Turbulent Combustion: Theory and Modeling

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Lecture-3
Introduction to Combustion (Contd.,)

Welcome back. Let us continue our discussion on turbulent combustion.

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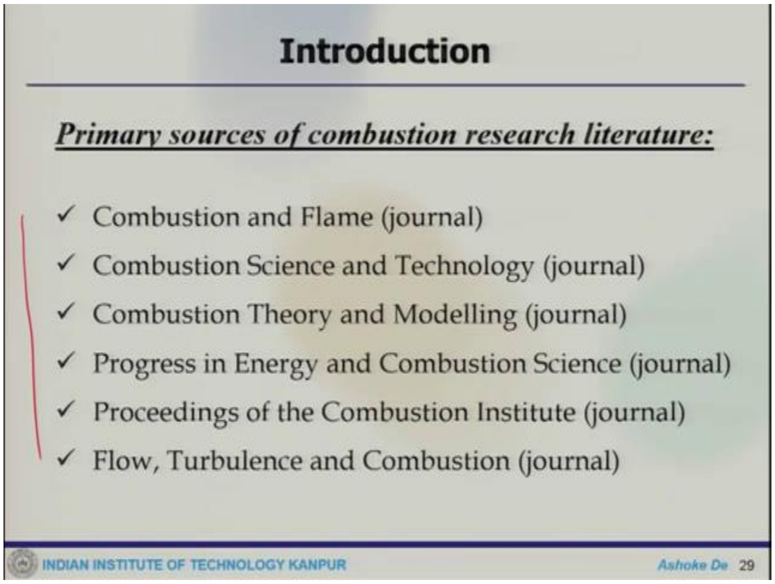

Introduction

Primary sources of combustion research literature:

- ✓ Combustion and Flame (journal)
- ✓ Combustion Science and Technology (journal)
- ✓ Combustion Theory and Modelling (journal)
- ✓ Progress in Energy and Combustion Science (journal)
- ✓ Proceedings of the Combustion Institute (journal)
- ✓ Flow, Turbulence and Combustion (journal)

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So this is where we actually stopped in the previous lecture that the looking at the different sources of combustion related research where one can find apart from all the textbook and other things, one may look at these resources to see the ongoing work and the advanced topics and combustion related research.

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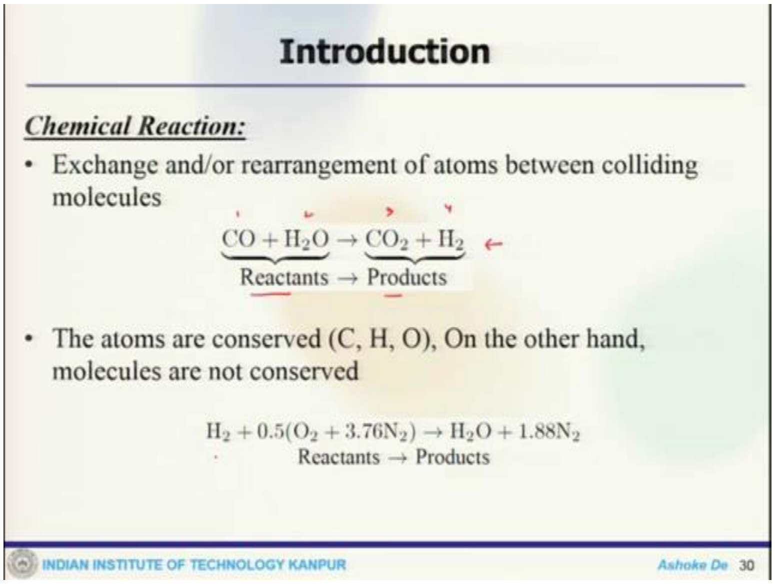

Introduction

Chemical Reaction:

- Exchange and/or rearrangement of atoms between colliding molecules

$$\underbrace{\overset{1}{CO} + \overset{2}{H_2O}}_{\text{Reactants}} \rightarrow \underbrace{\overset{3}{CO_2} + \overset{4}{H_2}}_{\text{Products}} \leftarrow$$

- The atoms are conserved (C, H, O), On the other hand, molecules are not conserved

$$H_2 + 0.5(O_2 + 3.76N_2) \rightarrow H_2O + 1.88N_2$$
$$\text{Reactants} \rightarrow \text{Products}$$

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Now moving ahead, we can look at some of the fundamentals of this combustion process where we look at first the chemical reaction. So, what happens this is in sample chemical reaction, which is happening and there are multiple species. This is 1, 2, 3, 4. So, if one look at this particular system, so there are 4 number of species which are involved here and one side you call it reactant and the other side you product. So, here the C 1, H 2 they are reactant they react to each other and finally you get the products in terms of CO_2 and H_2O there are different species. So in this kind of chemical reaction takes place. So it is a rearrangement of atoms between colliding molecules. So, if you look at both the sides of this particular equation your atoms are sort of maintained or balanced. So, where the atoms are conserved at the same time molecules are not conserved.

So, you look at this particular one, which is containing with hydrogen when it reacts to air so this whole thing one can treat as air where you have oxygen and nitrogen by different percentages and here you can look at it the molecules are not conserved.

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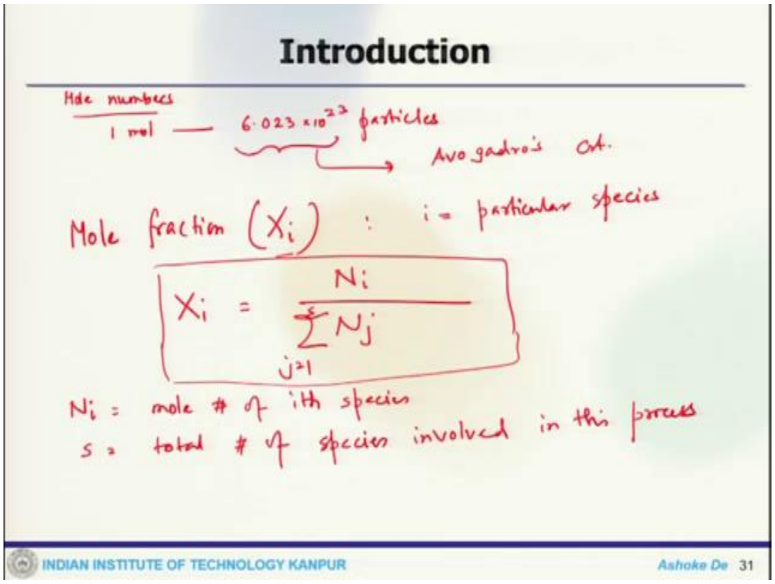

Introduction

Mole numbers

1 mol — $\underbrace{6.023 \times 10^{23}}$ particles $\rightarrow$ Avogadro's Cst.

Mole fraction (X_i) : i = particular species

$$\boxed{X_i = \frac{N_i}{\sum_{j=1}^{s} N_j}}$$

N_i = mole # of ith species

s = total # of species involved in this process

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So, there are few things one has to know. One of the important things is the mole number. So how do you define these things? Typically one mole corresponds to a number which is 6.023×10^{23} particles. So this could be atoms molecules or any chemical species. See this particular number is known as Avogadro's constant. So, every, one molecule of the species now one can define the important thing is the Mole fraction which will terminate like X_i, where i stands for that particular species.

So, the mole fraction of ith species is represented as X_i and it will be defined as:

$$X_i = \frac{N_i}{\sum_{j=1}^{s} N_j}$$

Now, N_i here is the mole number of the ith species and s is total number of species involved in this process. So, what happens if you have s number of species which are involved then their individual mole number is corresponding to N_j. So, the mole fraction is the particular species mole number with the ratio with the total mole of the all the reacting species they are involved there. So, you can find out the mole fraction in that way.

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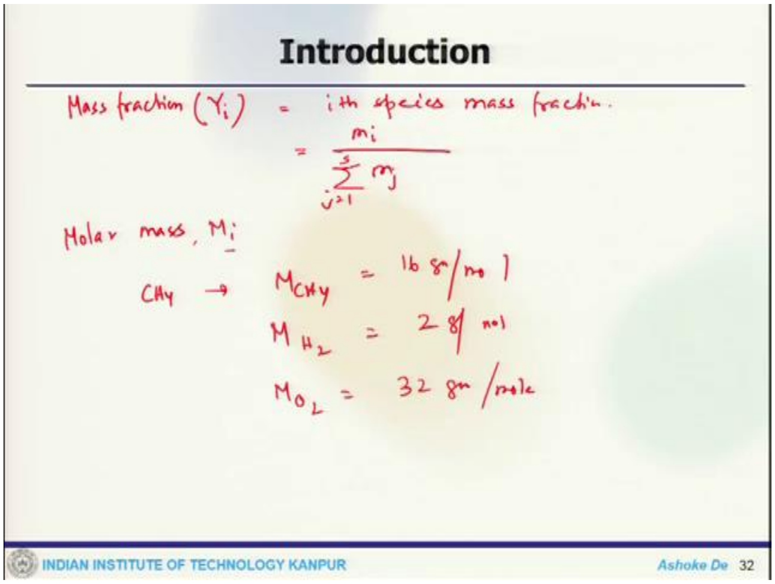

Introduction

Mass fraction (Y_i) = i th species mass fraction.

$$= \frac{m_i}{\sum_{j=1}^{s} m_j}$$

Molar mass, M_i

CH_4 → M_{CH_4} = 16 gm/mol

M_{H_2} = 2 g/mol

M_{O_2} = 32 gm/mole

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Now another important definition is the mass fraction. Because these are some of the fundamental definition one would require well, we move along with the other definition. So, this is again i^{th} species. Mass fraction how we Define it? It is:

$$Y_i = \frac{m_i}{\sum_{j=1}^{s} m_j}$$

So it is a particular mass of that species i divided by the total mass of the system. So that is how you define the mass fraction. Now one can define the molar mass or M_i which would be basically the molar mass is for example, if you have CH_4 the molar mass of CH_4 is 16 gram per mole. Similarly molar mass for hydrogen is 2 gram per mole, molar mass of for example O_2 is 32 gram per mole. Okay? So the molar mass for a particular species is represented as M_i. So, one should not get confused with the molecular weight here with the molar mass. Okay. So that would get you the definition of this molar mass and all these things.

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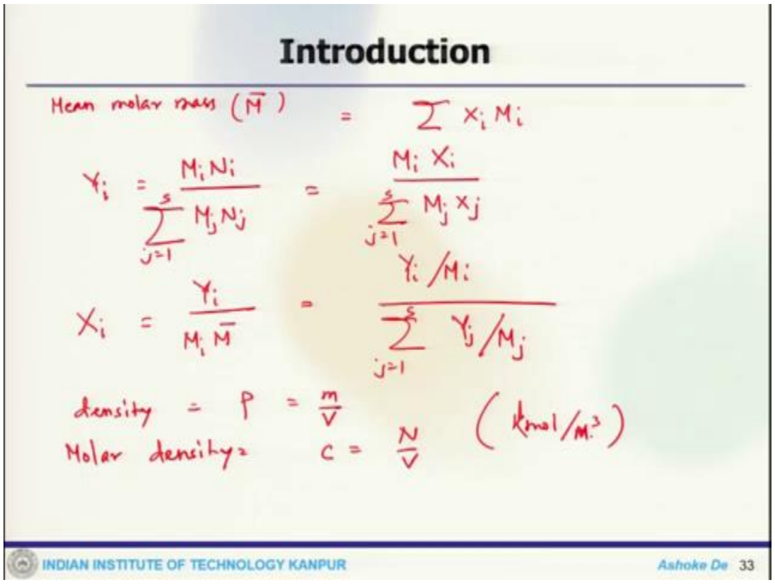

Introduction

Mean molar mass ($\bar{M}$) $= \sum X_i M_i$

$$Y_i = \frac{M_i N_i}{\sum_{j=1}^{s} M_j N_j} = \frac{M_i X_i}{\sum_{j=1}^{s} M_j X_j}$$

$$X_i = \frac{Y_i}{M_i \bar{M}} = \frac{Y_i / M_i}{\sum_{j=1}^{s} Y_j / M_j}$$

density $= \rho = \frac{m}{V}$

Molar density $=$ $C = \frac{N}{V}$ $(kmol/m^3)$

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Now, one can find out one more thing is the mean molar mass, which is mean molar mass. That is $\bar{M}$. So this should be the mixture of species which are involved in that particular system and you get the total so mean molar mass that will be:

$$\bar{M} = \sum X_i M_i$$

That means individual species molar mass multiplied with its individual molar mass to the mole fraction will get you the mean molar mass. So where always uses the number of species which are involved in the system. So, one can correlate this mole fraction and Mass fraction nicely. So one can write:

$$Y_i = \frac{M_i N_i}{\sum_{j=1}^{s} M_j N_j}$$

That is the mass fraction. Nicely can be correlated with:

$$Y_i = \frac{M_i X_i}{\sum_{j=1}^{s} M_j X_j}$$

Or alternatively

$$X_i = \frac{Y_i}{M_i \breve{M}}$$

So which can be represented as:

$$X_i = \frac{Y_i / M_i}{\sum_{j=1}^{s} Y_j / M_j}$$

So, one can find out that thing in that fashion. So, there are some more things which one can define is the one is the density that is another important things which will come into the picture which is mass divided by volume. Then you have Molar density which will be:

$$C = \frac{N}{V}$$

That means if you look at the unit kilo mole per volume cube or meter cube.

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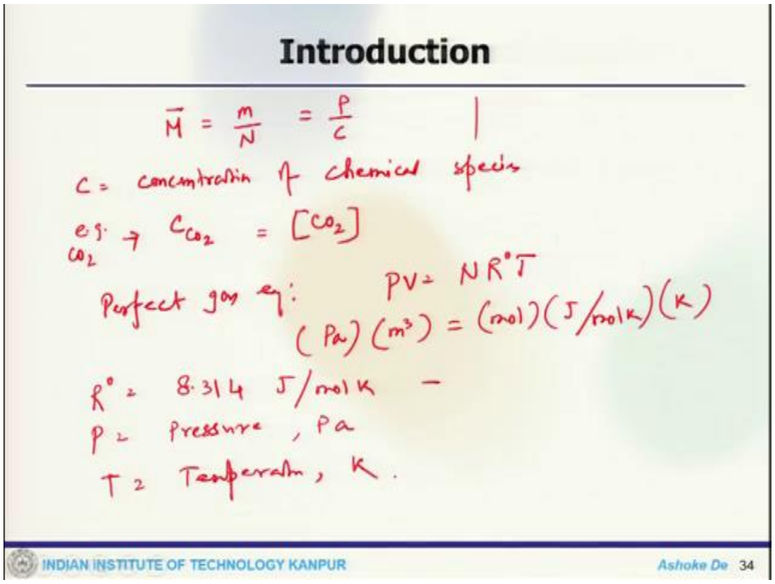

Introduction

$$\bar{M} = \frac{m}{N} = \frac{\rho}{C}$$

C = concentration of chemical species

e.g. CO_2 → $C_{CO_2} = [CO_2]$

Perfect gas eq: $PV = NR^{\circ}T$

$$(Pa)(m^3) = (mol)(J/molK)(K)$$

R° = 8.314 J/mol K

P = Pressure, Pa

T = Temperature, K.

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So, mean molar mass one can estimate as:

$$\bar{M} = \frac{m}{N} = \frac{\rho}{C}$$

So now the convention in chemical kinetics is the concentration, so the concentration C of chemical species are usually shown by the symbol. So if I say, this is the concentration of chemical species then C for particular species. Let us say for example CO_2. One can write it would be concentration of CO_2 like this. So, this is very common in definition of the kinetics that usually one defines the concentration of a particular species. For most condition, which are involved in the combustion it is quite satisfactory to use the perfect gas equation. So that is one of the equation that one can use is the equation of state or perfect gas equation where:

$$PV = NR^0T$$

And if you do the unit balancing, this should be Pascal. This is meter cube. This is mole. This is Joule per mole Kelvin, and this is Kelvin and there are values for R Naught is 8.314 Joule per mole

Kelvin, which is known as universal gas constant. P is essentially your pressure, unit is Pascal and T is Temperature which is in kelvin.

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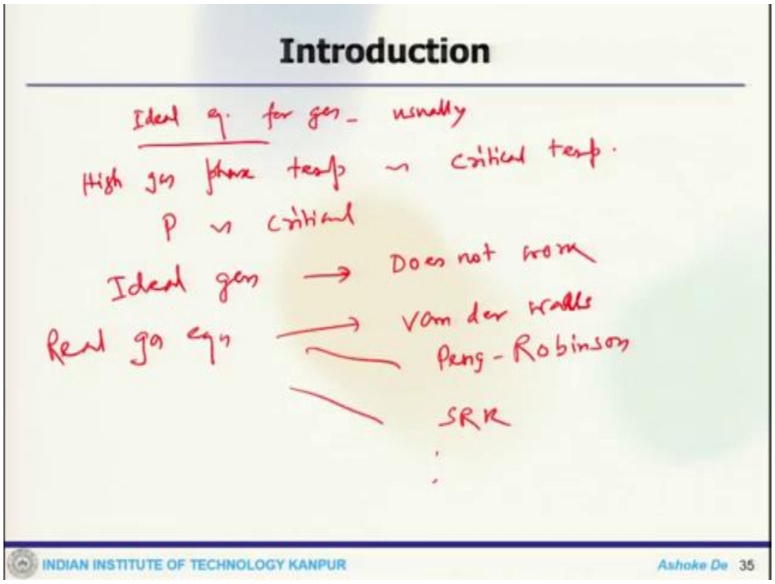

Introduction

Ideal eq. for gas – usually

High gas phase temp ~ critical temp.

P ~ critical

Ideal gas → Does not work

Real gas eqn → van der Walls

Peng - Robinson

SRK

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Now the thing is that I mean most of the time one uses the ideal equation for gas this is usually which is used but when the combustion process encounters high temperature gas phase temperature, which is near or least so high gas phase temperature which is almost close to the critical temperature or pressure are near or above the critical pressure. So, another case could be the pressure and the density or concentration is not then correctly predicted by the ideal gas law.

So there are two conditions where temperature is quite high which is nearly close to a critical temperature or pressure is also close to the critical pressure. So here the ideal gas does not work. So one has to take the real gas equation, which could be in terms of either Van Der Walls equation or there are one Peng Robinson or SRK model. So, there is some of this real gas equation of state which one can use and get the situation. So, depends on the particular process temperature pressure and all these things. So whether the equation of State could be ideal or real that one has to decide.

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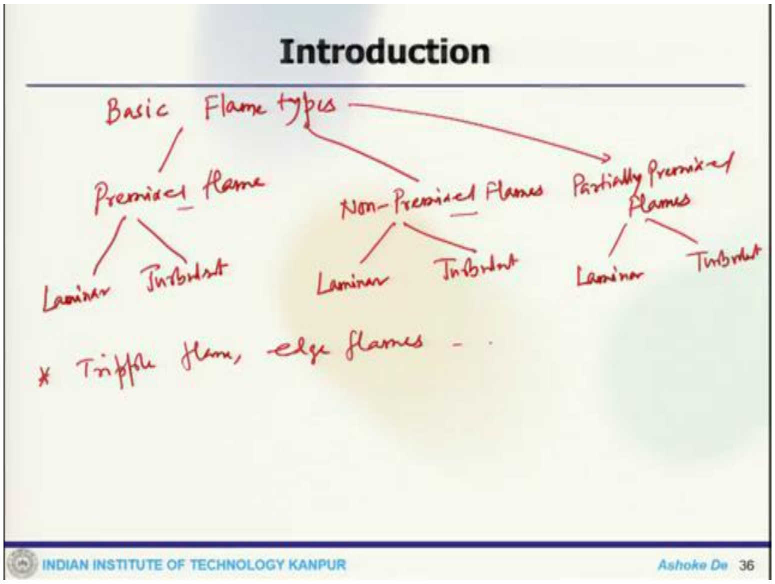

Introduction

Basic Flame types

Premixed flame

Laminar

Turbulent

Non-Premixed Flames

Laminar

Turbulent

Partially Premixed Flames

Laminar

Turbulent

* Triple flame, edge flames - .

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Now we can come to some of the basic flame types. So the basic flame types; so one of the system could be pre-mixed flame that is one of them then one can have non-premixed flame. So we will talk about these flames in details that so now we are getting into the classification of different flame types. This could be one of these partially premixed flames. So, these are the three primarily broad categories of flame where you have one premixed non-premixed, partially premixed.

Now depending of the situation whether the fluid dynamical behavior is quite nice in that case the premixed flames can be of two types one could be laminar or other ways it could be turbulent. Similarly this is also a case for other two flames. Non-premixed flame also could be of two types depending on the laminar or turbulent. And this case also it could be laminar or turbulent. Now why we are broadly categorizing these flames into different regimes because the characteristics of pre-mixed flame is quite different from the non-premixed flames.

And at the same time partially premixed flames are different from these two. So apart from this classification, there could be other flames like triple flames, edge flames. So these are some of the other information one can actually have regarding the flame classification.

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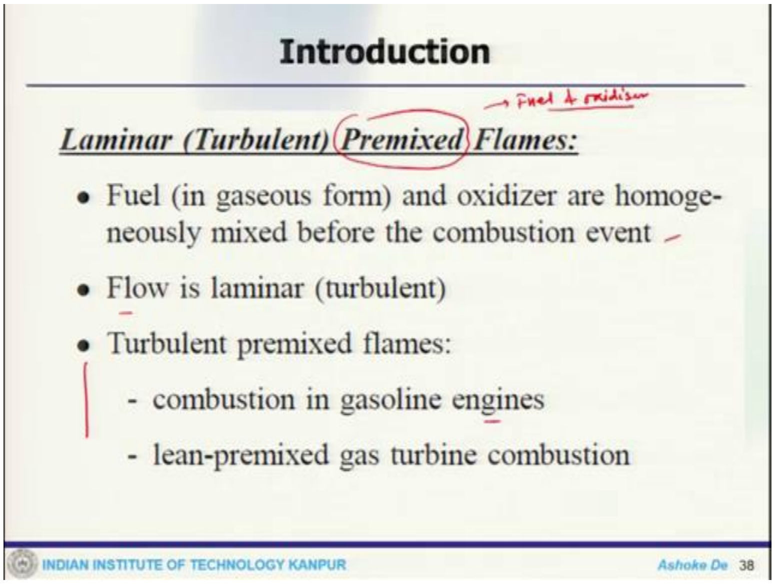

Introduction

→ Fuel & oxidiser

Laminar (Turbulent) Premixed Flames:

- Fuel (in gaseous form) and oxidizer are homogeneously mixed before the combustion event
- Flow is laminar (turbulent)
- Turbulent premixed flames:
  - combustion in gasoline engines
  - lean-premixed gas turbine combustion

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Now if we get to the details of this laminar or turbulent pre-mixed flame what it exactly it is so as the name suggests the pre-mixed that means, your reactants are of two types one it will have the fuel so that means your fuel and oxidizer. So, they are pre-mixed before they are injected into the combustion chamber. So that is why the premixed comes into the picture where things are previously before injection they are mixed.

So one can think about the proportion is nice so you can have nice combustion and all these details will see so as the name suggest homogeneously mixed because the combustion event. Now depending on the fluid behavior the flow could be laminar or turbulent. So either you can have laminar pre-mixed flame or turbulent pre-mixed flame. So, for example, turbulent premixed flame you can have in gasoline engine then Lean premixed gas turbine combustion. So, these are the example of your turbulent regime.

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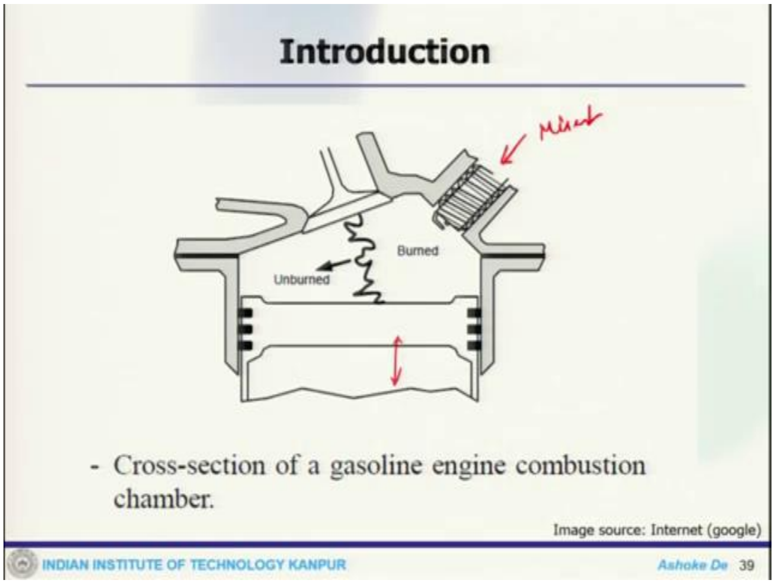

Introduction

- Cross-section of a gasoline engine combustion chamber.

Image source: Internet (google)

And this is one of the cross section of your gasoline engines. So essentially your spark ignition engines, which are used in your specifically the engines either two-wheelers or four wheelers cars and somewhere the petrol based engine. These are sort of pre-mixed engine. So this is one of the cross section where you can see the mixture comes through this and then there, an ignition takes place. So and then there would be unmanned product and bond product and then finally there is a movement of the Piston. So that is how you have this combustion process, which we will get into the different cycles and the cycle stands out to your forces.

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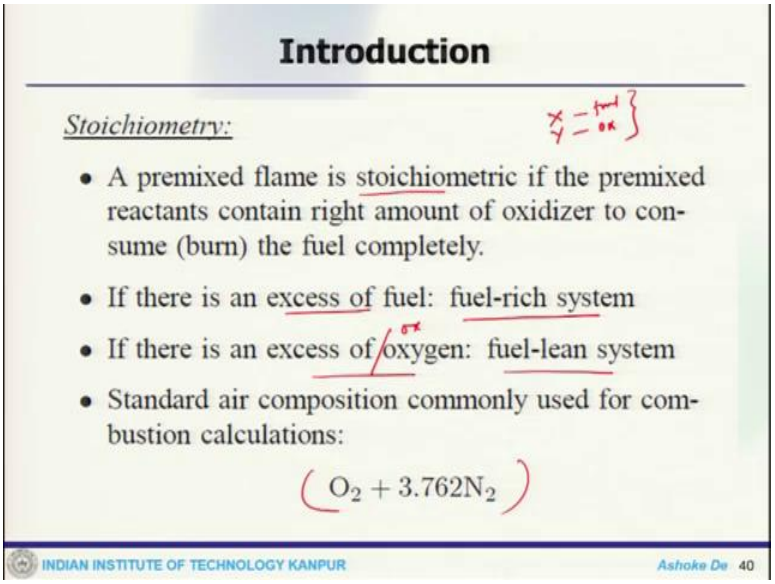

Introduction

Stoichiometry:

$\left.\begin{array}{l} x = \text{fuel} \\ y = \text{ox} \end{array}\right\}$

- A premixed flame is stoichiometric if the premixed reactants contain right amount of oxidizer to consume (burn) the fuel completely.
- If there is an excess of fuel: fuel-rich system
- If there is an excess of $\overset{\text{ox}}{\text{oxygen}}$: fuel-lean system
- Standard air composition commonly used for combustion calculations:

$$(O_2 + 3.762N_2)$$

Now another definition is that when you talk about the pre-mixed flame is the stoichiometry. So, typically the pre-mixed flame is stoichiometric if the flame reaction contents right amount of oxidizer to consume the fuel completely that means if I mix X amount of fuel with Y amount of oxidizer? So the proportion is rightly mentioned so that you get stoichiometric situation. If for example, the fuel is excess then one can say it is fuel rich system.

If there is an excess of oxygen or I would say oxidizer because it could be burning in oxygen or the fuel could be burned in oxidizer. So, it is fuel lean system. And typically the standard air composition as we have seen this is oxygen and nitrogen by volume which it contains.

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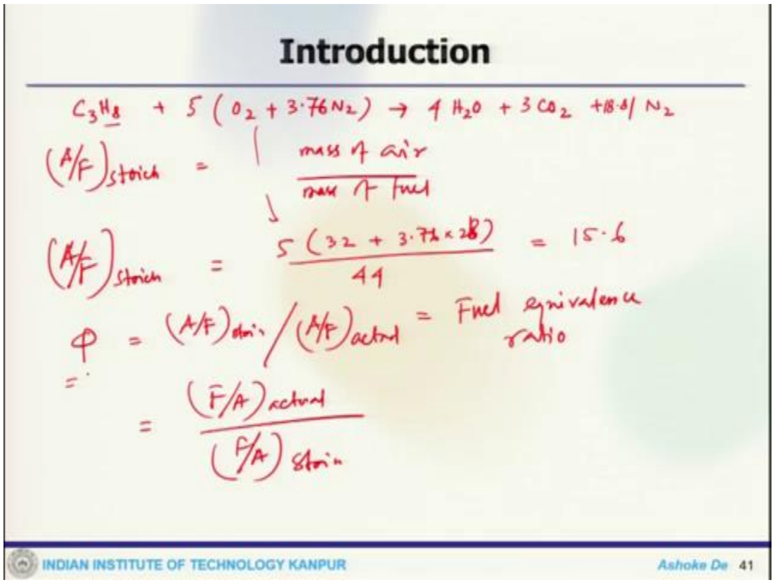

Introduction

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 4H_2O + 3CO_2 + 18.81N_2$$

$$(A/F)_{stoich} = \frac{\text{mass of air}}{\text{mass of fuel}}$$

$$(A/F)_{stoich} = \frac{5(32 + 3.76 \times 28)}{44} = 15.6$$

$$\phi = (A/F)_{stoic} / (A/F)_{actual} = \text{Fuel equivalence ratio}$$

$$= \frac{(F/A)_{actual}}{(F/A)_{stoic}}$$

So, we can see an example. For example, let us say we taken hydrocarbon C_3 H_8 and bonds with air and you get H_2O plus CO_2 plus the extra amount of nitrogen because if the nitrogen remain as an inert gas, most of the time nitrogen remain as inert gas unless or otherwise depending on the temperature where you get the NO_x and all these things. So, if you balance out these things so looking at the system here you put 5 so this will lead 2, 4 so this will become then 3 CO_2 and the rest of the things which will around 18.81 would be nitrogen.

Now, one can find out the stoichiometric air fuel ratio. So it is:

$$\left({}^{A}\!/_{F}\right)_{stoich} = \frac{mass\ of\ air}{mass\ of\ fuel}$$

So, one can calculate this air fuel stoichiometry. So here:

$$\left(A/_{F}\right)_{stoich} = \frac{5(32 + 3.76 \times 28)}{44}$$

So that will get you around 15.6. So, the Phi ($\emptyset$) is $\left(A/_{F}\right)_{stoich}$ divided by $\left(A/_{F}\right)_{actual}$ is called as fuel equivalence ratio. So, this is what or one can reversely define $\left(F/_{A}\right)_{actual}$ to $\left(F/_{A}\right)_{stoich}$ so that will give you the actual situation where one can find out the equivalence ratio in a pre-mixed flame.

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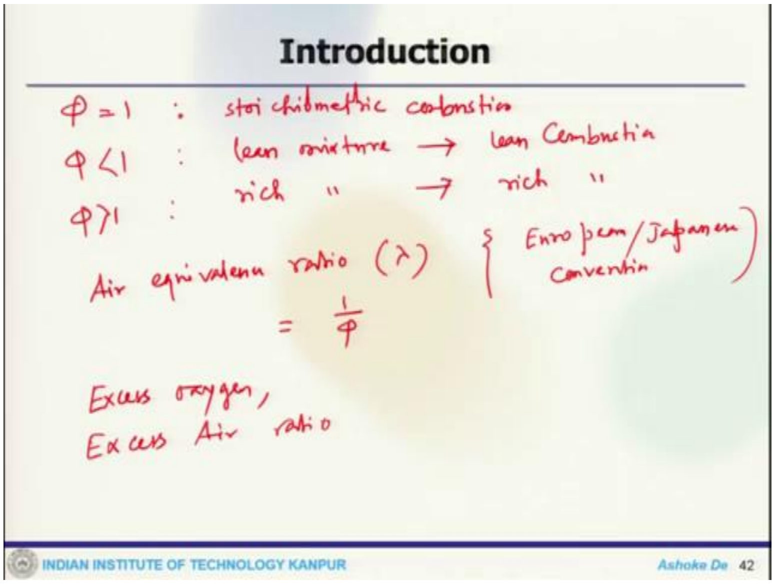

Introduction

$\phi = 1$: stoichiometric combustion

$\phi < 1$: lean mixture → lean Combustion

$\phi > 1$: rich " → rich "

Air equivalence ratio (λ) { European/Japanese convention)

$= \frac{1}{\phi}$

Excess oxygen,

Excess Air ratio

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Now depending on the $\emptyset$ for example $\emptyset$ is 1 obviously it is a stoichiometric combustion when Phi is less than 1 this should be a lean mixture. So, lean mixture into lean combustion at the same time if $\emptyset$ is greater than 1 it could be rich mixture to rich combustion. Now, typically different countries they use some of the different convention, European convention and to a certain extent to Japanese also use the air equivalence ratio.

So, they call it as air equivalence ratio, which is call is Lambda (λ). This is in a nutshell European + Japanese convention. So, that is nothing but $\left(1/_{\emptyset}\right)$ all certain industries also use excess air ratio, excess oxygen or similar terminologies are also used sometimes the people use excess oxygen. Sometimes they use excess air ratio. So these are the different terminologies which are available and people do use that thing.

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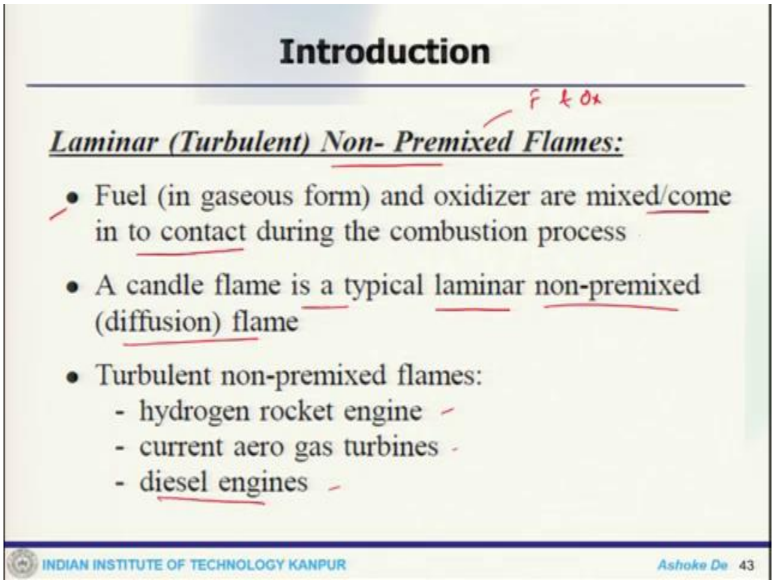

Introduction

F & Ox

Laminar (Turbulent) Non- Premixed Flames:

- Fuel (in gaseous form) and oxidizer are mixed/come in to contact during the combustion process
- A candle flame is a typical laminar non-premixed (diffusion) flame
- Turbulent non-premixed flames:
  - hydrogen rocket engine
  - current aero gas turbines
  - diesel engines

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So, those are which are required for a premixed system. Now what happens when you come down to non-premixed system, so that means clearly as the name suggests the reactants like your fuel and oxidizer they are not mixed a priory before the combustion takes place. So which is the point here that the fuel and oxidizer are mixed when they come in contact during the combustion process. That means priory like your pre-mixed combustion they are not mixed and injected to the combustion chamber here they are directly or to be very specific they are separately injected to the combustion chamber and they come in contact during the combustion process.

So, one of the examples is the candle flame which we usually burn almost in our daily life the candle burning. So that is a typical example of laminar because the flow is so calm and nice non-premixed diffusion flame and there are some examples of your non-premixed turbulent flames which are hydrogen rocket engine current aero gas turbines diesel engines. This is also from your automobile sector.

So these are some of the examples of your non-premixed system. So the combustion takes place in the furnace and all these also comes under non pre-mixed combustion. So these are some of the turbulent application of that.

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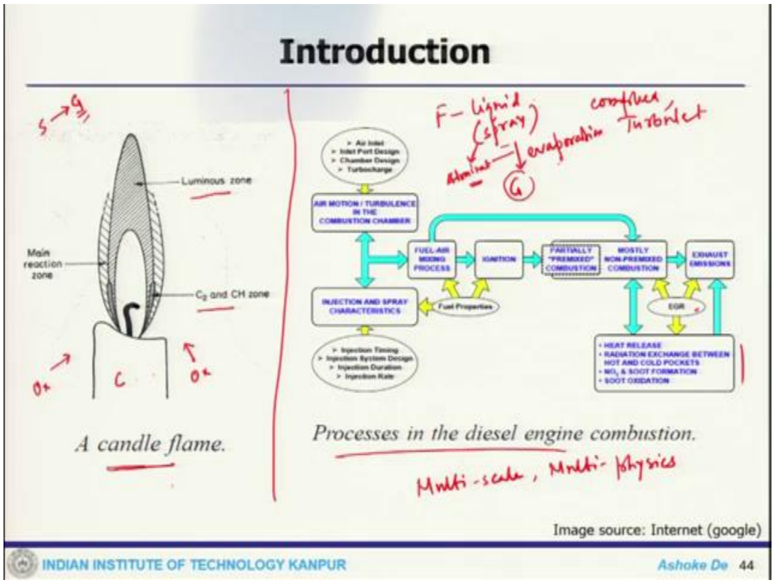

Introduction

A candle flame.

Processes in the diesel engine combustion.

Image source: Internet (google)

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This is a typical image of a candle flame where this candle is essentially your Solid fuel this is your carbon and then obviously from sides you get the oxidizer. That means once you get the air then keep on burning but one important things people has to mind it here is that any combustion whether it is simply makes non-premixed, partially premixed or multi-phase the combustion takes place in gaseous mode only.

Even then we are burning candle as a solid then there is a paralysis takes place. So immediately solid transform into gas and that time scale is so small and that is why as we have been talking that combustion has a multiscale problem because now here first solid fuel, it transforms to gas and then the combustion takes place and it happens instantaneously that is why in a visual normal eye we cannot see that thing happening rather we see the candle is burning and you get the luminous zone where you get the light and there would be other reaction zone which you call it C_2 and CH zone.

Now another example if you see so this is typically happen in a diesel engine combustion, which is turbulent in nature. And obviously as you can see that is also quite complex in nature. So, this is turbulent complex. So there are different situations to it. You have intake port and all these things that comes in turbulence is there then here one more thing is that diesel engine combustion is that are your fuel is in liquid state?

That means you have some spray. So the previous example in the candle flame we have seen the solid burning here. So solid means solid actually immediately due to the paralysis it goes to gaseous state and the burning takes place here your liquid has to evaporate. Now when you have a liquid this has to again form to gas through evaporation. So, before even evaporation there is a state which goes to atomization that means the liquid has to break into the smaller droplets and those droplets evaporates and finally you get a gas and that gas only takes into participation of the combustion process.

So, there is a complicated process and then top of that you have some exhaust re-circulated through air. You have heat release, radiation then other complicated stuff like soot and all these things. These are the things which will see as we go along. But the thing is that as soon as you move from one simple example of candle burning to a diesel engine situation, which is a more or less like an your realistic situation the complications actually increases and increases in a different manifold. It increases in a different time scale one case you solid has to go to gas and then burn here your liquid has to go through the atomization process. So, this clearly example of your multi scale, Multiphysics problem because liquid has to atomize then it has to go to mean basically evaporate and finally forms in forms of fuel gas and then the burning takes place and all these things happens.

So it essentially multi-scale like a problem. So that gives you an idea about how this turbulent and real life problems actually differs from the simple problem. So we will stop here and then we will discuss and continue the discussion in the next lecture. Thank you.