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Module No # 04
Lecture No # 19
Combustion Reactions: An Introduction

Hello everybody welcome to today's lecture on combustion reaction as I had mentioned in the last class there are certain specific reactions which are of interest for chemical engineers and bio chemical engineers. Combustion reaction is a very common reaction seen in most of the chemical industries and in many bio-chemical industries also. So it is very important for us to understand what this reaction are and what are the terminologies associated with such combustion reactions.

So in this lecture we will go through some of these concepts and try to solve some example problems which helps us understand this terminologies better.

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Combustion

- What is combustion?
- Reaction of a substance with oxygen
- Release of product gases – CO₂, CO, H₂O, SO₂ etc.
- Products are usually cheaper than reactants
- Importance – Release of energy
- Common examples: Coal, heating oil, natural gas to generate electricity, engines using combustion of petrol or diesel

What is combustion? Combustion is a process when some substance reacts with oxygen to form combustive gases which are basically the product gases namely carbon dioxide, carbon monoxide, water vapor and sulfur dioxide etc. So the product which is formed here the carbon dioxide, carbon monoxide and all are usually cheaper than the reactions this is because the reactant which are taking part in the reaction are usually fuels and the fuels are very expensive.

So why is this important this is because the fuel which is burnt release energy this energy which is released is used for different processes in many of the industries. Some common example would be where coal or heating oil or natural gas is burnt to generate electricity engines where combustion of petrol or diesel is happening so that it can be converted to kinetic energy. So these are certain process where combustion reaction are of critical important.

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Combustion

- Air is the common source of oxygen
- For ease of calculations, air can be assumed to be 79% N_2 and 21% O_2
- Average MW of air = 29
- N_2 is treated as non-reacting component by neglecting oxidation of N_2 to for NO_x
- Terminologies are specific

In addition to fuel combustion can happen only in the presence of oxygen air used as the common source of oxygen. Purified oxygen is more expensive for this reason the cheaper alternative which is used in most chemical and bio chemical processes for combustion of fuels. So for ease of calculations air is considered to be 79% nitrogen and 21% oxygen.

So the molecular weight of this particular composition of air would be 28.84 grams per mole to be accurate or 29 grams per mole roughly. So nitrogen which is present in this air is treated to be inert component during the combustion reaction in reality some amount of nitrogen can actually gets converted to NO_x gases which are pollutant these are usually very small quantities because of this they are considered to be negligible and are usually ignored by form this calculation.

So this particular process has specific terminologies which is associated with combustion process for this reason it is important for us to learn and remember what this terminologies are and apply

them appropriately. So here are some of the terminologies which are commonly used in combustion reaction.

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Terminologies

- Flue or stack gas – All gases resulting from combustion including water vapor, also called wet basis
- Orsat analysis or dry basis – All gases resulting from combustion *not including water vapor*
- Complete combustion – Complete reaction of fuel to form CO_2 , SO_2 and H_2O
- Partial combustion – Combustion of fuels that produces at least some CO

Flue or stack gas so flue or stack gas is the combination of all the gases that are resulting from the combustion this includes from the water vapor which is formed it is also called as wet basis based on which calculation can be performed.

You also have another terminology which is Orsat analysis or dry basis here all the combustion gases taken into account except for water vapor you have complete combustion which represents that all the carbon is converted to carbon dioxide sulfur is converted to SO_2 and hydrogen is converted to water vapor.

Only when this reaction goes to completion these particular product gases are formed you have partial combustion where some of the carbon can be left as carbon monoxide instead being converted carbon dioxide.

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Terminologies

- Theoretical air or theoretical oxygen – Minimum amount of air or oxygen required for complete combustion
- Excess air – Air provided in excess of that required for complete combustion
 - Excess air is calculated based on how much fuel can be burned, not on how much fuel is actually burned
- If both CO and CO₂ is formed in the reaction, theoretical air and excess air are calculated assuming all of carbon is burned to form CO₂

Another terminology which is commonly used combustion reaction this theoretical or oxygen. Theoretical air or oxygen is the minimum amount of air or oxygen which is required for complete combustion to occur. Which means all of carbon should be converted to carbon dioxide sulfur to be converted to sulfur dioxide and hydrogen to be converted to water vapor you have something called excess air which is basically the air which is provided in excess to what is required for complete combustion.

In general fuel is lot more expensive than air so this would mean supplying air in excess would ensure that fuel which is the limiting reactant which fully consumed. So there by utilizing most out of the fuel for this reason air almost always supplied in excess. So excess is actually calculate based on how much fuel can be burnt basically how much fuel is available for the combustion reaction rather than how much fuel is actually burnt during the combustion reaction it is being studied.

These two terms theoretical air or oxygen and excess air or actually calculated based on the assumption that complete combustion happen this means even if carbon monoxide and carbon dioxide are both formed in a reaction in reality however we should calculate this theoretical terms of theoretical air and excess air based on reaction happening in a way that all of carbon is converted to carbon dioxide which is what complete combustion.

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Wet and dry basis

- Compositions on wet basis – Commonly mole fractions or percentages of a gas including water vapor
- Compositions on dry basis - Commonly mole fractions or percentages of the same gas not including water vapor
- Example – A gas with 33.33% N₂, 33.33% O₂ and 33.34% H₂O (wet basis) is written as 50% N₂ and 50% O₂ (dry basis)

So we also mentioned wet and dry basis when we looked at this what do we mean by this. Wet basis is basically composition of a gas which is leaving the system which includes water vapor. So usually mole fraction or mole percentages are given so the total number of moles includes the number of moles of water vapor which is leaving the system you also have dry basis in which the composition are given as mole fractions or mole percentages where the same gas is accounted for total moles does not accounted for the moles of water vapor.

Here is an example just to illustrate this if you have a gas which contains 33.33% nitrogen, 33.33% oxygen and 33.34 % water vapor then this is called as the wet basis. So you can also be written as 50% nitrogen and 50% oxygen based on dry basis this is because if you were to assume 100 moles of total gas you would have add 33.33% nitrogen sorry 33.33 moles nitrogen and 33.33 moles of oxygen and 33.34 moles of water vapor.

So when calculate dry basis we ignore the 33.34 mole of water vapor and we perform the composition calculations only based on the amount of nitrogen and oxygen which would be 33.33 moles each this would results in 33.33 divided by 67.6 for both nitrogen and oxygen giving you mole fractions of 0.5 or mole percentages of 50% which is what in the dry basis.

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Orsat analysis

- Traditional technique to analyze flue gas
- Fixed volume of sample gas is passed through specific solutions that can absorb a certain gas
- After complete absorption, the difference in volume is used to measure the concentration of the gas
- Caustic potash – CO_2 , Mix of pyrogallic acid, caustic potash and water – O_2 , Solution of cuprous chloride – CO

Orsat analysis mole fractions of 0.5 or mole percentages of 50% which is what in the dry basis Orsat analysis is a traditional technique which is used for analyzing flue gases so this technique will only give you dry basis so what happens here is a fixed volume of a sample gas is passed through specific solutions which can absorb certain gases.

So when these goes through this chamber the particular gases absorbed by the solutions and after complete absorption the difference in the volume is measured to actually identify the concentration of particular gas in the product as which is leaving the system. So caustic potash is used for absorbing carbon dioxide a mix of pyro Gallic acid and caustic potash in water is used for absorbing oxygen and a solution of cuprous chloride is used for absorbing carbon monoxide.

So by this method we can actually use orsat analysis to actually get the dry basis composition of the different flue gas which is leaving the system. Now that we have understood and learnt the terminologies let us perform certain example problem to ensure that we have fully understood that we have the grasp for performing calculation related to combustion reaction.

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Example #1

- The composition of a gas on wet basis is 60% N₂, 15% CO₂, 10% O₂ and rest is H₂O. Calculate the molar composition of the gas on a dry basis.

Basis - 100 mol of wet gas

$$\begin{array}{r} \Rightarrow 60 \text{ mol N}_2 \\ 15 \text{ mol CO}_2 \\ 10 \text{ mol O}_2 \\ \hline 85 \text{ mol} \\ \Rightarrow 15 \text{ mol of H}_2\text{O (v)} \end{array}$$

Dry basis:

$$\begin{array}{l} \text{N}_2 : \frac{60}{85} = 0.706 \frac{\text{mol}}{\text{mol}} \\ \text{CO}_2 : \frac{15}{85} = 0.176 \frac{\text{mol}}{\text{mol}} \\ \text{O}_2 : \frac{10}{85} = 0.118 \frac{\text{mol}}{\text{mol}} \end{array}$$

Problem adapted from Felder and Rousseau, Elementary Principles of Chemical Processes, 3rd edition, Wiley-India

Here is the first example problem the composition of a gas on wet basis is given as 60% nitrogen 15% carbon dioxide 10% percent is oxygen and the rest is water vapor. You are asked to calculate the molar composition of gas on the dry basis how do we go about performing this calculation the first thing we need to do is we need to calculate the number of moles of each of the component so that we actually ignore the number of moles of water to get the dry basis.

So for this we will assume a basis for the composition which has been given to us let us assume 100 moles of gas wet gases present so that would be basis would be given as 100 moles of wet gas. So this implies you have 60 moles of nitrogen 15 moles of carbon dioxide and 10 moles of oxygen and the rest is water so this adds up to 85 moles not accounting for water. So based on the information given 15 moles of water vapor is also present.

So when we calculate the wet basis what we would have done is we would have accounted for this 15 moles also and had a total moles of 100 which was the basis as assumed and from there we would have calculated the percentages. So now to calculate the dry basis we would not include the number of moles of water vapor present in the mixture. So the total number of moles which will be used for calculations to be 85 moles.

So using this we can calculate the dry basis composition as for nitrogen it would be 60 divided by 85 which is 0.706 moles per mole and you have carbon dioxide as 15 divided by 85 which is equal to 0.176 moles per mole and oxygen would be 10 by 85 giving you 0.118 moles per mole.

So the values we have calculated here would be the dry basis because you have ignored the number of moles of water vapor which is present in the gas perform calculations for the composition.

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Example #2

- Orsat analysis yields 65% N₂, 14% CO₂, 11% CO and 10% O₂. Humidity measurement shows that mole fraction of H₂O is 0.0700. Calculate the molar composition in wet basis.

$$\begin{aligned} \text{Basis} &= 100 \text{ mol DA} \\ \text{Mole fraction of H}_2\text{O} &= 0.0700 \frac{\text{mol H}_2\text{O}}{\text{mol Wet air}} \\ \Rightarrow & 0.930 \frac{\text{mol DA}}{\text{mol WA}} \\ \Rightarrow & \frac{0.0700}{0.930} = 0.0753 \frac{\text{mol H}_2\text{O}}{\text{mol DA}} \end{aligned}$$

Problem adapted from Felder and Rousseau, Elementary Principles of Chemical Processes, 3rd edition, Wiley-India

So here is the second example orsat analysis yields 65% nitrogen 14% carbon dioxide 11% carbon monoxide and 10% oxygen humidity measurement shows that mole fraction of water vapor is 0.0700 you asked to calculate the molar composition in wet basis. So the information you get from orsat analysis would be the dry orsat analysis is the technique for measuring the composition of flue gas based on absorption of gases.

And this can be done for gases other than water vapor so the value you get for the composition are on dry basis you have also been given how much water is present in the form of water based on the humidity. So that tells you the amount of water which is present and your dry basis will give you the information of the other components now that we have all this we have been asked to calculate how much each of these is present in terms of wet basis.

So let us go about and try to do this calculations for performing this calculations let us assume a basis of 100 moles of dry air entering into the system. So basis would be 100 moles of dry air so based on the humidity data we know that mole fraction of water = 0.0700 moles of water per mole of wet air. So this can be converted to moles of water per moles of dry air because only then you will be able to use the values for the basis easily.

So we have the information for amount of water which means the amount of fraction of other components in the wet air would be 0.930 moles of dry air per mole of wet air. So using this we can calculate the mole fraction of water per using this we can calculate the mole ratio of water to dry air so which would be 0.0700 divided by 0.930 giving you a value of 0.0753 moles of water per mole of dry air.

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Example #2

- Orsat analysis yields 65% N₂, 14% CO₂, 11% CO and 10% O₂. Humidity measurement shows that mole fraction of H₂O is 0.0700. Calculate the molar composition in wet basis.

$100 \text{ mol DA} = 0.0753 \times 100 \text{ mol H}_2\text{O}$ $= 7.53 \text{ mol H}_2\text{O}$ $100 \text{ mol DA} = 65 \text{ mol N}_2$ 14 mol CO_2 11 mol CO 10 mol O_2 $7.53 \text{ mol H}_2\text{O}$ <hr style="width: 100%;"/> 107.53 mol	<p style="margin: 0;">Wet basis:</p> $\text{N}_2 = \frac{65}{107.53}$ $\text{CO}_2 = \frac{14}{107.53}$ $\text{CO} = \frac{11}{107.53}$ $\text{O}_2 = \frac{10}{107.53}$ $\text{H}_2\text{O} = \frac{7.53}{107.53}$
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Problem adapted from Felder and Rousseau, Elementary Principles of Chemical Processes, 3rd edition, Wiley-India

Now that we know the amount of water present per mole of dry air we can calculate the number of moles of water present for 100 moles of dry air which is basis used so 100 moles of dry air would contain 0.0753 times 100 moles of water which is 7.53 moles of water. So based on the orsat analysis we know that the 100 moles of dry air actually is constituted by 65 moles of nitrogen 14 moles of carbon dioxide 11 moles of carbon monoxide and 10 moles of oxygen.

So now in addition to this we have 7.53 moles of water vapor so for performing wet basis we need to calculate the total number of moles of this mixture including so which adds up to 107.53 moles. So the wet basis calculation for each of these components would be as follows you have nitrogen which would be 65 / 107.53 carbon dioxide would be 14 divided by 107.53 and carbon monoxide would be 11 divided by 107.53 oxygen would be 10 divided by 107.53 and water vapor would be 7.53 divided by 107.53.

These fractions represent the moles fraction of each of the component on wet basis so performing this calculations we have converted dry basis into wet basis.

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Example #3

- 100 mol/h of butane and 5000 mol/h of air are fed into the combustion reactor. Calculate the percent excess air.



$$\text{Theoretical } O_2 \text{ req} = 6.5 \frac{\text{mol } O_2}{\text{mol } C_4H_{10}}$$

$$\Rightarrow 100 \text{ mol/h } C_4H_{10} = 650 \text{ mol/h } O_2$$

$$\text{Theoretical air req for } 100 \text{ mol/h } C_4H_{10} = \frac{650}{0.21} = 3094 \text{ mol.}$$

Moving on to the next problem here is the another example where you are asked to calculate percent excess of air as I mentioned air is usually supplied in excess and here you have been asked to calculate how much excess is the air which is being supplied 100 moles butane and 5000 moles per hour of air are fed into the combustion reactor you are asked to calculate the percent excess of air before we do that we need to understand the stoichiometric for this reaction.

Butane would be C₄H₁₀ you reacts with oxygen to form carbon dioxide and water vapor so we will assume complete combustion which means only carbon dioxide and water vapor are formed. You do not have carbon monoxide which is being formed. So this is not a balanced equation we now need to balance this equation so we have four atoms of carbon taking part in reaction.

So we need to have at least four atoms of carbon which is being produced so now carbon is balanced if where to balance hydrogen we would have to add as the five for stoichiometric coefficient for water thereby 10 atoms of hydrogen coming in and 10 atoms of hydrogen leaving. So oxygen now needs to be balanced here we have 8 + 5 13 atoms which are leaving the reaction so this means you would have 13 / 2 or 6 and half molecules of oxygen entering in the reaction.

So this is the balanced equation so this means theoretically how much oxygen is required theoretical oxygen is required would be 6.5 Moles of oxygen per mole of butane. So here you have 100 moles per hour of butane being supplied. So which means 100 moles hour of butane would require 650 moles of oxygen. So in this case you have 5000 moles of air which is supplied per hour so what does 650 moles of oxygen represent.

So based on this theoretical requirement for oxygen we now need to calculate the theoretical requirement of air. Air contains oxygen and nitrogen for simplicity we will use 79% nitrogen and 21% oxygen. So this 650 moles of oxygen would be present in how many moles of air that would be the theoretical requirement of air. So the theoretical air requirement for 100 moles per hour of butane would be equal to 650 divided by 0.21.

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Example #3

- 100 mol/h of butane and 5000 mol/h of air are fed into the combustion reactor. Calculate the percent excess air.

$$\begin{aligned}
 \% \text{ excess air} &= \frac{\text{Air fed} - \text{Air reqd}}{\text{Air reqd}} \times 100 \\
 &= \frac{5000 - 3094}{3094} \times 100 \\
 &= \boxed{61.6\%}
 \end{aligned}$$

So this would give the value of 3094 moles of air per hour now that we know the theoretical requirement of air we need to calculate the percentage excess of air so percent excess of air can be calculated as follows percentage excess of air would be equal to air fed – air required for theoretical complete combustion divided by air required times 100 so this could means 5000 moles is fed per hour – 3094 moles required per hour divided by 3094 moles required times 100 giving you a percentage excess of 61.6 % .

So with this we have calculated the percentage excess air that is being supplied to the system with that we have come to the conclusion of the introduction for combustion reaction. So this

introductory lecture gave us some information about the different terminology and some fundamental calculation so which are associated with material balances that would be done for combustion reaction now that we have this understanding in the next lecture we will look at performing material balance calculation for combustion reactions thank you.