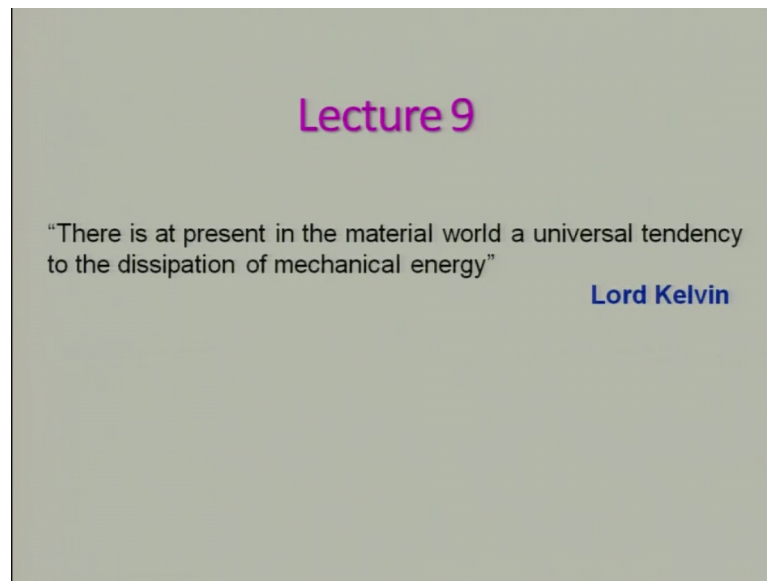


Fundamentals Of Combustion (Part 1)
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Lecture – 09
Stoichiometric calculations for air-gas mixture

Let us start this lecture with a thought process from Lord Kelvin.

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He says, There is at present in the material wall a universal tendency to the dissipation of mechanical energy and if you recall that we had basically initiated discussion on the various laws of thermodynamics; we just reviewed it, we did not derive those things. But keep in mind that we will be using the first law of Thermodynamics very profusely. And we will be using the second law of Thermodynamic whenever we are dealing with the equilibrium composition in combustion.

And towards the later portion of last lecture, we initiated discussion on Stoichiometric. Stoichiometry plays a very important role which indicates theoretical oxidizer required for the complete combustion of wealth; isn't it? And we will take an example and then, see how we will handle in a better manner and let us consider that we will take one mole of methane.

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Stoichiometry

Example: $\text{CH}_4 + 2(\text{O}_2 + 79/21 \text{N}_2) \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 3.76 \text{N}_2$

$\text{C}_x\text{H}_y + a(\text{O}_2 + 79/21 \text{N}_2) \rightarrow x\text{CO}_2 + \frac{y}{2}\text{H}_2\text{O} + 3.76a \text{N}_2$

$a = (4x+y)/4$ O: $2a = 2x + y/2 \Rightarrow a = \frac{4x+y}{4}$

For CH₄: $(A/F)_{\text{stoic}} = \frac{m_{\text{air}}}{m_{\text{fuel}}} = \frac{\{MW_{\text{air}} \cdot (n_{\text{O}_2} + (79/21)n_{\text{N}_2})\}}{\{MW_{\text{CH}_4} \cdot n_{\text{CH}_4}\}}$

$(A/F)_{\text{stoic}} = \{29 \times 2(1 + 79/21)\} / \{16\} = 17.26$

$(A/F)_{\text{stoic}} = 4.76a \{MW_{\text{air}} / MW_{\text{C}_x\text{H}_y}\}$

The actual (Ox/F) in a fuel-air mixture can be different than (Ox/F)_{stoic}.

Lean mixture: If $(F/Ox)_{\text{actual}} < (F/Ox)_{\text{stoic}}$ $\phi < 1$

Rich mixture: If $(F/Ox)_{\text{actual}} > (F/Ox)_{\text{stoic}}$ $\phi > 1$

Stoichiometric mixture: If $(F/Ox)_{\text{actual}} = (F/Ox)_{\text{stoic}}$ $\phi = 1$

Equivalence Ratio: $\phi = \frac{(F/Ox)_{\text{actual}}}{(F/Ox)_{\text{stoic}}} = \frac{(F/Ox)_{\text{actual}}}{(F/Ox)_{\text{stoic}}}$

Equivalence Ratio: The equivalence ratio is defined as the ratio of the actual fuel/air ratio to the stoichiometric fuel/air ratio.

$\% \text{ Stoichiometric air} = \frac{100}{\phi}$ $\% \text{ excess air} = \frac{(1 - \phi)}{\phi} \cdot 100$

And it is reacting with basically air; if you look at this is nothing but your air, oxygen and nitrogen; 21 percent oxygen is there in air and 79 percentage of nitrogen in the air. That we are assuming. However, air will be containing other constituents also, all composition also species also.

Now, and we are assuming that the product will be carbon dioxide, water and nitrogen. Keep in mind nitrogen is not participating in it; it is remaining as nitrogen. But in real situation there will be some n Ox; n o nitrous oxide, nitric oxide. Other things like s e n, but we are not assuming. Similarly it is not that product will do only carbon dioxide and water; it is a only theoretically. There will be carbon monoxide; there will be unburned hydrocarbon; there will be some other species; formaldehyde other things. But those are things, but here we are assuming theoretical or the something ideal situation.

Now, I want to basically find out how much air is required to burn 1 mole of methane. So, what I will have to do? I will have to do a balance. So, how I will do it? So, if you look at like, can you people do that? It is very easy and if you look at I can, I know put it here 2. Because CH 4. So, H 4 in the left hand side and water and that H is 4. So, similarly I can put here 2; because this is 4 O and this is 2 O in the water on the right hand side and O 2 in the carbon monoxide side and nitrogen is very easy, it will be into 79 by 21. If you look at 79 by 21 will be 3.76 kind of thing. So, this thing ratio will be 3.76.

Now, that means, this is basically (Refer Time: 03:57); that means, 1 mole of fuel will be burnt, you know 2 moles of air for complete combustion and which is theoretical. Now, if it is some other hydrocarbons, let us say propane or butane or pentane or hexane or any other hydrocarbons. So, how will deal with that? That is the question arisen, which will be little easier way of doing. So, for that let us represent the hydrocarbon as $C_x H_y$; x can be 1, H can be 4 that is methane. So similarly, x can be 2 and y can be some other things, you know it will be another. So, if will do that, how we are going to do this?

This is in a similar way. Is not it? For example, if it is $C_x H_y$, what I will do? I will put it here x and in this space, we can put it y by 2 and this will be, a will be what? That is the thing we need to find out and this will be nothing but $3.76 a$. We need to find out a. How we are going to do it? If I say that a will be equal to $4x$ plus y divided by 4; is it right? How can I derive it? It is a very simple one.

What I will have to do? I will have to take O and balance it. If I will do that, O is equal to on the left hand side $2a$ and on the right hand side for carbon dioxide term, if you look at that is $2x$ and for the water, it is y by 2 and then, that is nothing but your what you call, a is equal to $4x$ plus y divided by 4; that you can get very easily. Is not it? If you look at a is equal to $4x$ plus y divided by 4, that I am getting very easily.

So, if you remember this it will be very easy to do that, but there might be a situation, you know this would not be hold good. For example, if I say producer gas or a coke oven gas, this formula would not help. Will it help you? Even if you are remember it would not work because it will be not only containing hydrocarbon, it will be containing CO; it will be containing nitrogen; it will be containing hydrogen. You know then, this formula would not be helpful. We will take an example little later on, just to find out, how we can handle, this mixture which is not represented by $C_x H_y$, hydrocarbons.

Now, we need to find out what will be this, you know of air fuel stoichiometric? Air fuel stoichiometric, basically by mass we consider; that means, mass of air divided by mass of fuel; is equal to, what is the mass of air? And keep in mind in this expression or the both the chemical reaction what I have shown here like which is generalized hydrocarbon, other is methane.

For both case it is the moles, but now we will have to convert into mass. Therefore, will have to multiply with the molecular weight of air into the air; air will be a into O_2 plus

79 divided by 21 N₂ that is basically number of moles of nitrogen. And this we know this is nothing but your 3.76 divided by number of moles into the molecular weight of methane; number of moles of the fuel or the methane into molecular weight of the methane.

Now, in this case a will be what, in this case? For, because we are talking about for methane. So, therefore, it will be 2. Is not it? a will be 2 and if we will generalize this A by F stoichiometric, we will get that, but before that let us look at like we will substitute these values; a molecular weight of air I have taken as 29. It may be little bit different and then into 2 1 plus 79 divide by 2. Then divided by 16; it happens to be 17.26 air fuel ratio. That means, for 1 kg of fuel, you need to supply 17.26 kg of air for complete combustion. Now if it is I say propane, what it would be? Any idea? Will it be more or it will be less, what it would be, air fuel ratio you will?

Student: Less.

It will be less. So, how much it will be? Any idea?

Student: More.

It will be more; that means, because it is, why you are saying it is more?

Student: Hydrogen and (Refer Time: 09:24).

Hydrogen and carbon atoms are more.

Actually it is not true; it will be less. It will be around 15. If I say butane, it will be around 15 also. If I say you know let us say hexane, it will be around 15. So, only exception is the methane for which it will be 17.26 or 17. Keep in mind that it is 15 means does not mean it is 15. It is 14.98; in some case 14.89. It is like that not exactly 15, but therefore, we keep always a hydrocarbon means air fuel ratio will be around 15 in mind bulk pack number. Are you getting? You please do a calculation; then, you will know .

And let us say that we want to have this air fuel stoichiometric ratio for a generalized hydrocarbon that is C_x H_y. What it would be? If you can look at basically this portion is nothing but your, if you look at this portion, what it will be? This will be 1 plus 3.76

because number of moles. Then it will be 4.76 and molecular air divided by molecular weight of the fuel or the hydrocarbon. In this example basically hydrocarbon.

So, that is a very simple formula, you can remember provided it is a hydrocarbon; basically the stoichiometric is a theoretical value of air fuel ratio which is required for complete combustion or fuel-air ratio or fuel oxidizer ratio for complete combustion. But in real situation, if I will give that amount of air to burn 1 kg of fuel; let us say for methane I am supplying 17.26 kg of air for burning 1 kg of fuel. Whether the complete combustion will take place or not? Yes or no? Actually in case it is not; it is a theoretical. So, therefore, we need to give little more in practical situation.

And we will have to also give much more because emission is a big concern. So, therefore, we will have to reduce it and sometimes we give also the less amount of oxidizer or the air for combustion because that depends on what is the applications. For example, I want to have a sooty flame, naturally I will have to give less; whenever I am talking about (Refer Time: 12:16).

So, therefore, we need to look at whether it is a fuel Lean or it is a fuel Rich or is it a stoichiometric. So, if it is what do you mean by fuel Lean then? That means, the amount of fuel will be what? Less as compared to the requisite fuel for the stoichiometric for the same amount of oxidizer; that means, if fuel and oxidizer actually is less than fuel and oxidizer stoichiometric; then, we call it is fuel lean. Fuel is less and if it is Rich mixture it will be fuel and oxidizer actual will be greater than fuel and oxidizer stoichiometric; that is a Rich mixture and stoichiometric means it will be same.

Now, this is of course, qualitatively we will say, it is less or more, but now I need to express that in terms of certain numbers. So, that it will be easier for me to calculate or to determine. What will be, whether Lean fuel mixture or the Rich mixture, for that what I will have to do? I like to define a term which is known as Equivalence Ratio. So, equivalence ratio is basically if you look at it is oxidizer bio fuel Stoichiometric divided by the oxidizer by fuel actual. This is basically actual and that is same as fuel and oxidizer actual divided by fuel and oxidizer Stoichiometry.

That means if Equivalence Ratio is equal to 1, what is the thing? If ϕ is equal to 1; it is Stoichiometric. If ϕ is equal to less than 1, it will be Lean mixture. If it is ϕ greater than 1, it will be Rich mixture. Are you getting? And when you are talking about this, we

mean basically fuel rich; there can be oxidizer rich also. Is not it? I can say oxidize, but here, the what we are discussing is basically ϕ is greater than 1 means it is fuel rich more amount of fuel is there than the whatever the amount of oxidizer, stoichiometric oxidizer required for complete combustion.

So, that is basically equivalence ratio is defined as the ratio of actual fuel air ratio to the stoichiometric fuel air ratio. Keep in mind that this is a very useful you know term for analyzing the, which plane? Premix plane or the diffusion plane. This will be very useful for analyzing the premixed plane because there in case of premixed plane fuel and oxidizer are mixed before the combustion take place. So, therefore, you need to know what you are doing; that means, I can control the fuel air ratio or the equivalence ratio in other words so that I will get the good combustion.

But apart from that, there are other terms which are used to understand like how it is different from the stoichiometric? That means how the fuel air ratio or the oxidizer air ratio is different from the stoichiometric ratio? For that we will be talking about 2 terms; one is percentage of stoichiometric air which is nothing but 100 divided by ϕ , ϕ is your equivalence ratio. This is your equivalence ratio and similarly, I can find out what is the percent of excess air? That is nothing but 1 minus ϕ divided by ϕ and this ϕ also same as the equivalence ratio; that means, which will say that how much excess you are given? As I told that for complete combustion for, to reduce the emission we always give excess air.

So, now as I told that this will be a very useful for premixed plane, but we will have to handle also the diffusion plane. Where, the fuel and oxygen are not really mixed before the combustion takes place and for that we will look at it, you know how to handle that. But before getting into that, you know how we will handle, whether we will use equivalence ratio or not and how we can modify it or will be using, using some different term for to take care of that; we will take an example, how to carry out a stoichiometric calculation? And particularly, how we will handle some fuel which need not to be a simple hydrocarbon unsaturated hydrocarbon.

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Stoichiometry Calculation

Problem: Gasoline + dry air $\rightarrow$ Products (10.02% CO₂; 5.62% O₂; 0.88% CO; 83.48% N₂)
Determine (i) A/F ratio; (ii) Equivalence ratio; (iii) % of Stoichiometric air used

Solution: $\text{C}_8\text{H}_{18} + a(\text{O}_2 + 3.76 \text{N}_2) \rightarrow 10.2 \text{CO}_2 + 0.88 \text{CO} + 5.62 \text{O}_2 + 83.48 \text{N}_2 + b\text{H}_2\text{O}$

By mass balance:

N: $3.76a = 83.48$; $\rightarrow a = 22.2$

C: $8x = 10.02 + 0.88$; $\rightarrow x = 1.36$

H: $18x = 2b$; $\rightarrow b = 12.24$

O: $2a = 10.02 \times 2 + 0.88 \times 2 + 5.62 \times 2 + b$ $\rightarrow \text{LHS} = 44.4 = \text{RHS} = 44.4$ (checked)

Recasting the above reaction in terms of 1 mole of fuel as given below;

$\text{C}_8\text{H}_{18} + 16.32 (\text{O}_2 + 3.76 \text{N}_2) \rightarrow 7.37 \text{CO}_2 + 0.65 \text{CO} + 4.31 \text{O}_2 + 61.38 \text{N}_2 + 9 \text{H}_2\text{O}$

$(F/A)_{\text{actual}} = m_{\text{fuel}}/m_{\text{air}} = ((12 \times 8) + 18) / (16.32(32 + (3.76 \times 28))) = 0.05089$ $A/F = 19.65$

Stoichiometric Equation: $\text{C}_8\text{H}_{18} + 12.5(\text{O}_2 + 3.76 \text{N}_2) \rightarrow 8 \text{CO}_2 + 9 \text{H}_2\text{O} + 47 \text{N}_2$ $a = (32 \times 7.5) / 4 = 12.5$

$(F/A)_{\text{stoic}} = m_{\text{fuel}}/m_{\text{air}} = ((12 \times 8) + 18) / (12.5(32 + (3.76 \times 28))) = 0.06643$

Equivalence ratio (Φ) = $(F/A)_{\text{actual}} / (F/A)_{\text{stoic}} = 0.766$

Since $\Phi < 1$, the mixture is lean

% Stoichiometric air can be determined as:

% Stoichiometric air = $100 / \Phi = 100 / 0.766 = 130.5\%$

Now, for that we will take an example. This example is Gasoline. Gasoline, you know we call it basically petrol in our terminology or generally, is mixed with the dry air; that means, dry air means what? It does not contain moisture. But, however, you cannot avoid it moisture in the air. Suppose I say that you want to have a dry air in your lab, how you are going to get it, any idea? I want to have a dry air in my lab, in combustion lab; you know where you are conducting combustion. Explain how you will get it?

Student: (Refer Time: 18:13).

[FL].

Student: Sir, 100 percent [FL].

[FL] 100 percent [FL] I want to have, how I will do that? This question you think about it.

Student: Sir, silica gel.

Very good.

So, you can pass through the silica gel; it will absorb the moisture and then, you can do that; very good. It will go to the products; products I can measure you know like by various means and let's say the measured products is 10.02 percentage carbon dioxide;

5.62 oxygen and 0.88 CO, that is carbon monoxide and 83.48 nitrogen. These are the things you are getting.

And we will have to determine air fuel ratio equivalence ratio and percentage of stoichiometric air used in this mixture. So, if you look at gasoline can be represented as C_8H_{18} ; let's say the X moles of C_8H_{18} is reacting with a moles of air and giving the product of 10.2 carbon dioxide, 0.88 carbon monoxide, 5.62 oxygen. If you look at some oxygen is there. Here also, that means, it is remain unutilised; it remains unutilized and 83.48 nitrogen and of course, the water will be formed you cannot avoid water and assume that all are in gaseous form. Now, how we are going to do it? Because I want to balance I will have to find out what is a ? What is b ?

This is not known, I do not know also the x ; it may be 1 mole, it may be different than 1 mole because what is known is the product, but I am not aware how much is there in the reactant you know. So, therefore, I do not know. So, how we are going to do this, any idea? You have done all those things in plus 2. So, I am just trying to make you recall, no idea. Basically we will be doing mass balance.

So, what we will have to do? We will have to take the each element and then, try to balance. Let us do that that is very easy and they all already we have done and now, I am just asking you to. So, basically mass balance N, nitrogen we are taking element. If you look at left hand side is basically what it would be? I can say this will be N_2 , if 1 that will better; otherwise, you have to multiply it by 2 here, left hand side. Left hand side if you look at it is nothing but a and $3.76a$ is equal to this one.

Student: That should be equal to 83.

83.48. So, therefore, a you can get very easily. What is that a ? Is equal to 22.2 and similar manner I will go for C, if you look at it is basically left hand side $8x$ and from the right hand side carbon dioxide 10.2 and from carbon monoxide 0.88. So, I will get x right and x is equal to 1.36, see I have also not taken the after decimal, second digit after decimal point, but you may take for accuracy. If you round it up, it also and some error you may incur; but I have just taken round it up.

So, for H left hand side it is $18x$ and right hand side is the water only that is $2b$. So, you will get b is basically, how much it will be? 12.24 because x is 1.36; x is known I can this

is x . This is not multiplication sign. This x is basically the symbol x . I wish I could have used y . So, that is basically x , 18 into 1.36 divided by 2 will give you 12.24. Now, if you look at, I got all x values, a values and b values good enough.

But, however, you need to do another balance just to check whether it is right or wrong; for that what we will have to consider? Will consider O; in O it is $2a$ in the left hand side, right hand side it is from carbon dioxide is 10.02 into 2 because CO_2 plus carbon monoxide 0.88.

And oxygen is basically 2 into 5.62 and of course, b ; this is actually just to check because this good enough whatever we have done till now. So, you will find out left hand side is 44.4, right hand side is 44.4. So, therefore, whatever you are done is right; you are 100 percent sure. Then, you know what it is. So, now, what we are getting? We are getting 1.36 moles of C_8H_{18} is reacting with 22 point moles of air giving to the product of 10.2 carbon dioxide, 0.88 C, carbon monoxide; 5.62 oxygen and of course, 8.48 nitrogen and b is 12.24 water.

Now, what we will have to do, b is basically 12.24 and a is if you look at in this example, it is 22.2. Now I can divide all this thing with the 1.36. So, that I can convert into 1 mole of C_8H_{18} is you know, what it is. If you will do that; what I will do? I will divide this thing by 1.36. Why I am doing? With just to recasting the above reaction equation rather in terms of 1 moles of well as given below you will get in one terms. Are you getting? It will be just easy you need not to do that also, but it will be easier.

Now, what is the fuel air ratio? That is actual right this is m fuel divided by m oxidizer. What do you do m fuel is C_8H_{18} . So, this is nothing but your fuel and this is your oxidizer and you will get 0.05089. Now if we are having a calculator you do that, what will be air fuel ratio? Just let us do that what is coming? Something, 19.65.

Now, let us look at Stoichiometric Equation. That is very easy, 1 mole of C_8H_{18} is reacting with 12.5 of oxygen plus 3.76 nitrogen; 8 moles of carbon dioxide, 9 moles of water and 47 moles of nitrogen. If you look at you need to balance, I have just given this thing. Of course, it is very easy to do that from here.

Suppose here, now C 8. So, therefore, it is 8 and 18. Therefore, it is 18 by 2, 9 very easy and then of course, I need to know this. How I will know this? If you look at the formula

what we have used? a is equal to $4x$ plus y divided by 4 that is the f and x is what in this case? 8. So, 8 into 8 will be what? 32 plus y is 18 divided by 4; 32 plus 18 is 50; 50 divide 4 is nothing but your 12.5.

Now, the fuel air Stoichiometry is basically m_{fuel} divided by m_{air} . So, you will find out all these values, you substitute you will find out 0.06643. Now in this case, what will be air by fuel stoichiometric? It will be approximately 15, just can you please check? So, it is approximately 15. So, now, Equivalence Ratio, what it would be? It would be basically fuel by oxidizer, actual divided by fuel by oxidise stoichiometric; it happens to be 0.766; that means, what?

It is basically Lean mixture because ϕ is less than 1 and why you can say I mean because it product contains oxidizer, oxygen; therefore, it will be a Lean mixture. And if product will be containing fuel, it will be a Rich mixture and percentage of stoichiometric air can be determined as basically 100 divided by ϕ and that happens to be 130.5 percent; 130.5 percent. That means, 30 percent extra air is given in this, you know example. 30 percent extra is given for combustion of this gasoline.

So, now you have learnt how to basically do a Stoichiometric calculation in a very systematic manner; yes or no? So, if you do this, you would not make any mistake; any kind of fuel can be handled by this method. Then the what I, you know discussed earlier about hydrocarbon you know. So, with this we will stop over. In the next lecture we are going to discuss, how to handle the fuel air ratio you know in case of a diffusion flame.

Thank you very much.