Material and Energy Balance Computations
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Lecture –27
Combustion Reactions Balance (Contd.,)

Hello everyone, Welcome back once again in the NPTEL online certification course on material and energy balance computation. We were discussing the balances on combustion reactions, and we introduced a few terms that are necessary while dealing with the problem statement on combustion reactions and one of such was the percentage excess air or percentage excess oxygen. We have seen its definition.

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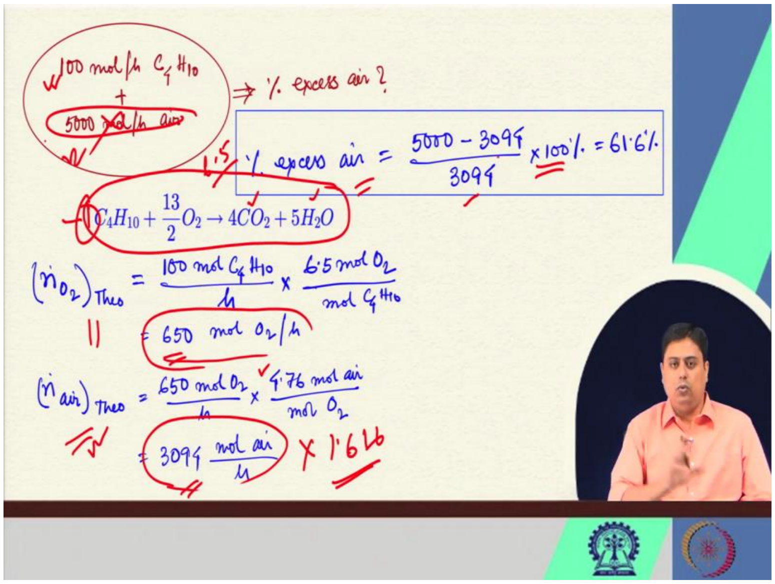

$100 \text{ mol/h } C_4H_{10} + 5000 \text{ mol/h air} \Rightarrow$ % excess air ?

$$\% \text{ excess air} = \frac{5000 - 3094}{3094} \times 100\% = 61.6\%$$

1.5

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$

$$(\dot{n}_{O_2})_{Theo} = \frac{100 \text{ mol } C_4H_{10}}{h} \times \frac{6.5 \text{ mol } O_2}{\text{mol } C_4H_{10}} = 650 \text{ mol } O_2/h$$

$$(\dot{n}_{air})_{Theo} = \frac{650 \text{ mol } O_2}{h} \times \frac{4.76 \text{ mol air}}{\text{mol } O_2} = 3094 \frac{\text{mol air}}{h} \times 1.616$$

Now see quickly, how do we calculate or how do we understand or how do we implement that concept while solving a problem. Now, it is said that we have 100 mol/h of C_4H_{10} it is there in a system. So, 100 mol/h of C_4H_{10} which is butane is combusted in presence of 5000 mol/h of air that is, these 2 are fed to a combustion chamber combustion reactor. We have to find out how much is the percentage excess air that we have fed.

So, for that, first we have to calculate what the theoretical air demand is or what a theoretical air requirement is. Now that air requirement would come from the oxygen requirement because essentially combustion is happening in presence of oxygen. So, the stoichiometry that we would write the reaction is butane + oxygen giving us CO_2 and H_2. Remember we are calculating theoretical oxygen requirement, which means we must write a complete combustion reaction equation.

And for that complete combustion, there will be carbon dioxide and H_2O because in this part, the reactant we have only C and H. So, carbon, after complete combustion, would create or generate CO_2 and hydrogen produce H_2O. So, now here before going into the air calculation, we need to understand how much is the oxygen requirement. Now the theoretical amount of air that is needed here, we can see that we have 100 mol/h of butane.

So 1 mole of butane requires 6.5 moles of oxygen from the stoichiometry it is clear for complete combustion. So, that means for 100 mol we would need 650 mol of oxygen/h. Now at the same time, we know that 1 mole of oxygen is there in 4.76 mole of air because you remember that 79 / 21 ratio from there, we knew that we have 4.76 mole of air contains 1 mole of O_2. So, which means the theoretical air that is fed to the system is basically 3094 this is the theoretical amount that that is required but we have fed 5000 moles of air/h.

So the percentage excess air is 5000 – the theoretical requirement / theoretical requirement × 100%, which is around 61.6% or say in a problem statement, if it is mentioned that 61.6% of excess air has been provided to the system, and this information is not there then we can also similarly calculate that our oxygen requirement is 650 mol/h for complete combustion, air requirement is 3094 moles of air/h.

So, this × 1.616 is the amount of air that has been supplied to the system which would be 5000 mol/h. So, 1 + this fraction in the percentage after converting into fraction 1 + that fraction that you have to multiply to the theoretical requirement to have the actual amount of flow or flow rate.

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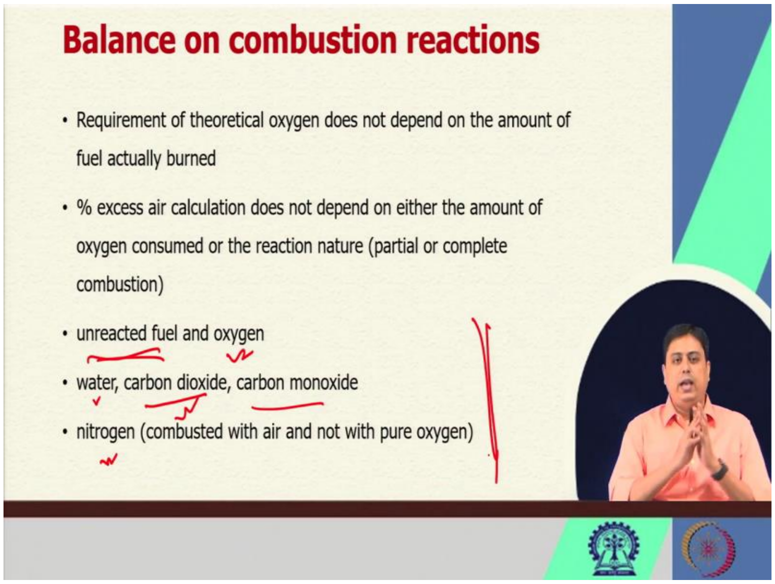

Balance on combustion reactions

- Requirement of theoretical oxygen does not depend on the amount of fuel actually burned
- % excess air calculation does not depend on either the amount of oxygen consumed or the reaction nature (partial or complete combustion)
- unreacted fuel and oxygen
- water, carbon dioxide, carbon monoxide
- nitrogen (combusted with air and not with pure oxygen)

So, when we come to the balance and combustion reaction we have to be very careful and not to confuse with the concept that theoretical oxygen requirement does not depend on the amount of fuel actually burnt because there will be a scenario where it could be mentioned that the percentage conversion of fuel or combustion of that fuel is this much that would not, or that should not influence the theoretical oxygen calculation, the amount of theoretical oxygen requirement because it always based on the complete combustion of that fuel.

Similarly, the percentage excess air calculation should not depend or it should not depend on either the amount of oxygen consumed or is it a partial or incomplete combustion that category. So, which means the percentage excess, air calculation always depends on the theoretical air requirement or in terms of theoretical oxygen requirement and the amount that has been fed to the system. It would never be calculated based on how much oxygen has been consumed or what is the type of reaction is it partial or complete combustion.

While doing the balance on the combustion reactions, you should be careful while writing the product stream that whether there is unreacted fuel or unreacted oxygen is there. Because unreacted oxygen means or because the excess oxygen if it is provided. Then in the product team there would be some oxygen. And if the combustion or say the conversion is not 100% then there will be unreacted fuel as well.

You should write water on the product stream, if there is partial or say incomplete combustion even if it is not mentioned and if the fuel is of hydrocarbon which is typically always happens the carbon dioxide, carbon monoxide, carbon dioxide would always be there for any hydrocarbon fuel and carbon monoxide depending on the nature of the reaction that is, whether it is a partial combustion or not. If there is partial combustion, there will be carbon monoxide.

And you must not forget about nitrogen which typically we consider as inert and the reason of focusing on nitrogen because most of the problem statement or in most cases if the combustion does not happen or it is, the pure oxygen is typically not provided. Pure oxygen is expensive instead, it is combusted with air, where the major portion is nitrogen. So, these things we have to be careful when we encounter any combustion reaction.

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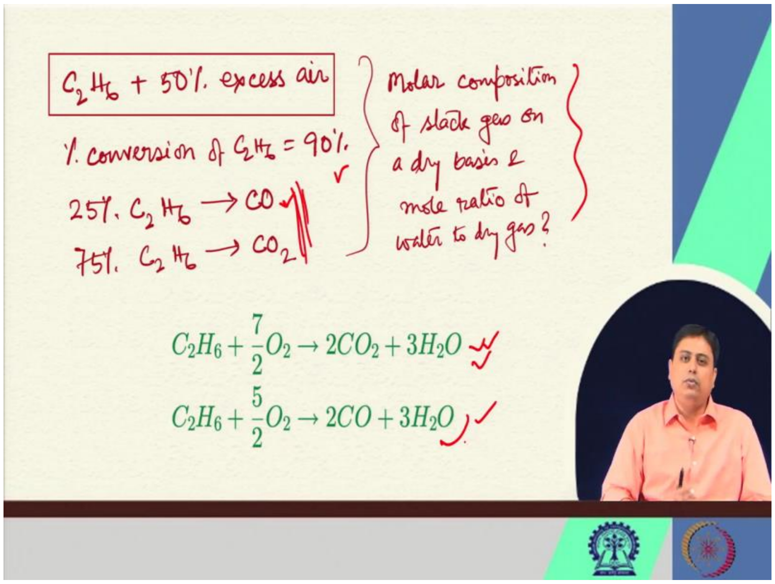

$\boxed{C_2H_6 + 50\%\ \text{excess air}}$

% conversion of $C_2H_6 = 90\%$ ✓

$25\%\ C_2H_6 \rightarrow CO$ ✓

$75\%\ C_2H_6 \rightarrow CO_2$

Molar composition of stack gas on a dry basis & mole ratio of water to dry gas?

$$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$$ ✓

$$C_2H_6 + \frac{5}{2}O_2 \rightarrow 2CO + 3H_2O$$ ✓

So, say this problem statement that we have here that we have ethane is burning in presence of 50% excess air the percentage conversion of ethane is 90% it is mentioned that the amount of ethane that reacts of which 25% of ethane generates carbon monoxide and the rest generates carbon dioxide. So, which means you have a known ratio of CO and CO_2 production. Our task is to find out the molar composition of the stack gas on a dry basis and more ratio of water to dry gas that means a kind of Orsat analysis.

So, first of all as per our previous understanding, what we should do, we should draw a flow chart. Now, before drawing the flow chart and writing the species on the inlet and the outlet and we have to identify at first that what are the things would be there on the outlet in case of combustion reaction, because just before this, I mentioned that we have to be careful in writing the product stream composition because here it is not explicitly mentioned that what would be the product composition in fact, that we have to find out.

So, now it is apparent that we have incomplete combustion because carbon monoxide is generated. So, we write the balanced stoichiometry or the balanced reactions or equations for these reactions. One is the incomplete one the other one is the complete combustion. For complete combustion we needed 3.5 moles of oxygen per 1 mole of ethane but in case of incomplete combustion, we need 2.5 mole of oxygen per mole of ethane that generates carbon monoxide and water.

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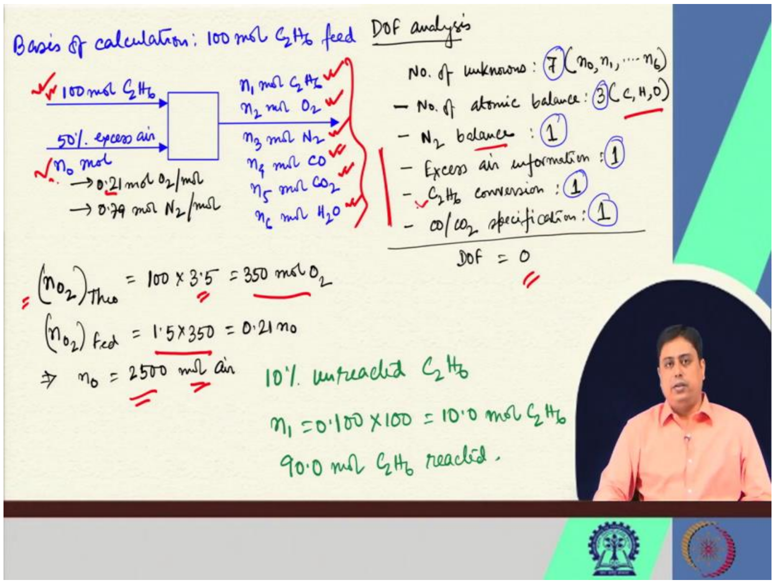

Basis of calculation: 100 mol C_2H_6 feed

DOF analysis

No. of unknowns : ⑦ $(n_0, n_1, \cdots n_6)$
– No. of atomic balance : ③ (C, H, O)
– N_2 balance : ①
– Excess air information : ①
– C_2H_6 conversion : ①
– CO/CO_2 specification : ①

DOF = 0

$(n_{O_2})_{Theo} = 100 \times 3.5 = 350$ mol O_2

$(n_{O_2})_{Fed} = 1.5 \times 350 = 0.21\, n_0$

$\Rightarrow n_0 = 2500$ mol air

10% unreacted C_2H_6

$n_1 = 0.100 \times 100 = 10.0$ mol C_2H_6

90.0 mol C_2H_6 reacted.

So, that means now we are clear that what would be there on the product stream because we have a certain percentage conversion of ethane so, which means there would be unreacted ethane we have 50% excess air, that means 50% excess oxygen is fed to the system the percentage excess air or percentage excess oxygen is the same because it is basically × a constant factor when it comes to the ratio.

So, there will be excess oxygen in the product stream that is unknown. The nitrogen would be there it is explicitly not mentioned that nitrogen is also getting oxidized that is why nitrogen is inert that assumption is there. And then we have the products that are carbon monoxide, carbon dioxide and the moisture or water. These are all unknown for us. Our basis of calculation depending on this analysis that has been asked this composition that is mentioned here that we consider 100 mole of ethane is fed in to the system.

So, if that is the case and 50% excess air is there and this 50% excess air we consider that, as n_0 mole of air is being fed to the system, and in 1 mole, we have 0.21 mole of oxygen and 0.79 mole of nitrogen because the air composition has not been explicitly mentioned. So, this is our flow chart and this is also labelled. The next step is the degree of freedom analysis. So, we see here that we have number of unknowns as 7 all the 6 + the n_0.

Now since here, we have multiple reactions involved as per our previous recommendation, we would go with the atomic species balance, where we have input is equal to output for all the species. Now here, the atomic species, the number of atomic species that are involved is 3 that is C, H and O these are the independent atomic species that we can write balances on it. We have 1 nitrogen balance because this is the unreacted species the molecular balance, we can write on N_2.

We have excess air information excess air gives us the relation between the n0 and the basis of calculation based on the stoichiometry. We also know another information from C_2H_6 conversion, that is ethane conversion and also, we know the CO and CO_2 production ratio that specification. So, based on these, we see the degree of freedom is basically zero for this problem, which means we can solve this with the given information.

So, first, we use this additional information to quickly reduce the number of unknowns and we see if we start with the excess air information, the amount of theoretical oxygen that is required here, based on this 100 mole of ethane, we see that it requires 3.5 mole, as I mentioned here theoretical oxygen calculation always involves complete combustion only. 1 mole of C_2H_6 required 3.5 mole of oxygen so, 100 moles that is, our basis of calculation requires 350 moles of oxygen.

So, which means the amount of oxygen fed is 1.5 times of 350, which is equal to 0.21 × n_0 because this is the amount of oxygen that is going into a system. So, from here we can easily find out what is n_0 that means the moles of air that is fed to a system. So, 2500 moles of air is fed to the system from the C_2H_6 conversion relation, we knew that we had 90% conversion, which means 10% is unreacted and that would come along with the product stream.

So, if 10% is unreacted of 100 mole, we have 10 mole of unreacted C_2H_6, which is going out of the system that means n_1 is 10 mole. So, which means 90 moles of C_2H_6 reacted.

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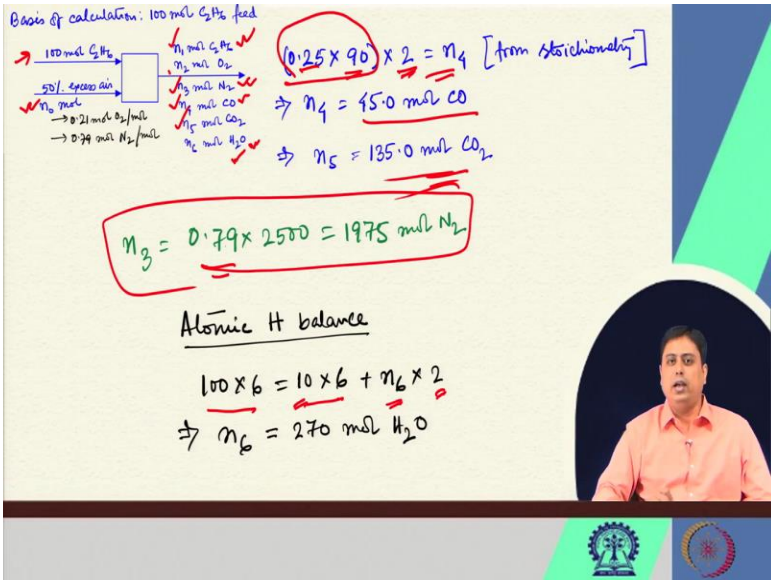

Basis of calculation: 100 mol C_2H_6 feed

$(0.25 \times 90) \times 2 = n_4$ [from stoichiometry]

$\Rightarrow n_4 = 45.0$ mol CO

$\Rightarrow n_5 = 135.0$ mol CO_2

$$\boxed{n_3 = 0.79 \times 2500 = 1975 \text{ mol } N_2}$$

Atomic H balance

$100 \times 6 = 10 \times 6 + n_6 \times 2$

$\Rightarrow n_6 = 270$ mol H_2O

So, if 90 moles reacted and then if we look at the carbon monoxide balance it says that 25% of ethane that has reacted, it generates carbon monoxide. So, 25% of the amount that has been reacted okay, so, there what we have if we look at the stoichiometry. So, 1 mole of ethane generates 2 moles of carbon monoxide. So, based on that from this stoichiometry the amount of ethane 25% of the amount of ethane that has reacted, that is, 90 mole.

It would generate × 2 that amount of carbon monoxide that is n_4. So, which means we have 45 mole of carbon monoxide. Similarly now here, what we have it is 3 : 1 that is the ratio that has mentioned okay. So, quite naturally, the n_5 the amount of carbon dioxide that is generated is this much, 3 times of that or one can calculate with the same concept that with 0.75 × 90 × 2 because 1 mole of it ethane generates 2 moles of carbon dioxide is equals to n_5 that would also give you the same result.

Now if we look at the molecular species N_2 balance, which is the inert we know the amount of air that has gone that is n_0 so, n_0 × 0.75 that would come out as N_2 because it is a inert it is a non-reactive species. So n_3 is also known. So, we have n_1, n_3, n_4, n_5, these are all now known. For the oxygen and for the moisture the first we can do is the atomic H balance because it is recurring or happening in a lesser number than the oxygen in the other species or the atomic oxygen.

So, atomic hydrogen is there only in 1 species in the inlet which is ethane. So, 1 mole of ethane contains 6 moles of hydrogen, atomic hydrogen, which is 100 × 6, equals to here we have in case of n_1 we can identify that hydrogen is occurring in 2 terms. 2 species, 1 is in unreacted C_2H_6, which is 10 moles × 6 + n_6, which is unknown, × 2 because 1 mole of water consists of 2 moles of atomic hydrogen. So, we can easily calculate what n_6 is.

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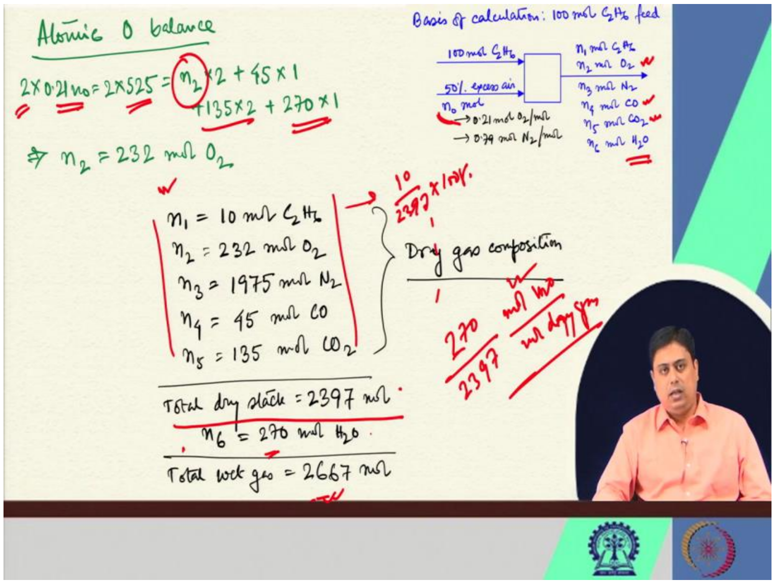

Atomic O balance

$2 \times 0.21 n_0 = 2 \times 525 = \boxed{n_2} \times 2 + 45 \times 1 + 135 \times 2 + 270 \times 1$

$\Rightarrow n_2 = 232$ mol O_2

Basis of calculation: 100 mol C_2H_6 feed

$n_1 = 10$ mol C_2H_6
$n_2 = 232$ mol O_2
$n_3 = 1975$ mol N_2
$n_4 = 45$ mol CO
$n_5 = 135$ mol CO_2

Total dry stack = 2397 mol.
$n_6 = 270$ mol H_2O.
Total wet gas = 2667 mol

$\frac{10}{2397} \times 100\%$

Dry gas composition

$\frac{270}{2397}$ mol H_2O / mol dry gas

Once it is known similarly, we apply atomic oxygen balance, oxygen balance this is the inlet or input 0.21 n_0 is the amount of oxygen fed to the system and 1 mole of oxygen consists of 2 moles of atomic oxygen this number is known n_0. So, that is equals to now n_2 × 2, because again 1 mole of molecular oxygen consist of 2 moles of atomic oxygen + n_4 × 1 + n_5 × 2 + n_6 × 1 these are all known values except n_2. So, we calculate the value of n_2.

So, which means now we have all the values n_1 to n_6 for dry basis composition, we would exclude water. So, that means on a total dry stack gas, these are the components will add up and from there the individual composition, we can easily calculate that is 10 / 2397 × 100% and like this for all the compositions all the species on a dry gas composition. And when we add to this, the water term, it becomes the total wet gas and the wet gas compositions can also be calculated by the similar manner.

So, here what we have the amount, the ratio that was asked also in the problem statement the water to dry gas composition is 270 / 2397 moles of water per mole of dry gas this would be the answer. So, this is how we apply balance on the combustion reaction.

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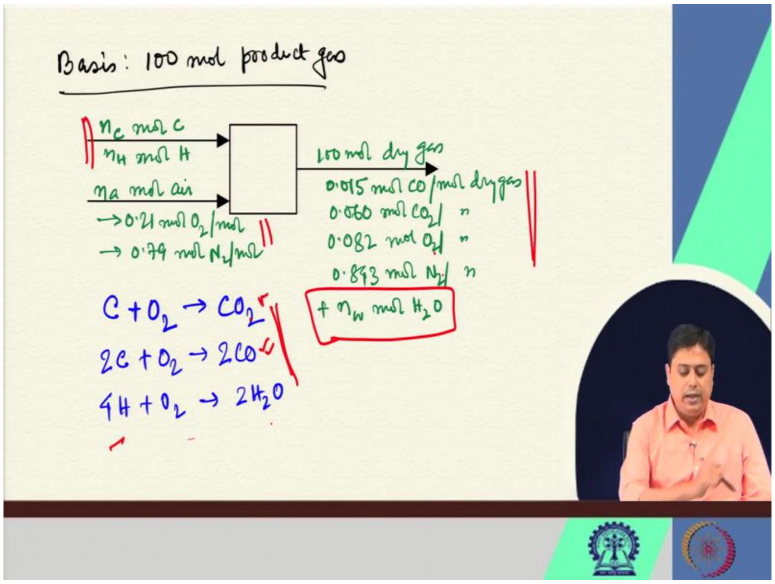

Basis: 100 mol product gas

n_C mol C
n_H mol H
n_a mol air
→ 0.21 mol O_2/mol
→ 0.79 mol N_2/mol

100 mol dry gas
0.015 mol CO/mol dry gas
0.060 mol CO_2/ "
0.082 mol O_2/ "
0.843 mol N_2/ "
$\boxed{+ n_w \text{ mol } H_2O}$

$C + O_2 \rightarrow CO_2$
$2C + O_2 \rightarrow 2CO$
$4H + O_2 \rightarrow 2H_2O$

Now sometimes the composition of the fuel gas is also not known, or in fact the fuel is unknown, but kind of fuel we are burning. Let us see such example that say 1 hydrocarbon gas is burnt with air okay, and this composition, this hydrocarbon gas does not contain any atomic oxygen, that means it is pure carbon and hydrogen mixture Now when it is burnt on dry basis, this composition has been analyzed CO, CO_2, O_2 and N_2, which means there is incomplete combustion is happening even though the air is there an amount of excess.

We have to find out what is how much is the excess air that has been fed to the system. So, we have to speculate what is the composition of this hydrocarbon gas and what is the percentage excess. So, for that we again assume a basis of calculation. which is based on the dry basis product compositions that means 100 moles of product gas because that those compositions are given. Now in the inlet, we do not know what is the fuel or the hydrocarbon.

So, we consider at the atomic level we have n_C moles of atomic carbon and n_H moles of atomic hydrogen, it is combusted with n_a mole of air, where this composition of oxygen and nitrogen is there which we safely assume that because explicitly it is not mentioned what is the composition of air. So, 21% oxygen, 79% nitrogen and the dry basis analysis shows that we have these values of carbon monoxide, carbon dioxide, oxygen, nitrogen.

Now it does not mean that there is no water there would be a certain moles of water in the product stream because hydrogen is there. So, what will happen the atomic carbon will react with oxygen to produce carbon dioxide and atomic hydrogen would react with oxygen to produce water does these reactions eventually will happen so, that we find out carbon monoxide, carbon dioxide and oxygen because carbon monoxide is mentioned specifically. So, we had to write this stoichiometry.

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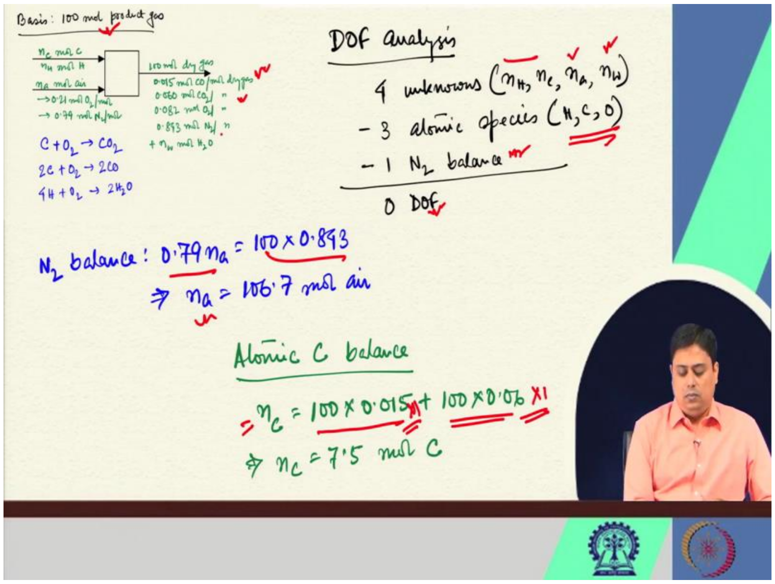

Basis: 100 mol product gas

n_C mol C

n_H mol H

n_a mol air

→ 0.21 mol O_2/mol

→ 0.79 mol N_2/mol

100 mol dry gas

0.015 mol CO/mol dry gas

0.060 mol CO_2/ "

0.082 mol O_2/ "

0.893 mol N_2/ "

+ n_w mol H_2O

$C + O_2 \rightarrow CO_2$

$2C + O_2 \rightarrow 2CO$

$4H + O_2 \rightarrow 2H_2O$

DOF analysis

4 unknowns (n_H, n_C, n_a, n_w)

− 3 atomic species (H, C, O)

− 1 N_2 balance

0 DOF

N_2 balance: $0.79 n_a = 100 \times 0.893$

$\Rightarrow n_a = 106.7$ mol air

Atomic C balance

$\Rightarrow n_C = 100 \times 0.015 \times 1 + 100 \times 0.06 \times 1$

$\Rightarrow n_C = 7.5$ mol C

Now once this is known or when we level this flow chart, we do the degree of freedom analysis. Here we have 4 unknowns, which the composition of the fuel the air amount and the water amount the moles of water, 3 independent atomic species C, H and O and 1 unreacted species, which is nitrogen balance we can write which means the degree of freedom is zero. Now we start with the nitrogen balance the additional information that has been given to which is 0.79 of n_a and if our assumption or the basis of calculation is 100 mole of product gas.

There, we have 84.3% of nitrogen, which means these moles of nitrogen that means we can easily calculate what is the air, the amount of air fed to the system. Then we apply atomic carbon balance. Atomic carbon balance this is the input is equals to output. Now the output is happening in terms of carbon monoxide and carbon dioxide this is the amount of carbon monoxide is living the system and 1 mole of carbon monoxide basically contains 1 mole of atomic carbon.

One mole of carbon dioxide contains 1 mole of atomic carbon these are known. So, we can easily calculate what is n_C.

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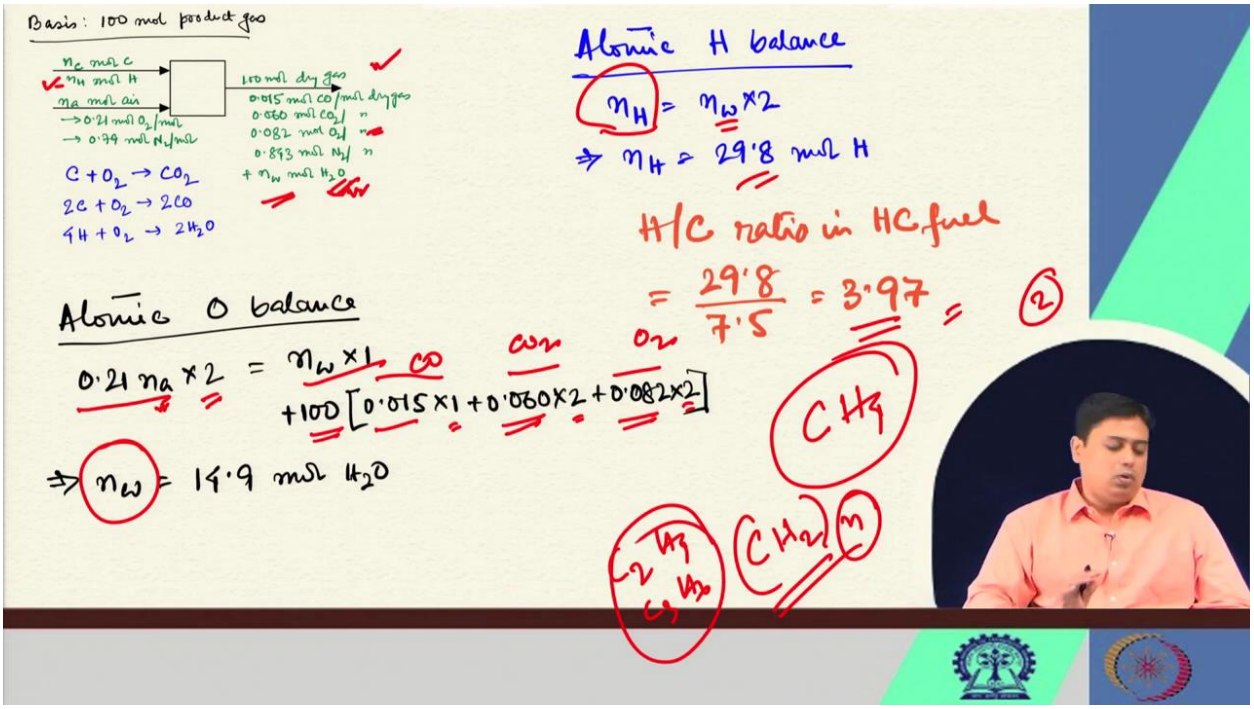

Basis: 100 mol product gas

$C + O_2 \rightarrow CO_2$

$2C + O_2 \rightarrow 2CO$

$4H + O_2 \rightarrow 2H_2O$

Atomic O balance

$$0.21\, n_a \times 2 = n_w \times 1 + 100\,[\underset{CO}{0.015 \times 1} + \underset{CO_2}{0.060 \times 2} + \underset{O_2}{0.082 \times 2}]$$

$$\Rightarrow n_w = 14.9 \text{ mol } H_2O$$

Atomic H balance

$$n_H = n_w \times 2$$

$$\Rightarrow n_H = 29.8 \text{ mol H}$$

H/C ratio in HC fuel

$$= \frac{29.8}{7.5} = 3.97$$ ②

CH_4

C_2H_8 C_3H_{12}

$(CH_2)_n$

Similarly, we apply atomic oxygen balances. Now here, the amount of oxygen fed to the system is 21% of the air this n_a is known to us × 2 because this is the molecular oxygen fed to the system and 1 moles of O_2 contains 2 moles of atomic oxygen that means that is equals to this much amount of water that is going out × 1 because 1 mole of H_2O contains 1 mole of atomic oxygen + 100 is the product gas 100 moles in which we have 0.015, this is the CO part carbon monoxide.

This is 1 stands for 1 mole of CO_2 consist of 1 mole of atomic oxygen this is the CO_2 part 1 mole of CO_2 contains 2 moles of atomic oxygen and this is the O_2 part, which is this much amount of O_2 consists of 2 moles of atomic oxygen, n_a is known. So, we can easily calculate what is n_w that is the amount of water. Similarly, we do the atomic hydrogen balance the atomic hydrogen is with only in 1 case.

So, atomic hydrogen in the inlet is n_H is equals to amount of water being produced × 2 because 1 mole of water contains 2 moles of atomic hydrogen. So, this is the amount of hydrogen. So which means what we have the H / C ratio. The atomic hydrogen by atomic carbon in the fuel we have 3.97 which is nearly 4 that means the fuel is possibly CH_4. So, this is the conclusion on the possibility of what would be the fuel for such case.

Now if it comes out to be say 2 then it could have been anything of this nature of say it could have been C_2H_4, C_3H_6 anything could have been there. You could not have possibly concretely tell, what is the actual fuel, but since it is nearly 4, the only possibilities CH_4.

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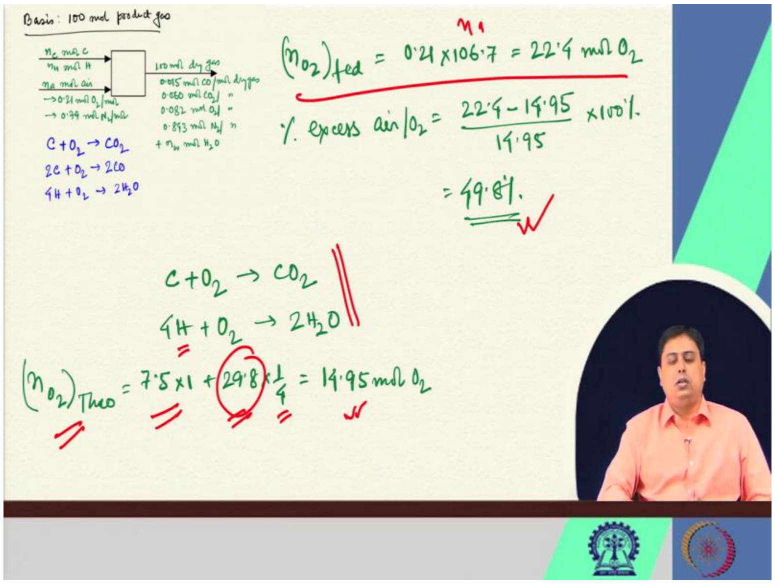

$C + O_2 \rightarrow CO_2$

$2C + O_2 \rightarrow 2CO$

$4H + O_2 \rightarrow 2H_2O$

$(n_{O_2})_{fed} = 0.21 \times \overset{n_a}{106.7} = 22.4$ mol O_2

% excess air/O_2 $= \frac{22.4 - 14.95}{14.95} \times 100\%$

$= 49.87\%$

$C + O_2 \rightarrow CO_2$

$4H + O_2 \rightarrow 2H_2O$

$(n_{O_2})_{Theo} = 7.5 \times 1 + 29.8 \times \frac{1}{4} = 14.95$ mol O_2

And the final thing that we have is the percentage excess air. Now percentage excess air for this

And the final thing that we have is the percentage excess air. Now percentage excess air for this

we need amount of theoretical oxygen requirement. For amount of theoretical oxygen requirement we have to look into the complete combustion that means there would be no carbon monoxide. So, the theoretical oxygen requirement is basically comes from the atomic carbon and the atomic hydrogen, 4 moles of hydrogen requires 1 mole of oxygen.

So, this much amount of hydrogen requires 1 fourth of that oxygen for the complete combustion, and that gives us this much amount of O_2. So, the O_2 fed to the system that we already knew it from the amount n_a which is 22.4. So, the percent excess air or oxygen as I mention when it comes to the percentage calculation, it is the same value 22.4 – 14.95 / the theoretical requirement × 100%.

So, this concludes this discussions and our understanding on the balances on chemical reaction stoichiometry based calculations and specifically on the combustion reaction. So, in the final module from my part in the next 3 lectures, I will discuss another topic until then, thank you for your attention.