain percentage.

So, the composition on wet basis and composition on dry basis. So, wet basis there must be some water in the product stream or the stream mixture and when it is mentioned dry basis, there is no water in that composition. And then sometimes you would find a stack gas or a flue gas, which is the gas that is coming out of a combustion chamber or a combustion chimney. That gas when it is analyzed, one of such technique is the Orsat analysis.

The Orsat analysis provides us the composition on a dry basis. It is a technique for stack gas analysis and provides always the composition in dry basis. So, if a problem statement says that product streams Orsat analysis gives us this, this component then there would be no moisture content mentioned or moisture composition or water composition would not be mentioned and separately, the moisture content would be explained or mentioned in the problem statement.

Let us say, if you are asked to calculate that what would be its dry basis composition that means you are calculating its or such analysis. And then there is theoretical and excess oxygen, and air theoretical oxygen and excess oxygen what happen that when we have some precious reactant okay, and we want its complete consumption, it is typically combusted with the excess amount of air or oxygen. Because oxygen combustion and combustion oxygen is essential mandatory.

Now, a free and a cheap source of oxygen is here it here, Air has a certain percentage of an oxygen. So, what happens that we provide whatever required theoretically. Now, that is the theoretical requirement of oxygen for that particular reaction we provide in excess of that amount 2 times, three times, five times of the theoretical required of oxygen. So, that the precious reactant or the complete combustion can take place.

Now, the point is the theoretical requirement or the theoretical oxygen requirement is basically depends on a balanced stoichiometric reaction or the calculation of theoretical oxygen demand or theoretical oxygen requirement. You at first have write the balance stoichiometry of the reaction and then you can find what is the theoretical demand based on the complete combustion. So, theoretical oxygen requirement is always related with complete combustion of that particular reaction.

And based on that calculation because we know the relation between the oxygen concentration and the air, or say the oxygen composition in air, amount of oxygen that is available in air. Based on that, we can find out the amount of air that is needed in order to supply that much amount of oxygen or the vice versa.

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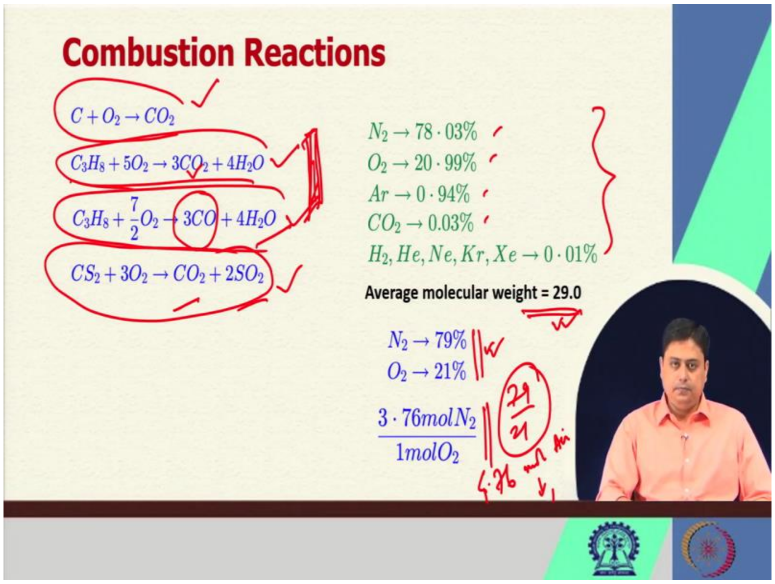

Combustion Reactions

$C + O_2 \rightarrow CO_2$

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

$C_3H_8 + \frac{7}{2}O_2 \rightarrow 3CO + 4H_2O$

$CS_2 + 3O_2 \rightarrow CO_2 + 2SO_2$

$N_2 \rightarrow 78 \cdot 03\%$

$O_2 \rightarrow 20 \cdot 99\%$

$Ar \rightarrow 0 \cdot 94\%$

$CO_2 \rightarrow 0.03\%$

$H_2, He, Ne, Kr, Xe \rightarrow 0 \cdot 01\%$

Average molecular weight = 29.0

$N_2 \rightarrow 79\%$

$O_2 \rightarrow 21\%$

$\frac{3 \cdot 76 mol N_2}{1 mol O_2}$

$\frac{79}{21}$

4.76 mol Air

So this set of reactions, the first one is C + O_2 giving CO_2, this is an example of complete combustion. The second one as well, this is also an example of complete combustion, but the third one is the partial or incomplete combustion of propane and the fourth one as well it is the complete combustion of carbon disulphide it is creating CO_2 and SO_2. So, this standalone reactions or individual reactions here that is mentioned.

So, first one is complete combustion, second one is complete combustion, third one incomplete or partial combustion fourth one is the complete combustion. Now, say propane is combusted and the problem statement says that you have these 2 reactions that are involved in the system which means there is incomplete combustion of propane is happening because one of the reactions is producing carbon monoxide. So, some part it is incomplete combustion as well as it is also free of generating CO_2.

So, whenever CO is involved in a hydrocarbon fuel, you can safely in imagine that there is incomplete combustion is happening. Now in order to find out what is the air composition or whenever that is mentioned, it is combusted with air typically, what happens the air composition is not mentioned, as I mentioned in my previous lectures, when it is not mentioned we typically consider the composition as this following that nitrogen is 79% mole percent and oxygen is 21 mole percent in the air.

Otherwise, a detailed composition analysis of air shows that this is the percentages of several different gaseous components which has an average molecular weight of 29. So, it is recommended that you remember that the average molecular weight of air is 29 and when it is explicitly not mentioned, the composition of air we assume or we take the composition of nitrogen and oxygen as 79% and 21% which means if we see that 3.76 moles of nitrogen and 1 mole of oxygen because it is basically 79 / 21 in this ratio nitrogen and oxygen is present in air.

So, 79 / 21, it is 3.76 : 1 in this ratio, which means 4.76 moles of air contains one mole of oxygen and 3.76 mole of nitrogen this ratio or this relation you can easily calculate or you can remember like this. Because it would be necessary when we will calculate the percentage excess air from percentage excess oxygen or say the excess oxygen and excess air calculation. So, 79 / 21, which is 3.76 that means 4.76 moles of air contains 1 mole of oxygen and 3.76 mole of nitrogen.

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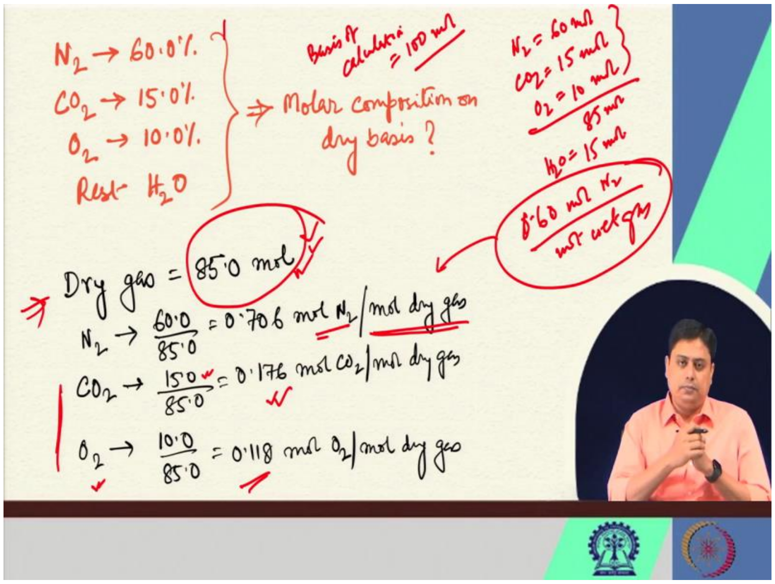

$N_2 \rightarrow 60.0\%$
$CO_2 \rightarrow 15.0\%$
$O_2 \rightarrow 10.0\%$
Rest H_2O

$\Rightarrow$ Molar composition on dry basis ?

Basis of calculation = 100 mol

$N_2 = 60$ mol
$CO_2 = 15$ mol
$O_2 = 10$ mol
85 mol
$H_2O = 15$ mol

0.60 mol N_2 / mol wet gas

$\Rightarrow$ Dry gas = $\boxed{85.0 \text{ mol}}$

$N_2 \rightarrow \frac{60.0}{85.0} = 0.706$ mol N_2 / mol dry gas

$CO_2 \rightarrow \frac{15.0}{85.0} = 0.176$ mol CO_2 / mol dry gas

$O_2 \rightarrow \frac{10.0}{85.0} = 0.118$ mol O_2 / mol dry gas

Now, as we mentioned that if we have a composition on wet basis how do we calculate the same for on a dry basis because sometimes it would be necessary to convert these dry basis to wet basis or wet basis to dry basis analogous to what we have done earlier from mass fraction to the mole fraction that kind of calculation. So, here, if you see that a composition the gas stream composition is mentioned that you have nitrogen 60% these all in mole percent, carbon dioxide

15%, oxygen 10% and rest water or moisture.

So, we have to calculate what is the molar composition on a dry basis? So, how do we convert such problem or such information? So, here, clearly we can see that if our basis of calculation is say 100 mole of this gas stream then we have nitrogen as 60 mole, CO_2 as 15 mole, O_2 we have 10 mole and the rest is water, which means water is the amount we have it is 15 mole that means the total dry gas that we have is basically a summation of these three except water, which is 85 mole.

The amount of dry gas we have for our basis of calculation of one hundred mole of wet gas. So, if this is the amount of dry gas, then we can easily find out what is the nitrogen based on this amount or with respect to this amount, how much or what is the wet mole fraction of nitrogen we have which means 60 / 85, that is 0.706 mole of nitrogen per mole of dry gas that we have. We had 0.60 mole of N_2 per mole of wet gas.

But when it is converted to dry gas, it is we have 0.706 mole of nitrogen per mole of dry gas because we have the total amount of dry gas as 85 mole. So or similarly, we can easily calculate what is the molar composition of carbon dioxide and oxygen because carbon dioxide was present as 15 mole per 100 mole wet gas or per 85 mole of dry gas that means we have this much mole of CO_2 per mole of dry gas.

So, the mole fraction is 0.176 and same for the O_2, we have the rest of the amount. So, which means we can easily find out from the wet analysis or wet basis composition to a dry basis composition by deducting the water component which is quite straightforward.

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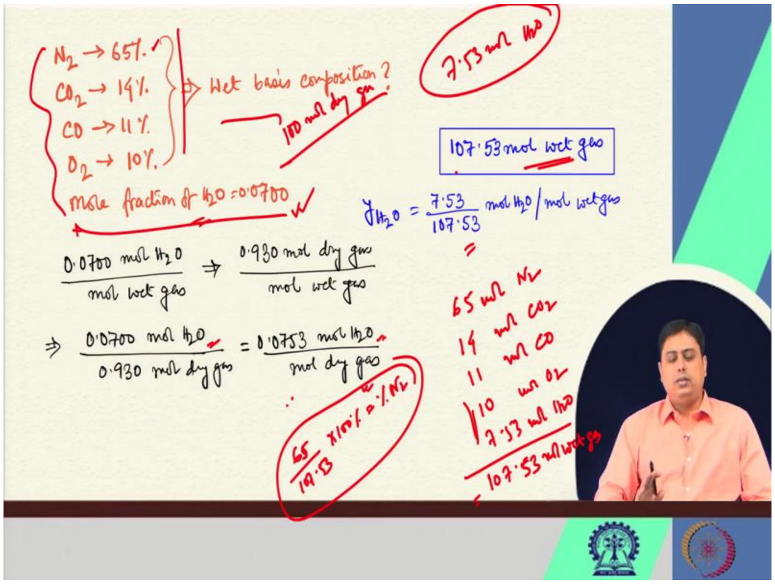

$N_2 \rightarrow 65\%$
$CO_2 \rightarrow 14\%$
$CO \rightarrow 11\%$
$O_2 \rightarrow 10\%$
mole fraction of $H_2O = 0.0700$

$\Rightarrow$ Wet basis composition?

100 mol dry gas

7.53 mol H_2O

107.53 mol wet gas

$$\frac{0.0700 \text{ mol } H_2O}{\text{mol wet gas}} \Rightarrow \frac{0.930 \text{ mol dry gas}}{\text{mol wet gas}}$$

$$\Rightarrow \frac{0.0700 \text{ mol } H_2O}{0.930 \text{ mol dry gas}} = \frac{0.0753 \text{ mol } H_2O}{\text{mol dry gas}}$$

$$y_{H_2O} = \frac{7.53}{107.53} \text{ mol } H_2O/\text{mol wet gas}$$

$\frac{65}{107.53} \times 100\% = \% N_2$

65 mol N_2
14 mol CO_2
11 mol CO
10 mol O_2
7.53 mol H_2O
107.53 mol wet gas

But when we go to the other aspect or when we go to the on a different way, that is from a dry basis composition to wet basis composition. So, say gas mixture analysis tells us that this is the or say this is it is mentioned Orsat analysis. Orsat analysis provides us this composition and it mentions that you have a mole fraction of water is 0.0700. So, Orsat analysis would typically provide this kind of information.

Now, the task is to convert this information on a wet basis composition that what would be the wet basis composition of this analysis or this mixture. So, for that what we should do again, we can consider or we must consider a basis of calculation okay, and say that basis of calculation is based on the dry gas analysis. So, so we have hundred mole of dry gas that means what we have that 65 moles of nitrogen in the 100 moles of dry gas.

We have 14 moles of carbon dioxide, 11 moles of carbon monoxide and 10 moles of oxygen. The mole fraction of H_2O is provided which means that we have 0.07 moles of water per mole of wet gas. So, in one mole of wet gas, we have 0.07 mole of water because it is mentioned that the mole fraction of H_2O is 0.07. So, that means we have 1 – 0.07, which is 0.93 mole of dry gas per mole of wet gas.

So then what we can understand or what we can realize here, that 0.07 mole of H_2O and 0.93 mole of dry gas in this ratio, we have in the composition when it comes for the wet basis analysis. So, the wet basis composition of this gas would consist of 0.07 moles of water and 0.93 mole of dry gas which means 0.0753 mole of water is there per mole of dry gas that means 0.0753 mole of water is there per mole of dry gas or should would be there per mole dry gas in that wet basis composition if that has to consist the mole fraction of water as 0.07.

So, which means our basis of calculation, we took 100 mole of dry gas. If 100 mole of dry gas is there that means there, we have 7.53 mole of water which means we have total 107.53 mole of wet gas that means the fraction of water that we have is basically 7.53 / 1.07 this is the fraction of the mole fraction of water in the wet basis composition. Now, the final answer would be if we have to convert now, to wet basis, we know we have 65 mole of nitrogen, 14 moles of CO_2, 11 mole of CO, 10 mole of O_2 and 7.53 mole of water, which means we have 107. 53 mole of wet gas.

Now we take each and every component to find out its percentage it would be our percentage nitrogen in the composition. So, 65 divided by this total amount would be our percentage of nitrogen in wet basis composition or analysis. Similarly, for carbon dioxide, 14 / 100 × 7.53 ×100 that would be that much percentage of carbon dioxide of that much percentage in the product gas or that way basis composition similarly, for the other components.

So, I hope it is now clear, that how this wet basis and dry basis analysis can be interchangeably expressed that if one is known we should be able to calculate the other analysis.

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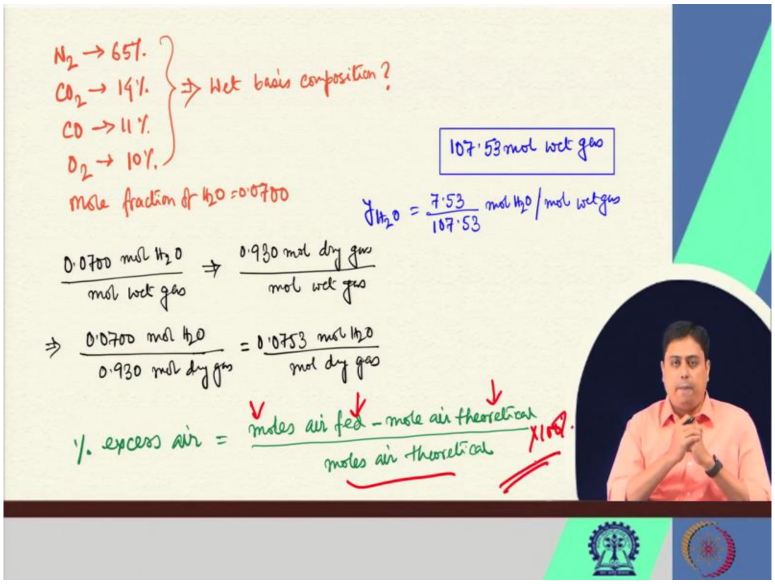

$N_2 \rightarrow 65\%$

$CO_2 \rightarrow 14\%$

$CO \rightarrow 11\%$

$O_2 \rightarrow 10\%$

$\Rightarrow$ Wet basis composition?

Mole fraction of $H_2O = 0.0700$

$\boxed{107.53 \text{ mol wet gas}}$

$$y_{H_2O} = \frac{7.53}{107.53} \text{ mol } H_2O/\text{mol wet gas}$$

$$\frac{0.0700 \text{ mol } H_2O}{\text{mol wet gas}} \Rightarrow \frac{0.930 \text{ mol dry gas}}{\text{mol wet gas}}$$

$$\Rightarrow \frac{0.0700 \text{ mol } H_2O}{0.930 \text{ mol dry gas}} = \frac{0.0753 \text{ mol } H_2O}{\text{mol dry gas}}$$

$$\% \text{ excess air} = \frac{\text{moles air fed} - \text{mole air theoretical}}{\text{moles air theoretical}} \times 100$$

Now, when we do or when we find out what is the percentage excess air, the percentage excess air like the other definitions we have seen, it is analogous to such concept that percentage excess is the moles of air fed to the system minus the theoretical amount that is required for complete combustion divided by this theoretical amount that is required for complete combustion. So, remember once again that theoretical oxygen required is for complete combustion.

And for complete combustion, you have to write a balanced stoichiometry, where on the right hand side for any hydrocarbon, there will be carbon dioxide and water and then we find out by stoichiometry that for one mole of that hydrocarbon how much mole of oxygen is necessary and then we cross check or check with how much it is being fed to the system, that is the excess divided by the moles of theoretical air × 100% is the percent excess air.

So, these are basically few jargons few things acronyms or say the few necessary terms that we require in order to solve certain problems or solve all the problems that is related to combustions and which we will take this up in the next lecture. So, in the next lecture, we will solve couple of problems on combustion. We will see how the balance can be applied on these combustion reactions and then we will be done with this module of chemical reaction stoichiometry and the combustion reaction. So, till then, thank you for your attention.