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Module - 05 Combustion and Thermochemistry Lecture - 19 Thermodynamic Considerations of Combustion

Deal learners, greetings from IIT, Guwahati. We are in the MOOCs course Advanced Thermodynamics and Combustion. Today, we are going to start a new module that is Module V, 5th module and the title of this module is Combustion and Thermochemistry. So, from now onwards we will move towards the combustion part of this course and we will see how our understanding in thermodynamics are helpful for combustion studies.

This combustion is very vital in our day to day life and in fact, it is in existence since human civilizations. So, the very basic intention for this module is to introduce the thermodynamic concepts in combustion applications.

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So, in this module we will have four important lectures. The first one is thermodynamic considerations of combustions. Here we will be discussing about fundamental aspects of combustion and various terminologies that are used while dealing with the combustion studies.

Then we will apply the conservation of energy for reacting systems; the word reacting means; that means, there is a chemical reaction that takes place when combustion happens. We will try to see how our understanding of e energy conservation will be useful for chemical reactions. Then we will try to introduce some important parameters which are very familiar in the combustion studies.

First thing is adiabatic flame temperatures; then entropy; of course, entropy we have used in our thermodynamic course, but how that entropy is an important phenomena which will decide the direction of chemical reactions. Now, in addition to this we have another thermodynamic parameter which we have introduced in Module 3 which is Gibbs functions and here we will see that how Gibbs function finds it is applications in reacting systems.

In the last lecture, we will be talking about the products of combustions and effective energy utilizations means that during a combustion process by considering the constituents of combustion products we can predict whether we have effectively utilized the fuels energy or not. Now, if not then what is the methods in which we can effectively use the energy utilizations during a combustion process.

So, this is about overall introduction about the Module 5 that is Combustion and Thermochemistry. Now, we will start the first lecture on this module that is thermodynamic considerations of combustions.



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So, in this lecture that is we are in the lecture number 19 that is overall lecture number and first lecture of module 5 is the thermodynamic considerations of combustions where we will be dealing with the combustion fundamentals, some terms like stoichiometry, equivalence ratio, products of combustion and we will see that how thermodynamics properties can be evaluated for a reacting system.

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Now, let us start the first segment that is combustion fundamentals. As I mentioned that combustion is in existence since human civilization and in fact, it is one of the important ancient discovery. So, basically during that point of time people used to think of fire of woods, but in reality what happens during the fire process, there is a fuel and there is a oxygen and as a results we have the heat that is going to be generated.

In fact, till today there is a self sustained heat release mechanism that happens in the sun. So, if you will look at suns view point you can see that it is the infinite source of fuel which keeps on burning and because of which we are in the receiving end in terms of light. And, of course, during this combustion process, there is some exhaust emissions which might have occurred in the deep space or in the vicinity of sun and many a times we call this as a solar storm.

So, they are nothing but the exhaust that comes out during self sustained combustion for which happens in the sun. So, just to give the importance or of the topic combustions and in our view point we will view it as a chemical reaction between a fuel and air. So, fuel and air means it is an oxidizer. So, when they react we get a combustion products. So, in totality we say there is some reactants and there are some products.

So, by definition one can say rapid oxidation to generate heat or light or both or slow oxidation accompanied by little heat or no light is regarded as the basic definition of combustion.

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Now, when you say this combustions, it can occur in a flame mode or non flame mode. We all know that when the combustion happens in engines; SI engines or CI engines we can say there are some flame generated and that keeps on propagating that is in the SI engine combustions whereas, in the diesel engines there are auto ignition of fuel and because of this we get a diffusion flame in the CI engine combustions.

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	Combustion Fundam	entals
•	The mechanism of combustion transforms energy sto	red in chemical bonds to heat
	that can be utilized in variety of ways.	
•	The internal energy of monoatomic species consists of	of translational (kinetic) energy
	while the diatomic species internal energy results from	n translational together with he
	energy from vibration (potential and kinetic energy) an	d rotation (kinetic energy).
	The combustion of hydrocarbon fuel occurs in most	power-producing devices. So,
	the objective of this module is study systems i	nvolving chemical reactions,
	dissociation and their thermodynamic analysis.	
	The above principles will also allow to determine the	e equilibrium composition of a
	mixture of chemical substances.	Translation
		0
		Monatomic species
	Reactants \rightarrow Products	Translation Kotation
	Fuel + Oxidizer \rightarrow Combustion products	
		Vibration

Then moving further, to another side of this combustion process in reality what happens? Basically, fuel and oxidizer they mix or they form as reactants and when there is an ignition then what happens? Fuel is burnt. So, by fuel is burnt what do you mean is that internal energy for the fuel is broken. So, in totality what we can say that there are bonds, that happens when you consider a diatomic species or monoatomic species.

Now, when we consider this a monoatomic species, we will have a transnational kinetic energy, when you look at the diatomic species, the internal energy results from the transnational together with energy from the vibrations. So, basically speaking, by adding through this combustion process we are trying to break the chemical bonds. Now, as a results we get the heat release that we realize.

So, ultimately what fuels that we are been using till today they are typically hydrocarbon fuels and by using this fuel energy we are producing the power. So, our main intention of this combustion studies is to look at this chemical reactions, its dissociation process, studies this thermodynamic analysis when such a combustion takes place. And this these fundamental principle will also allow us to determine the equilibrium compositions of mixture.

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Combustion Fundamentals				
<u> </u>	Reactants, products and stoichiometric coefficient			
	When a chemical reaction occurs, the bonds within molecules of <i>reactants</i> are broken and the atom/electrons rearrange to form <i>products</i> .			
	The rapid oxidation of combustible elements of the fuel results in energy release as the combustion products are formed.			
	Combustion reactions are expressed in terms of chemical equations. The mass of reactants should be equal to mass of the products. The total mass of each <i>chemical element</i> of the products must be same on both side of the equation. However, the number of moles of products may differ from the number of moles of reactants.			
	In a chemical reaction, the numerical coefficients which precede the chemical symbols to give equal amounts of each chemical element on both sides of equation, are called as 'stoichiometric coefficients". Reactants \rightarrow Products			
	$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$ (Total number of moles in reactants and products are not equal)			
	$(1 \text{ kmol})H_2 + (\frac{1}{2} \text{ kmol})O_2 \rightarrow (1 \text{ kmol})H_2O; (2 \text{ kg})H_2 + (16 \text{ kg})O_2 \rightarrow (18 \text{ kg})H_3O$ 7			

The next important topic that we are going to discuss is the reactants, products and stoichiometric coefficients. We mentioned that during a combustion process there has to be some reactants and there has to be products. For example, in a hydrogen combustion; that means, when hydrogen and oxygen they mix, we get water and it is a chemical reactions.

So, what we say? The reactants consist of hydrogen and oxygen products, is the water. So, we have we got the definition means what is reactants and what is products. Now, when you write these things in the equation form we call it as a chemical equations. So, all the combustion reactions are expressed in terms of chemical equations and the way we say that mass balance is applicable for thermodynamic analysis, we also have the mass of reactants and mass of the products should be equal.

And, if you look at this particular reaction hydrogen and oxygen it gives water. So, the number of species that are involved here is hydrogen, oxygen and we have to see number of hydrogens which is there in the reactant side should match with the number of hydrogen in the product side. Also, hydrogen may not exist in its own form, but it has mixed with oxygen to form water, but this hydrogen exists in water in the product.

So, what it says is that total mass of each chemical element of the products must be same on both sides of the equations. But, however, one important thing is that if you talk in terms of moles, the moles may be different. If you look at here maybe you can say 1 kilo mole of hydrogen, half kilo mole of oxygen and when they mix, so, the total kilomole will be one and half kilo mole, but when you see the product it is only 1 kilo mole of water.

So, the coefficients that is stoichiometric coefficients; that means, what we say is that in a balanced chemical reactions, the stoichiometric coefficients they are not same. That means in this equation 2 kg is the stoichiometric coefficient for hydrogen; 16 kg would be the stoichiometric coefficient for oxygen, but if you say 2 kg and 16 kg they are going to match as 18 kg of water.

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Apart from this, then we have another parameter which is fuel. So, fuel till date we have fuels which is available in the form of hydrocarbon fuels. Now, when I say fuels they are nothing but the mixture of combustible chemical elements mainly, carbon, hydrogen and they both are called together as hydrocarbons, then we have also sulphurs. But, however, this sulphur has least contributor in the energy productions, but it is the main source of pollution and other corroding environment.

Now, when I say complete combustions so, fuel must burn with oxidizer. So, for this thing, there will be a complete combustions, it can takes place when all the carbons in the fuel is burnt to carbon dioxide; that means, during a complete combustion process. The carbon in the fuel should form carbon dioxide, the hydrogen should form water; sulphur will form sulphur dioxides. So, this is how we have to get. If not then it is a incomplete combustion.

So, in totality we try to avoid the incomplete combustions. Now, coming back to the fuel so, fuel is nothing but a combustible substance which mainly contains hydrogen and carbon commonly known as hydrocarbon and they exist in three phases – first is liquid phase in the form of gasoline, diesel, kerosene, fuel oil, so, they are nothing but the liquid hydrocarbons derived from the crude petroleum products through distillation and cracking processes.

Then we also have fuels in the gaseous form – one such example is methane, where gaseous hydrocarbons are obtained from the natural gas through certain chemical process and we also have solid hydrocarbon fuels, which is nothing but the coal. So, the fuels are available in the liquid, solid and gaseous form, and mostly till now we are very used with respect to liquid fuels that is gasoline, diesel and kerosene.

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Oxidizer Combustion Fundamentals
 Oxygen is required in every combustion reaction. But, usage of pure oxygen is not possible in combustion applications rather air provides required oxygen.
 The approximate composition of dry air in terms of mass fraction are as follows: N₂ (78.08%), O₂ (20.95%), Ar (0.93%), CO₂ (0.03%) and others (0.01%).
 For combustion analysis, all minor components of dry air is lumped together with nitrogen and air is considered to be 21% oxygen and 79% nitrogen on molar basis with molar ratio of 3.76 i.e. every mole of O₂ is accompanied by 3.76 moles of N₂.
Nitrogen present in combustion air does not undergo the chemical reaction and hence regarded as inert for combustion.
 But, due to the increase in temperature during the reaction, nitrogen is prone to form nitric oxide (NO) or nitrogen dioxide (NO₂). In fact, these are source of air pollution during a combustion process.
Fuel + Oxidizer \rightarrow Products Oxygen : $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$
Air: $CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 2(3.76)N_2$ 9

Then moving further fuel as a whole it cannot burn. So, we need oxidizer, that means, for every reaction oxygen is required for a combustion process. But, what happens is that the usage of oxygen is not possible in combustion applications; usage of oxygen means I mean it is a pure oxygen.

So, pure oxygen deriving from atmosphere is very critical task, but normally what you do? We use air as a mode of supplier of oxygen. So, if you look at the composition of dry air in terms of mass fractions nitrogen is close to 78.08 percent, oxygen is 20.95 percent, argon is 0.93 percent, carbon dioxide is 0.03 percent and rest of the other gases is 0.01 percent.

Now, if you see the major constituents of air is nitrogen and oxygen. So, for the combustion study in a effective way; that means, instead of taking all other components like argon, CO_2 and which are very minor components they are merged with nitrogen. So, for the combustion analysis what we say is air consists of nitrogen and oxygen.

And, in terms of percentage we can write like this it is contains 21 percent oxygen and 79 percent nitrogen on molar basis with molar ratio of 3.75 which means if you want to take 1 mole of oxygen from air it is always accompanied by 3.76 mole of nitrogen. So, although you are using this nitrogen gas and this in a effective chemical reactions, the nitrogen becomes inert; that means, hydrogen has no role during the combustion process.

So, basically speaking if you look at here in a actual combustion process as I mentioned or complete combustion process all the fuel should burn; that means, carbon should come to carbon dioxide, hydrogen should come to form water. So, in a complete combustion process we will get CO_2 and water.

Now, in same reaction when you view with air, we can say in a complete combustion process we get same CO_2 and water, but what remains intact or inert is the quantity of nitrogen gases in the reactant and products. So, in a complete combustion process it is felt that nitrogen does not undergo in the chemical reactions or does not participate, although it is given, but it does not participate in the combustion process.

So, it is regarded as a inert gas for the combustion process, but what happens? During the chemical reactions the temperature goes up and this when temperature goes more than 1000 or 1500 K, then what happens? The nitrogen tries to break bonds that means, nitrogen gas tries to dissociate.

So, when it dissociates during this process, it is more likely to react with the oxygen and prefer to form the compounds like nitric oxide, nitrogen dioxide and these are nothing but the source of air pollutions; that means, they are essential culprits for the combustion process, this needs to be avoided and why this happens because we do not get pure oxygen. We do not have pure oxygen during a combustion process.

So, we have to very careful while dealing with this nitrogen and when it reacts what type of compound it forms.

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The next important segment in the combustion process is a stoichiometry. The word stoichiometric means it is a parameter that is very common and basically the reactants in the in a combustion process consists of fuel and air. And, when I say a complete combustion process; that means, fuel requires adequate amount of air or exact quantity amount of air for a complete combustion process.

If this happens, then we call it is a stoichiometric conditions that means, in a complete combustion process stoichiometric air has to be supplied. So, for that reasons there are two parameters that pops up, one is air-fuel ratio and the fuel-air ratio. Air-fuel ratio in a chemical reaction is the ratio of the amount of air to the amount of fuel and this ratio also can be written either in mass basis or in the molar basis.

Now, the minimum amount of air that supplies oxygen for a complete combustion of the fuel is known as theoretical amount of air and many a times you also use the theoretical amount of air which is same as the stoichiometric quantity of air or that means stoichiometric quantity of oxidizer is needed for a complete combustion process. When I say stoichiometric combustion; that means, there is no free oxygen that appears.

Now, not necessarily that always a combustion process has to happen in a complete mode or stoichiometric air is being supplied, now when more than stoichiometric quantity of oxidizer is supplied then the mixture is said to be fuel lean; that means, it is rich in air, lean in fuel. While supplying less than the quantity of stoichiometric oxidizer, it results fuel rich mixtures.

Now, in a fuel rich mixture always free oxygen appears. We will see later point of time how the free oxygen appears in the products in a fuel-lean combustions. Alternatively when I say theoretical amount of air we also call as percentage excess air. So, theoretical amount air and stoichiometric they are same. Now, we say percent excess air; that means, if I say 100 percent theoretical air; that means, we are in the stoichiometric conditions.

If I say 150 percent theoretical air; that means, we have 50 percent excess air or oxidizer. Now, if I say 80 percent theoretical layer which means 100 percent is theoretical air, but when we are putting air for stoichiometric conditions it means it is equivalent to 20 percent deficit air or we say the fuel is rich.

So, it is a rich fuel or lean fuel they are very common which have been using we have been using during our IC engine course as well in the basic thermodynamic course. So, how to quantify this? So, first number what we say air-fuel ratio $AF = \frac{m_a}{m_f}$.

Now, for this mass of air if you represent in terms of number of moles $AF = \frac{n_a M_a}{n_f M_f}$. And, when I put this, instead of air-fuel ratio we say molar air fuel ratio; that means, number of moles of air to the number of moles of fuel into its molecular weight ratio.

So, this is how the relation between air-fuel ratio on mass basis and air-fuel ratio on molar basis $AF = \overline{AF} \frac{M_a}{M_f}$.

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Equivalence Ratio	
completely. This unburnt fuels ends up as pollution.	
In actual combustion, the equivalence ratio is the measure of fuel-air ratio relative to	
stoichiometric conditions. It is the ratio of the actual fuel-air ratio to the fuel-air ratio	
for complete combustion with theoretical amount of air.	
• The reactants form lean mixture when equivalence ratio is less than unity while rich	
mixture will have equivalence ratio greater than unity.	
$\phi = \frac{(FA)_{act}}{(FA)_{isol}} = \frac{(AF)_{isol}}{(AF)_{act}}; \ AF = \frac{m_a}{m_f} \& FA = \frac{m_f}{m_a}$	
$\phi < 1 \Rightarrow$ Lean fuel (oxygen in products); $\phi > 1 \Rightarrow$ Rich fuel (CO and unburnt fuel in products)	
$\phi = 1 \Rightarrow$ Stoichiometric fuel (Release of maximum energy from fuel)	
Methane-Air Combustion : Lean fuel (150% stoichiometric air)	
$CH_4 + 3O_2 + 3(3.76)N_2 \rightarrow CO_2 + 2H_2O + 3(3.76)N_2 + O_2$	
Isoctane-Air Combustion : Rich fuel (80% stoichiometric air)	
$C_8H_{18} + 10O_2 + 10(3.76)N_2 \rightarrow 3CO_2 + 9H_2O + 10(3.76)N_2 + 5CO_2 + 9H_2O_2 + 9H$	
Stoichiometric (Methane-Air): $CH_4 + 2O_2 + 2(3.76)N_2 \rightarrow CO_2 + 2H_2O + \frac{1}{2}(3.76)N_2$	п
Stoichiometric (Isoctane-Air): $C_8H_{18} + 12.5O_2 + 12.5(3.76)N_2 \rightarrow 8CO_2 + 9H_2O + 12.5(3.76)N_2$	

Now, next parameter that we are going to discuss is the equivalence ratio. So, you already told about the excess air, deficit air. Now, during an actual combustion process how do you take a decision which parameter we need to regulate. So, basically instead of talking about air-fuel ratio or fuel-air ratio another parameter is defined which is equivalence ratio and it is the measure of fuel-air ratio relative to the stoichiometric conditions.

And, we have discussed about the complete combustion process and incomplete combustion process. When there is a complete combustion process it refers to a stoichiometric chemical reaction between fuel and air. Now, when you have incomplete combustions it is a non-stoichiometric situations. Now, to define this non-stoichiometric situations, the equivalence ratio is chosen as the one of the non-dimensional parameters.

In fact, it is main advantage is that it says whether the mixture is rich in fuel or lean in fuel, the reactants form lean mixture when the equivalence ratio is less than unity and they form rich mixtures when they have equivalent ratio greater than unity. And, the parameter that is used is ϕ that is equivalence ratio fuel-air ratio actual divided by fuel-air ratio stoichiometric and when it is represented in terms of air fuel, it is air-fuel ratio stoichiometric by air-fuel ratio actual.

And, we also know what is their air-fuel ratio, we also know what is the fuel-air ratio. $AF = \frac{m_a}{m_f}$; $FA = \frac{m_f}{m_a}$. Now, from this equation it is clear that when $\phi < 1$, it is a lean fuel which means oxygen remains in the product. If you look at these equations methane-air combustion in a lean fuel let us start with a stoichiometric methane air combustions.

$$CH_4 + 2O_2 + 2(3.76N_2) \rightarrow CO_2 + 2H_2O + 2(3.76N_2)$$

If you see here nitrogen remains inert and the combustion product is CO_2 and H_2O . So, it is a stoichiometric methane-air combustions. Now, if it is lean fuel; that means rich in air; rich in means it is 150 percent theoretical or stoichiometric air. So, 150 percent means that means, 1.5 times higher. So, when I say 1.5 times higher the air becomes 1.5 times higher.

$$CH_4 + 3O_2 + 3(3.76N_2) \rightarrow CO_2 + 2H_2O + 3(3.76N_2) + O_2$$

And, here when I make this reaction to happen, in the products we have CO_2 , H_2O_2 , nitrogen, but what lands up is that free oxygen which is available in a lean fuel situations for a methane air combustions. Now, another scenario we can have the rich fuel. Now, when you have rich fuel we will have carbon monoxide and unburnt fuel in the products. Let us see how it happens.

If you consider the stoichiometric reaction of iso-octane air; that means, it is another fuel iso-octane is the fuel air is the oxidizer. If you do that and a balanced chemical reactions it says that $C_8H_{18} + 12.5O_2 + 12.5(3.76N_2) \rightarrow 8CO_2 + 9H_2O + 12.5(3.76N_2)$. But, what we require is rich fuel; that means, rich fuel means 80 percent of stoichiometric air; that means, it is air in deficit.

So, if that is the case, $C_8H_{18} + 10O_2 + 10(3.76N_2) \rightarrow 3CO_2 + 9H_2O + 10(3.76N_2) + 5CO$. And, we can have a balanced chemical equations that forms CO₂, water, nitrogen and here we have carbon monoxide as well as we will have unburnt fuels that remains; that means, fuel did not get sufficient quantity of air.

An ideal situation would be $\phi = 1$ which refers to a stoichiometric fuel which means at this situation we will have release of maximum energy from the fuel.

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Now, next segment that we are going to discussed is the products of combustion. Till this point of time we have seen fuel mixes with oxidizer to give combustion products. But, what are the products that comes and an ideal situation the products will be carbon dioxide, water and nitrogen.

Now, that means, this is a complete combustions to obtain the balanced chemical reaction. But, what happens in an actual scenario? None of the combustion process is a complete combustion process. It is always will have incomplete combustions. So, to quantify that whether it is incomplete depends on the whether we are rich in fuel or lean in fuel and in the parameters like NO, NO_x, CO all these constituencies are likely to be present.

Now, to quantify such parameters there are several devices that measures the composition of combustion products namely Orsat analyzer, gas chromatography, infrared analyzer, flame ionization detectors and all these things they are reported as dry product analysis and they are represented in terms of mole fraction.

So, basically all combustion products if you look at these products CO_2 , nitrogen, except water, we call this as a dry product analysis in terms of mole fraction. Here the question mark that comes in what happens to water.

Now, depending on the temperature of the exhaust products, water may exist in a vapour form or what happens if the vapour is exhausted to atmosphere it gets cooled. And, during

this cooling process, the vapour may turn back to liquid. So, water vapour changes its phase to liquid form, it has to pass through a temperature which we commonly use the word in psychrometrics which is called as dew point temperatures.

So, initially the gaseous products of combustions, they are already at elevated higher temperatures and when they are cooled to the atmospheric pressure, the water which was existed as a vapour form, it changes its phase and they are likely to condensate and this condensation has to pass through the dew point temperature.

And, this temperature depends at what partial pressures water vapour exist that we can find out from number of mole fraction of that constituents. The very basic point is that when the vapours begins to condensate or liquid droplets are formed, they effectively create corrosions in the metal parts, duct pipes.

So, this is the downside of the combustion process that continuous exposure of water in the metallic parts leads to corrosion and further damaging of surface.

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The last segment of this part is to study the thermodynamic property analysis for a reacting systems. So, here the first basic assumption that we are going to make is that till this point of time before this combustions we have exhaustively discussed the multi component systems and they are treated as an ideal gas mixtures.

So, the reference line for the combustion study is that as if it is a mixture of reactants and products and we have to find out the each constituents, their mole fractions, their individual parameters and we have to multiply that with respect to their respective mole fraction or mass fraction to get the effective thermodynamic parameters like w internal energy, enthalpy, entropy.

And, this analysis we have to recall it as a reference view point, we have to recall them as an ideal gas mixture to calculate these properties. For example, if you say internal energy is the summation of the molar specific internal energy multiplied by the mole fractions for all the components and same logic applies for enthalpy as well.

Now, for entropy similar philosophy is used. But, entropy is calculated at temperature t and pressure because it is a function of temperature as well as pressures, but here to calculate this temperature and pressure, people use the concept of absolute entropy where we assign this reference value of given constituents at reference pressure p_{ref} and temperature T_{ref} .

And, as we did in the ideal mixture analysis the reference value was taken as 1 atmosphere reference temperature was 25 C. So, the concept of absolute entropy is used to find the entropy of the ideal gas mixture.

Numerical Problems Q1. Determine the air-fuel ratio on both molar and mass basis for complete combustion f octane: (a) theoretical air; (b)120% theoretical air. Find the d Na + 00, 1.2) (12.5) (02+3.76 N2) (6) 15 (02 + 3.76 M2) 11

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With this we have come to the end of this contents of the today's lectures. Now, we will based on the lecture contents or whatever contents we have covered will try to solve some numerical problems. The first problem is based on air-fuel ratio calculation or fuel-air ratio calculation on molar and mass basis for a complete combustion process.

And, here we have used the word octane as the fuel, we have to calculate this air-fuel ratio for a theoretical air situation, excess air situations and when you are using the excess air we have to find out the equivalence ratio. So, when such a problems comes, first thing you have to write two equations; one is balanced chemical reaction between fuel and oxidizer, other is unbalanced equations; unbalanced equation means when we have excess air or excess fuel.

So, it is a octane oxygen combustion. So, balanced reaction we can write as $C_8H_{18} + a(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dN_2$. So, first thing we have to do balance; balancing the components.

Balancing components: Carbon: b = 8; Hydrogen (H₂): 2C = 18, C = 9Nitrogen: d = 3.76 a; Oxygen: 2b + c = 2a, a = 15 & d = 47.

So, the balanced reaction now becomes $C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 47N_2$, then we are now in a position to calculate the mole fractions and as well as the mass fractions. So, before that, for this fuel we can write molecular weight of fuel that is $C_8H_{18} = 12 \times 8 + 18 \times 1 = 114$.

So, molecular weight of fuel is 114, we all know molecular weight of air is 28.97. So, we are now in a position to calculate air-fuel ratio on molar basis that is $\overline{AF} = \frac{n_a}{n_f} = \frac{(12.5+(12.5\times3.76))}{1} = 59.5 \text{ kmol air/kmol fuel}$

$$AF = A\overline{F}\left(rac{M_{air}}{M_{fuel}}
ight) = 15.1 \, kg \, air/kg \, fuel$$

So, this is what happens it is a stoichiometric conditions. Now, second part which you are going to study when you have 120 percent theoretical air; that means, this coefficient has to be increased by 20 percent.

So, the reaction will now become $C_8H_{18} + 1.2 \times 12.5(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dN_2 + eO_2$. So, this coefficient needs to be calculated. So, now from this equations this reactant side all known parameters, product side we have unknown parameters.

By repeating same principle balancing the components we can get b = 8; c = 9; d = 56.4; e = 2.5. Now, after putting this we rewrite this equation as $C_8H_{18} + 15(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 56.4N_2 + e2.5O_2$.

So, here air-fuel ratio we can write $\overline{AF} = \frac{n_a}{n_f} = \frac{(12.5 \times 1.2 + (12.5 \times 1.2 \times 3.76))}{1} = 71.4 \text{ kmol air/}$ kmol fuel. So, this parameter is for oxygen, this parameter is for nitrogen. Now, once we know air-fuel ratio we can write $AF = A\overline{F}\left(\frac{m_{air}}{m_{fuel}}\right) = 18.15 \text{ kg air/ kg fuel}.$

Now, last parameter what is the equivalence ratio. $\phi = \frac{AF_{stoich}}{AF_{actual}} = \frac{15.1}{18.15} = 0.833$. So, this is about 0.833. Other way to find out is $\phi = \frac{\overline{AF}_{stoich}}{\overline{AF}_{actual}} = 0.833$ which means phi is less than 1.

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Now, next problem is the data analysis for a methane air combustions. When this methane is combusted with air and we get the combustion products and those combustion products consist of CO_2 , CO, O_2 and N_2 with their respective compositions. We need to find out airfuel ratio on molar and mass basis percentage of theoretical air and dew point temperature.

So, for this case also we say $a CH_4 + b(O_2 + 3.76N_2) \rightarrow 9.8 CO_2 + 0.6 CO + 86.6 N_2 + 3O_2 + c H_2O$.

So, basically unknown are stoichiometric coefficients of methane, air and water. So, we have to do the balancing of stoichiometric coefficients and it will result what a = 10.4, b = 23.5, c = 20.8.

Now, once we have this then we are in a position to write this complete balanced equations that is $10.4 CH_4 + 23.5(O_2 + 3.76N_2) \rightarrow 9.8 CO_2 + 0.6 CO + 86.6 N_2 + 3O_2 + 20.8 H_2O$. Now, we have M of CH 4 as 16 and M of air 28.97.

Then we can calculate air-fuel ratio $\overline{AF} = \frac{n_a}{n_f} = \frac{25(1+3.76)}{10.4} = 10.75 \ kmol \ air/kmol \ fuel.$ Then we can find AF on mass basis, $AF = A\overline{F}\left(\frac{M_{air}}{M_{fuel}}\right) = 19.47 \ kg \ air/kg \ fuel.$ So, we get air-fuel ratio on molar and mass basis percentage of theoretical air.

So, if it is a balanced chemical reaction what would have been? That $CH_4 + 2O_2 + 2(3.76N_2) \rightarrow CO_2 + 2H_2O + 2(3.76N_2)$. Then in that case $\overline{AF} = \frac{n_a}{n_f} = \frac{2(1+3.76)}{1} = 9.52 \ kmol \frac{air}{kmol} fuel$. So, percentage of theoretical air would be like $\frac{\overline{AF}}{\overline{AF}_{stoichio}} \times 100 = \frac{10.75}{9.52} = 113\%$. So, that is 13 percent excess air.

Third point is calculate the dew point temperature of the products mixture where equal to 1 bar. So, basically the products that water is forming dew. So, what is the mole fraction of this number? So, you can say water is available as component stoichiometric coefficient 20.8.

So, we can say mole fraction of water vapour as $Y_v = \frac{20.8}{100+20.8} = 0.172$. Now, partial pressure of water vapour is $p_v = Y_v p = 0.1744 \ bar$. So, we know this partial pressure and corresponding to this partial pressure we refer saturated pressure table for water and this will give you temperature as about approximately 60 C.

So, it means when these temperature products are cooled at 1 bar water will form dew and this dew to point temperature is 60 C at that partial pressure. So, you can see here one is on stoichiometric situation, other is a non stoichiometric situations.

With this I come to the end for this lecture today. Thank you for your attention.