Turbulent Combustion: Theory and Modelling

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Lecture – 11
Combustion Chemistry (Contd.,)

Okay, welcome back and let us continue the discussion on combustion chemistry, so different aspect of kinetic mechanism. Elementary reactions and the impact of the free radicals when they are present in the system so and then we have looked at a particular example of hydrogen-oxygen reaction.

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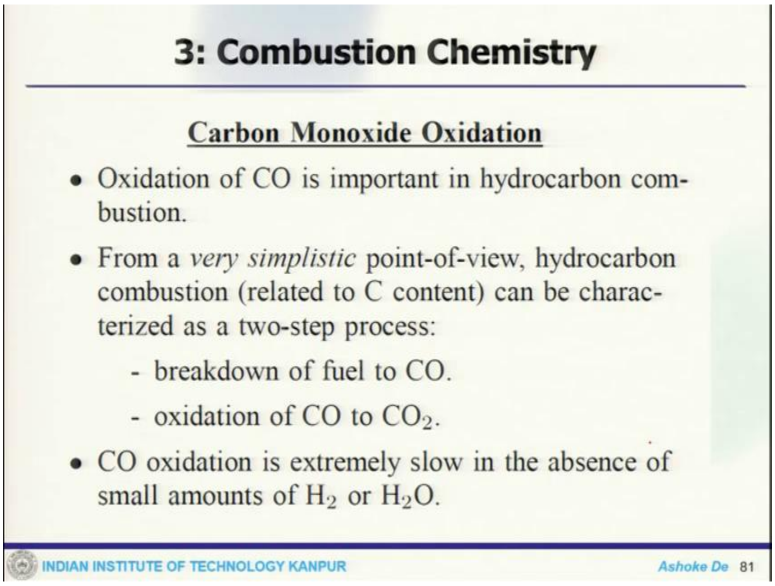

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Carbon Monoxide Oxidation

- Oxidation of CO is important in hydrocarbon combustion.
- From a *very simplistic* point-of-view, hydrocarbon combustion (related to C content) can be characterized as a two-step process:
  - breakdown of fuel to CO.
  - oxidation of CO to CO_2.
- CO oxidation is extremely slow in the absence of small amounts of H_2 or H_2O.

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So now we will look at some more examples, like carbon monoxide oxidation and CO oxidation. So, this is another or important reaction that CO oxidation because any hydrocarbon fuel that we burn for example C_xH_y any hydrocarbon of these series whatever you burn intermediate radical one of the important radical is this CO radical. And CO, if it is completely burnt or oxidized it will give you a CO_2. It does not then it will remain CO and it is one of the major concerns of your emission.

Now also very simplistic point of view; can you have 2 step this can happen for a hydrocarbon fuel one is the breakdown of fuel to CO that means where C_xH_y from CO then as I said, CO forms CO_2. The combustion is complete and there is nothing exists and everything goes smoothly as per expectation then he will get away in product as CO_2. Those CO_2 also has problem in the environmental issues but here it is much more problematic. So another issue what is kind of challenging is CO oxidation is extremely slow in the absence of small amounts of H_2O and H_2.

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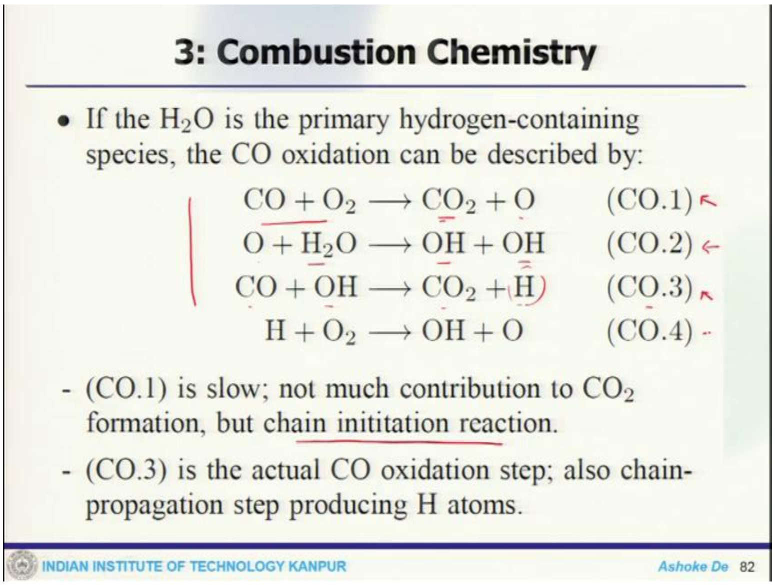

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- If the H_2O is the primary hydrogen-containing species, the CO oxidation can be described by:

$$\begin{aligned} CO + O_2 &\longrightarrow CO_2 + O && (CO.1) \\ O + H_2O &\longrightarrow OH + OH && (CO.2) \\ CO + OH &\longrightarrow CO_2 + H && (CO.3) \\ H + O_2 &\longrightarrow OH + O && (CO.4) \end{aligned}$$

- (CO.1) is slow; not much contribution to CO_2 formation, but chain inititation reaction.
- (CO.3) is the actual CO oxidation step; also chain-propagation step producing H atoms.

So, H_2O is the primary hydrogen containing species one can describe the CO oxidation by this set of mechanism. The first reaction for CO oxidation, CO will combine with oxygen and form CO_2 and form O radical then O will react to H_2O from OH and OH radical these are again some of the highly reactive radical as we have seen earlier. Then again, the CO react with OH to form radical H will react to O_2 to form OH and so this is the series of oxidation steps.

Now if you look at each of individual reactions CO1 is slow and also contributes quite a bit of CO_2 formation. So this is sort of a one can say it is chain initiation reaction? On the third reaction is actually the CO_2 oxidation state. So this is sort of an chain propagating step producing H atoms now you got this one and this one and then remaining reaction 2 and reaction 4, so they are sort of chain branching reaction which produces OH and H.

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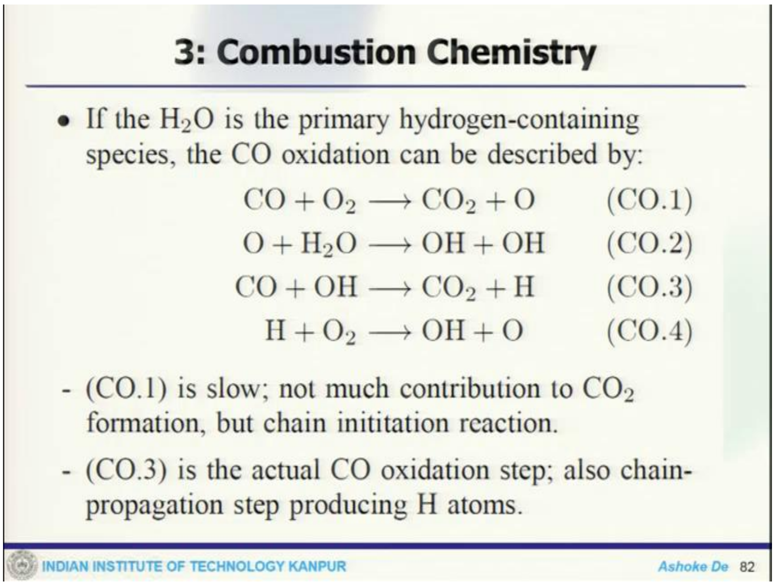

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- (CO.1) is slow; not much contribution to CO_2 formation, but chain inititation reaction.
- (CO.3) is the actual CO oxidation step; also chain-propagation step producing H atoms.

And CO_2 oxidation is the key for your CO oxidation. Now if hydrogen is present then some of these steps are also involved. There will be few more steps oxidation state of CO 5, 6, 7 where O react to H_2 to get OH plus H. And then OH to H_2 due to get H_2O and H mind it these are free radicals. So these radicals are highly reactive and they do take part in this reaction process aggressively and then finally CO react with HO_2 to get CO_2 and OH. Now, when you have H_2 inter H_2-O_2 reaction system should be included in the CO oxidation.

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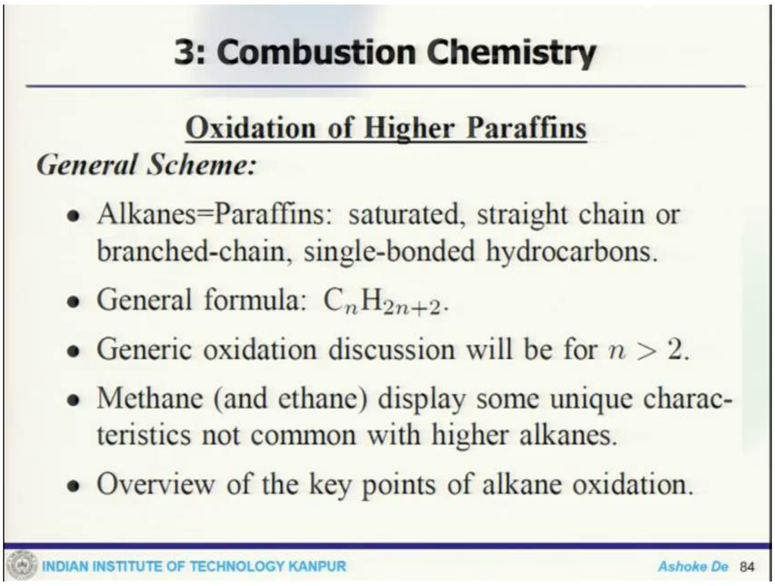

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Oxidation of Higher Paraffins

General Scheme:

- Alkanes=Paraffins: saturated, straight chain or branched-chain, single-bonded hydrocarbons.
- General formula: C_nH_{2n+2}.
- Generic oxidation discussion will be for $n > 2$.
- Methane (and ethane) display some unique characteristics not common with higher alkanes.
- Overview of the key points of alkane oxidation.

Now look at the general system of listings of paraffin’s where alkenes and paraffin's, these are saturated straight chain or branched chain single bonded hydrocarbons, so one can actually represent them in series C_n H_{2n+2}, for example CH_4 where n is 1 so you get 4, C_2H_6 then C_3H_8

and so on which will be methane, ethane, propane and like that. Now generic oxidation discussion will be for n > 2 that means we start from propane and butane. Methane or ethane, display some unique characteristics not with higher alkenes. So, these two where n1 and n2 show some different characteristics compared to higher order hydrocarbon. So the whole idea is that how you will look at the alkenes oxidation here.

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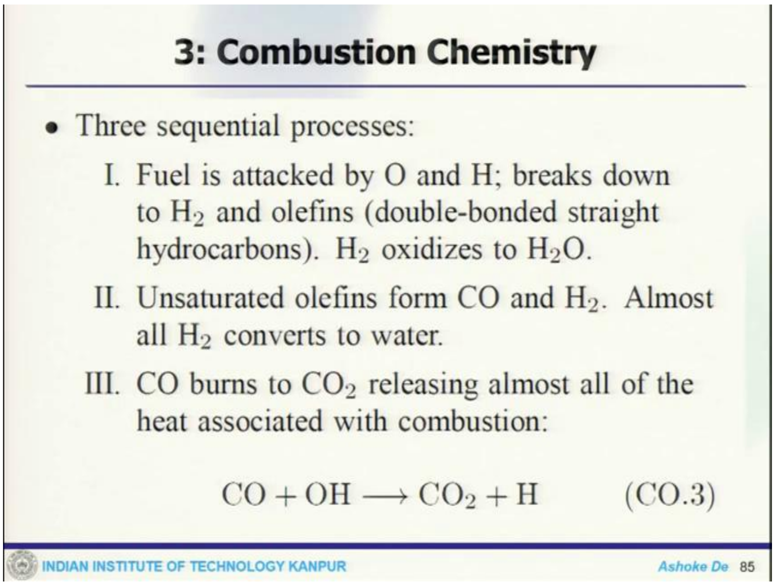

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- Three sequential processes:
  I. Fuel is attacked by O and H; breaks down to H_2 and olefins (double-bonded straight hydrocarbons). H_2 oxidizes to H_2O.
  II. Unsaturated olefins form CO and H_2. Almost all H_2 converts to water.
  III. CO burns to CO_2 releasing almost all of the heat associated with combustion:

$$CO + OH \longrightarrow CO_2 + H \qquad (CO.3)$$

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Now there are three sequential process here first fuel is attacked by O and H and then when that happens, it breaks down to H_2 and olefins so which is a double bonded state hydrocarbon and then H_2 oxidized to H_2O that is step number one. Where you first fuel is attacked by O and H. Then next step all this unsaturated olefins form CO and H_2 almost all H_2 convert to water by that time. So that is happens at 2nd state.

And then the third stage, CO bonds to CO_2. Releasing almost all of the heat associated with combustion. This is the state which is quite important that happens at the third stage.

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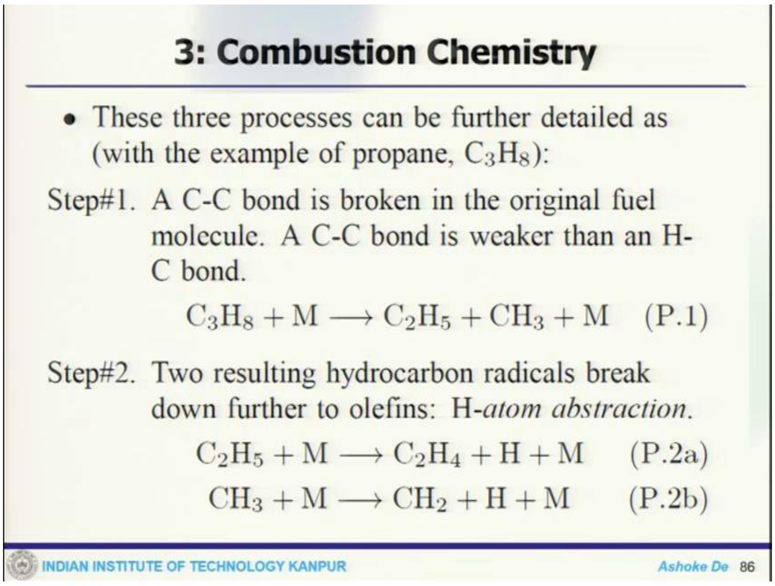

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- These three processes can be further detailed as (with the example of propane, C_3H_8):

Step#1. A C-C bond is broken in the original fuel molecule. A C-C bond is weaker than an H-C bond.

$$C_3H_8 + M \longrightarrow C_2H_5 + CH_3 + M \quad (P.1)$$

Step#2. Two resulting hydrocarbon radicals break down further to olefins: H-*atom abstraction*.

$$C_2H_5 + M \longrightarrow C_2H_4 + H + M \quad (P.2a)$$

$$CH_3 + M \longrightarrow CH_2 + H + M \quad (P.2b)$$

So, now we can look at these three things with an example, for example as we said n has to be greater than 2, so the simple one, one can take is the propane which is C_3H_8. Now with the propane faster the CC bond is broken into original fuel molecule. So, this is C_3H_8 and this should be broken into C_2H_5, CH_3 and M. So that is your step number one where fuel is sort of attacked. You know why that is possible that because the CC bond is weaker than the HC bond. Second step to result in hydrocarbon radical break down further to olefins H-atom of abstraction.

So this is called atom abstraction. So, here one is the C_2H_5 reacts to M form C_2H_4, M and C_2H_5 which also reacts to M. So, these are the two important steps which happens or takes place at step number two which is obtain from the breaking of the fuel bond.

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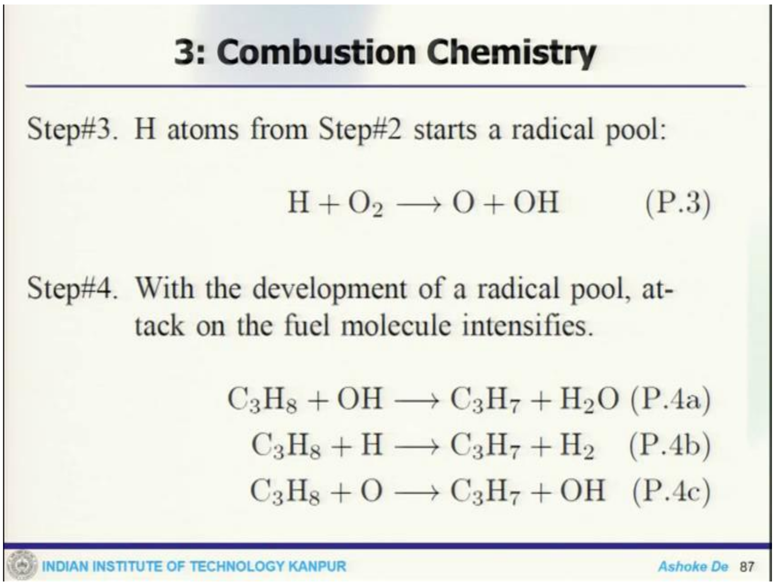

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Step#3. H atoms from Step#2 starts a radical pool:

$$H + O_2 \longrightarrow O + OH \qquad (P.3)$$

Step#4. With the development of a radical pool, attack on the fuel molecule intensifies.

$$C_3H_8 + OH \longrightarrow C_3H_7 + H_2O \quad (P.4a)$$
$$C_3H_8 + H \longrightarrow C_3H_7 + H_2 \quad (P.4b)$$
$$C_3H_8 + O \longrightarrow C_3H_7 + OH \quad (P.4c)$$

Then step three whatever you get H atoms of H radicals at step 2 they will start a radical pool, so H will now start with O_2 form O and OH. That means now you start getting more and more reactive radical in the system. Initially when these bonds are broken you get H. Now H will start reacting to O_2 which is part of your oxidizer. It starts forming more and more reactive radicals like O, OH and so on.

So when you start having more and more pool so the fuel molecule intensified. So, C_3H_8 again reacts with OH start forming these, it reacts with H form this. So these are multiple steps go on having a reaction with the fuel.

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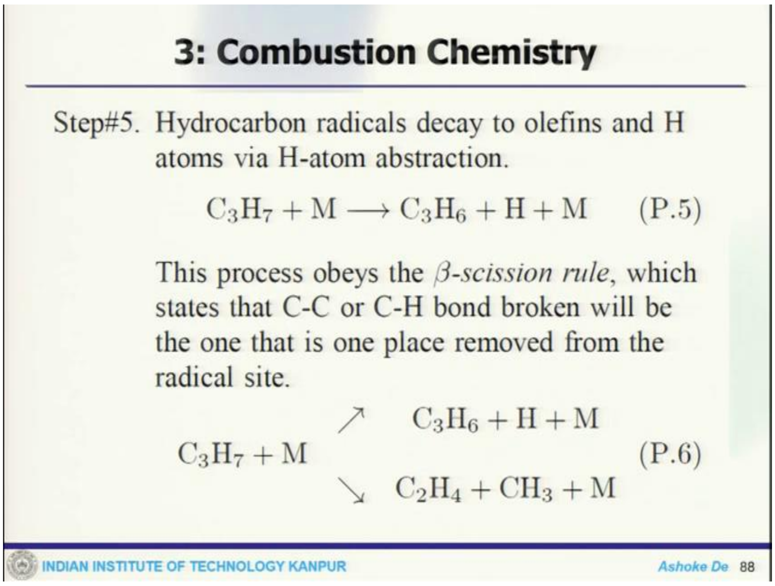

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Step#5. Hydrocarbon radicals decay to olefins and H atoms via H-atom abstraction.

$$C_3H_7 + M \longrightarrow C_3H_6 + H + M \qquad (P.5)$$

This process obeys the *β-scission rule*, which states that C-C or C-H bond broken will be the one that is one place removed from the radical site.

$$C_3H_7 + M \begin{array}{l} \nearrow \; C_3H_6 + H + M \\ \searrow \; C_2H_4 + CH_3 + M \end{array} \qquad (P.6)$$

Step five what you get is; now this hydrocarbon radicals decay to olefins and H atom where H atom abstraction. So, this is C_3H_7 which will get you C_3H_6, H and M? So this process obeys the one of the common rule is that beta scission rule which state that C-C or C-H bond broken will be the one that is one place removed from the radical site, which is C_3H_7 will react to M, so C_3H_6, H and M.

Or it can form C_2H_4, CH_3 and M so this C-C and C-H bonds are broken and one get to form this basically these broken bonds to form the olefins.

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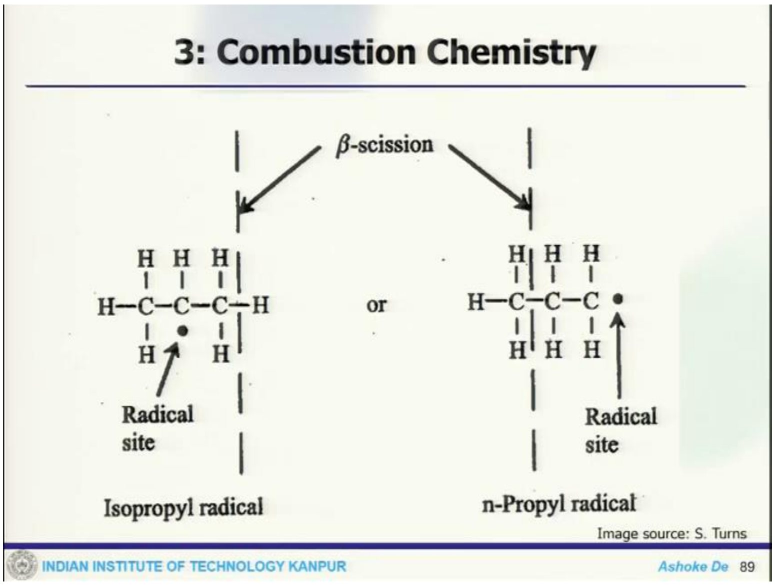

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Image source: S. Turns

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So, if you look at this image, which we just discussing this particular state, which is as per the step 5 as per the rule of beta Scission rule. You can see what happened this is isopropyl radical and this is n-propylene radical this is the C_3H bond. So, this is radical site and this is radical site and then due to the decay you get the olefins.

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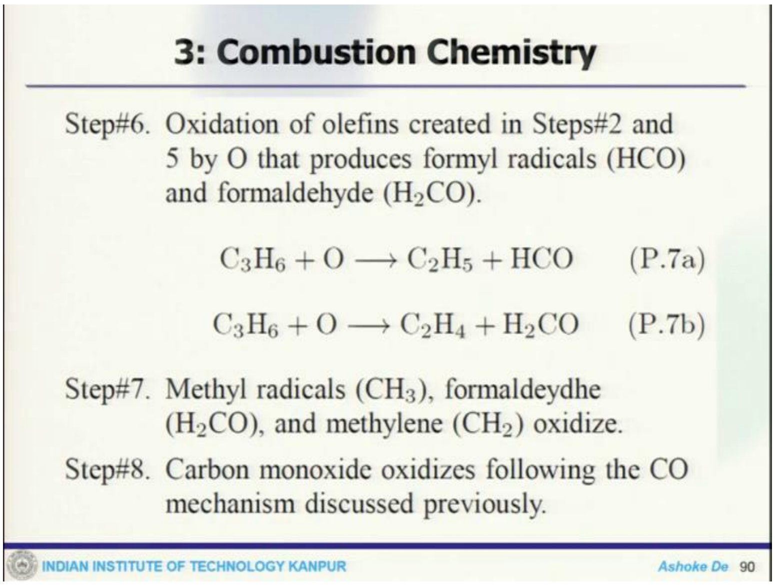

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Step#6. Oxidation of olefins created in Steps#2 and 5 by O that produces formyl radicals (HCO) and formaldehyde (H_2CO).

$$C_3H_6 + O \longrightarrow C_2H_5 + HCO \qquad (P.7a)$$

$$C_3H_6 + O \longrightarrow C_2H_4 + H_2CO \qquad (P.7b)$$

Step#7. Methyl radicals (CH_3), formaldeydhe (H_2CO), and methylene (CH_2) oxidize.

Step#8. Carbon monoxide oxidizes following the CO mechanism discussed previously.

Now, there after you go to step 6 where the olefins are now getting oxidized and then produces some other radicals like HCO and formaldehyde H_2CO. Now these are radicals now form when this olefins are reacted to the O radicals now C_3H_6 which will react to O will form C_2H_5, HCO or C_3H_6 and O form C_2H_4 H_2CO. So, these components produce due to the oxidation of the olefins. Now this methyl radical or formaldehyde H_2CO or methylene CH_2 oxidise at step 7, so these radicals actually do not stay longer and get oxidized. And then finally carbon monoxide oxidizes following the fuel mechanism as we discussed earlier. So that is what you get the CO_2.

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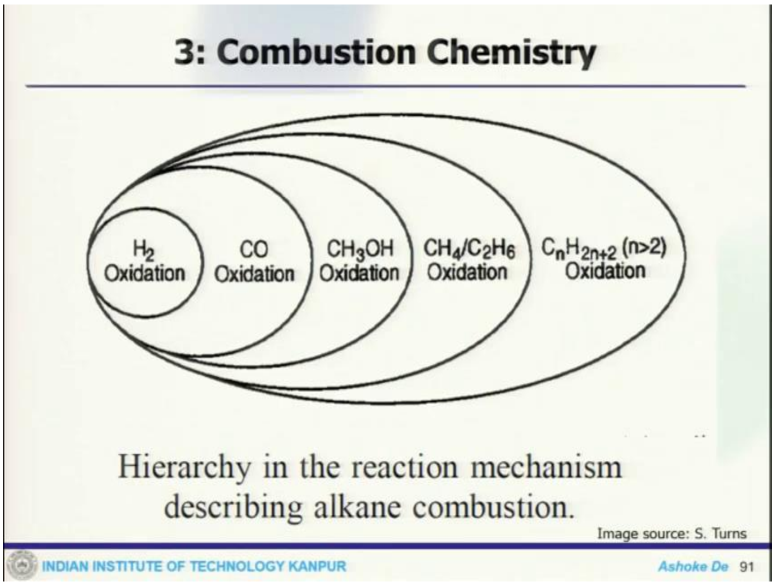

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Hierarchy in the reaction mechanism describing alkane combustion.

Image source: S. Turns

And if you put them in a figure you can see, what the hierarchy of the reaction mechanism, describing alkane combustion is. So this is your fuel higher order hydrocarbon C_nH_{2n+2} that first oxidise then you get CH_4, C_2H_6 that means it breaks down to the lower hydrocarbon. And you get more like olefins and then olefins actually produces this other radicals and those radicals oxidized and then finally gets CO oxidation.

And at the core you get H_2 oxidation. So, essentially if you go in a loop, this is how it actually goes on in straight line fashion that we have already discussed. So, first ones happen first. So, this is where step 1 to step 8 goes in this way. So, what happens first and then what like this.

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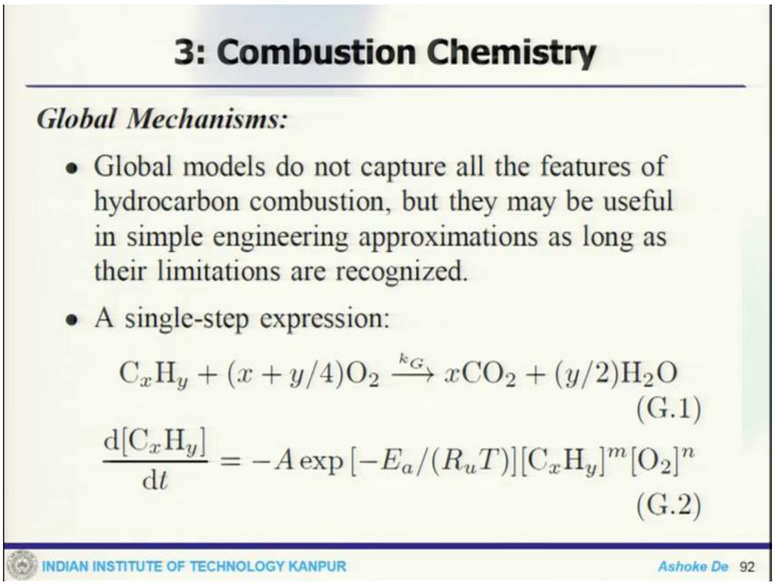

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Global Mechanisms:

- Global models do not capture all the features of hydrocarbon combustion, but they may be useful in simple engineering approximations as long as their limitations are recognized.
- A single-step expression:

$$C_xH_y + (x + y/4)O_2 \xrightarrow{k_G} xCO_2 + (y/2)H_2O \qquad (G.1)$$

$$\frac{d[C_xH_y]}{dt} = -A\exp\left[-E_a/(R_uT)\right][C_xH_y]^m[O_2]^n \qquad (G.2)$$

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Now when you come down to the global mechanism all this features that you get to see when you are looking at a detailed mechanism that means which has all intermediate species send radical features which forms in elementary reaction. By global models do not capture all the feature of hydrocarbon combustion. They are quite useful for simple engineering problem and as long as you can use them with their limitation.

For example, if you look at C_xH_y it is a single step of the expression for this much is burning. This is your reaction rate it will form CO_2, H_2O and the rate you can define as this expression to the Arrhenius expression.

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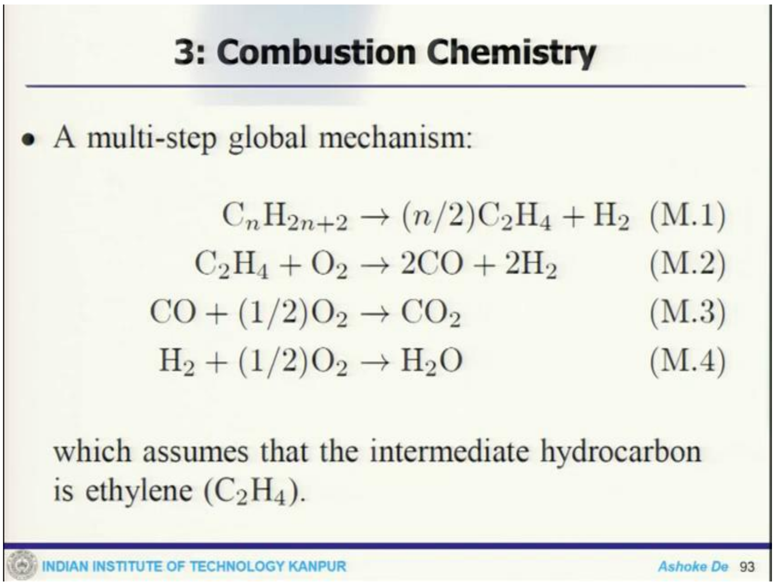

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- A multi-step global mechanism:

$$C_nH_{2n+2} \rightarrow (n/2)C_2H_4 + H_2 \quad (M.1)$$
$$C_2H_4 + O_2 \rightarrow 2CO + 2H_2 \quad (M.2)$$
$$CO + (1/2)O_2 \rightarrow CO_2 \quad (M.3)$$
$$H_2 + (1/2)O_2 \rightarrow H_2O \quad (M.4)$$

which assumes that the intermediate hydrocarbon is ethylene (C_2H_4).

Now if you for the same methane rather C_nH_{2n+2} so you can go slightly detail that means some more step instead of single step there are multiple step like 4 step mechanism. So, in 4 step mechanism first you get is lower order Hydrocarbon and then that gets oxidized to form CO and CO to CO_2 and H_2 to H_2O. So finally you get the products species like H_2 and CO_2, so but the higher order hydrocarbon first break down to a lower order one.

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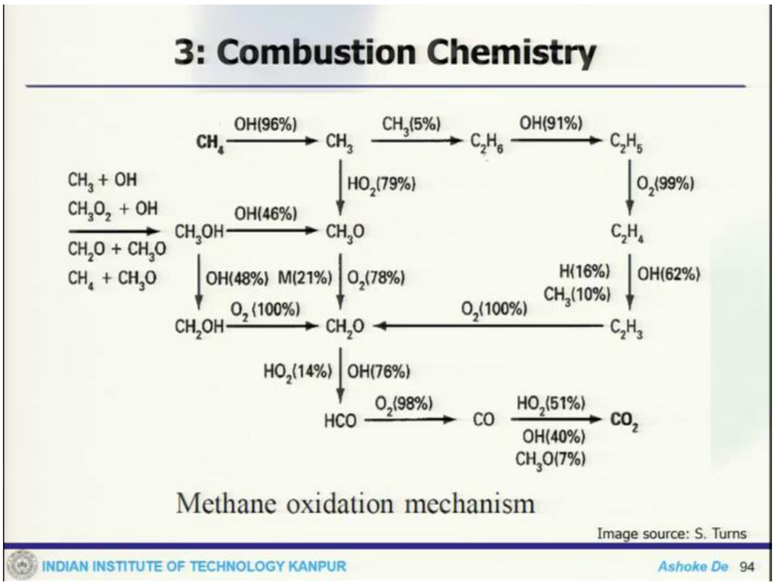

Methane oxidation mechanism

Image source: S. Turns

So, even if you take an example of a methane oxidation and how it goes and it goes in different ways. This is methane. So when it gets reacted to OH from CH_2 radical then CH_3 leads to C_2H_6, C_2H_5, C_2H_4, C_2H_3 then finally with the oxygen this radical or another part you can get CH_3 and CHCO or this side you can get CH_3OH which you can from that and you finally get to CH_2O.

Where again it will form a H_2O and then HO to CO and finally CO_2 so there is a big change this is called a skin or the reaction kinetics and this is a core research topic people who are working in the kinetics area where they form actually as a engineer you would be interesting to look at the kinetics only. So, because you need the mechanism so that you can actually handle or analyze your combustion process.

But the kinetics itself is an area of research where people look at and they develop different kind of kinetics and try to give you; I mean that is why Sorry for even a simple methane mechanism if one look at it, there are single step mechanism and two step mechanism, four step mechanism, 9 step and there are multiple step mechanisms. And every kinetics has its own limitation, but there has its own advantage and disadvantage.

So more and more detailed mechanism you include you can actually predict the minor species, intermediate radical. So these are species.

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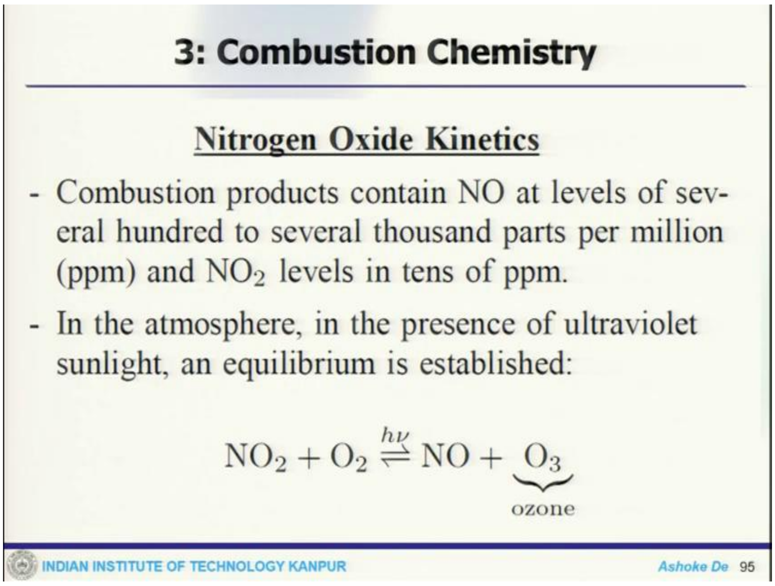

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Nitrogen Oxide Kinetics

- Combustion products contain NO at levels of several hundred to several thousand parts per million (ppm) and NO_2 levels in tens of ppm.
- In the atmosphere, in the presence of ultraviolet sunlight, an equilibrium is established:

$$NO_2 + O_2 \overset{h\nu}{\rightleftharpoons} NO + \underbrace{O_3}_{\text{ozone}}$$

Moving at one more thing that we would like to look at is the nitrogen oxide kinetics. This is another important issue the reason why because most of the combustion process as we have seen they are the source of air pollution. Pollution means CO, NO, this sort of gases, but NO does not sum so easily it is not a note that like in any normal combustion process you get to see a NO. To getting to NO, you need to have certain level of the process.

But if you look at the NO formation but this is no matter whatever it is. It has the presence of this NO as a serious health hazard or environmental concern. Now what happens when NO_2 oxidises with O_2, it forms NO and also the ozone gases. This is not something one would expect in the current scenario across the world that we are in Arrhenius form.

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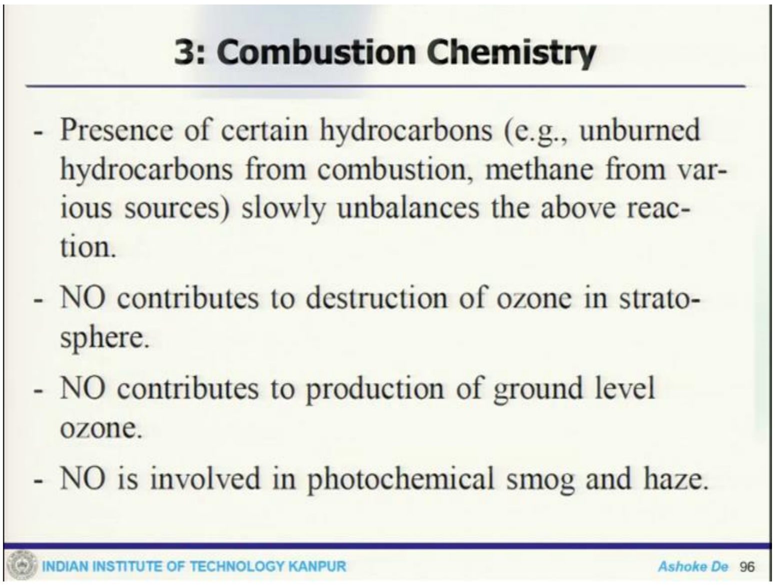

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- Presence of certain hydrocarbons (e.g., unburned hydrocarbons from combustion, methane from various sources) slowly unbalances the above reaction.
- NO contributes to destruction of ozone in stratosphere.
- NO contributes to production of ground level ozone.
- NO is involved in photochemical smog and haze.

Now presence of certain hydrocarbons like un-burnt hydrocarbons from combustion methane, so, slowly unbalances the previous reactions. What NO does, it has its series impact like it contributes to the destruction of the ozone in stratosphere. Secondly it contributes to the production of ground-level ozone also it is involved in smog and haze and all these things.

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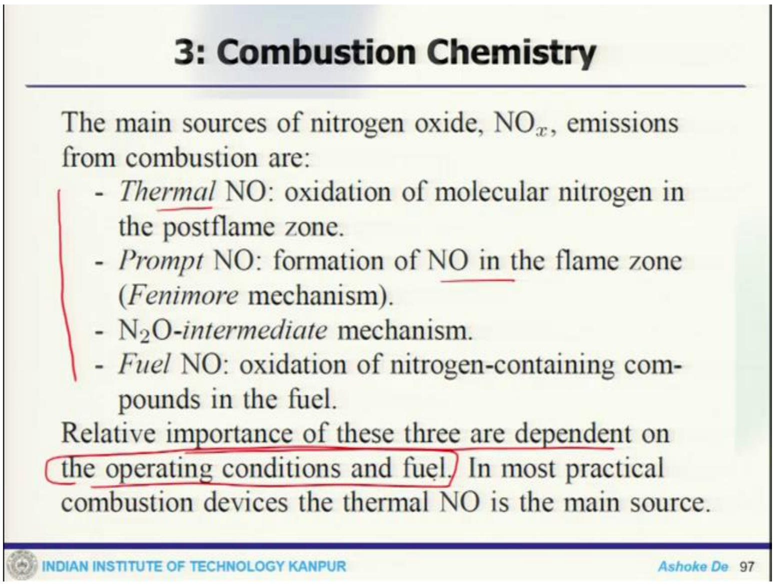

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The main sources of nitrogen oxide, NO_x, emissions from combustion are:

- *Thermal* NO: oxidation of molecular nitrogen in the postflame zone.
- *Prompt* NO: formation of NO in the flame zone (*Fenimore* mechanism).
- N_2O-*intermediate* mechanism.
- *Fuel* NO: oxidation of nitrogen-containing compounds in the fuel.

Relative importance of these three are dependent on the operating conditions and fuel. In most practical combustion devices the thermal NO is the main source.

So, this has a serious concern now if you see this NO forms it is a part of your pollution gas that NO_x formation from the combustion but there are different mechanism of the NO_x formation. It is not like that is what as I mentioned earlier that you cannot have NO_x from when your burning candle it may not be reforming and NO_x, but it will obviously from some CO to CO. So NO_x as some certain reason like there would be 3 different kind of NO_x or 4 different kind of NO_x.

One is the thermal NO_x which is oxidation of the nitrogen in the post flame zones that means when you have this flame or reaction zone it is in the post flame zone where thermal NO_x is formed that means it is highly dependent on the temperature. Then there is a prime NO_x this is the formation of flame within the flame zone. So, that forms between the flames. Then you can have also N_2O which is formed due to intermediate mechanism.

Finally, if your fuel contains some NO that will also can be into the combustion. So as I mentioned, this is an important thing the importance of these two depending on the operating conditions of the fuel. So depending on operating condition which kind of NO formation will there or there would not be any NO formation. It is highly dependent on the condition and the fuel. But as I mentioned most of the devices you get to see thermal NO that is the main source.

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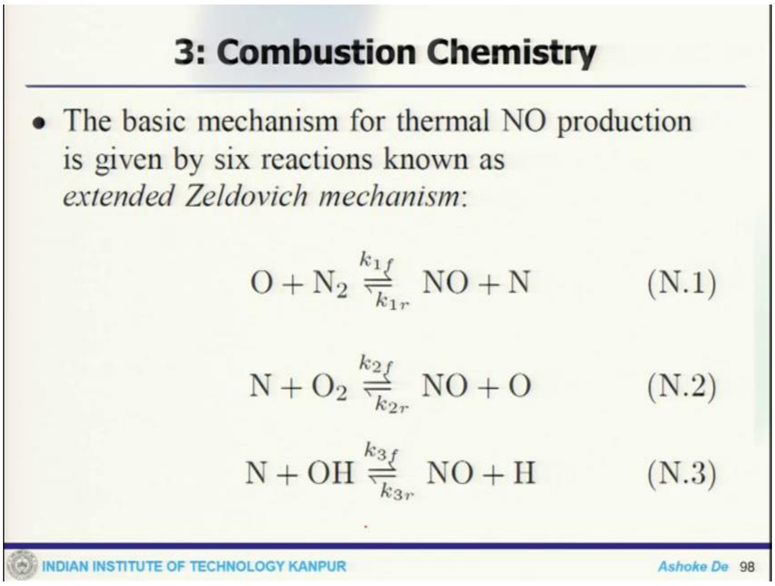

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- The basic mechanism for thermal NO production is given by six reactions known as *extended Zeldovich mechanism*:

$$O + N_2 \underset{k_{1r}}{\overset{k_{1f}}{\rightleftharpoons}} NO + N \qquad (N.1)$$

$$N + O_2 \underset{k_{2r}}{\overset{k_{2f}}{\rightleftharpoons}} NO + O \qquad (N.2)$$

$$N + OH \underset{k_{3r}}{\overset{k_{3f}}{\rightleftharpoons}} NO + H \qquad (N.3)$$

Now why this NO production is given by there is a mechanism by Zeldovich mechanism where there are different states through which the NO formation takes place. So these are the 6 reaction steps, these are forward and backward reaction. So, how O radical react to N_2 and form

NO, N form react to form NO, N react to O_2 to form NO and also the reverse reaction possible. Like NO with N can form these things.

But this is kind of thermal NO formation mechanism, now if you look at this contribution of the reaction is small for the mixture and for rich mixture it is considered. So, that means if the mixture is lean, then this contribution is small if the mixture is weak this is considerable. So this produces N of NO. Now when you look at the forward reaction of one it controls the system and it is slow at low temperature and high activation energy.

So this is also very effective in post flame regime where temperature is high T is high and also you get enough time that means these forward reaction, so, essentially the forward one, forward reaction. Now concentrations of 1000 to 4000 ppm are typically observed in uncontrolled combustion system and reaction 1, 2, 3 you can calculate the NO.

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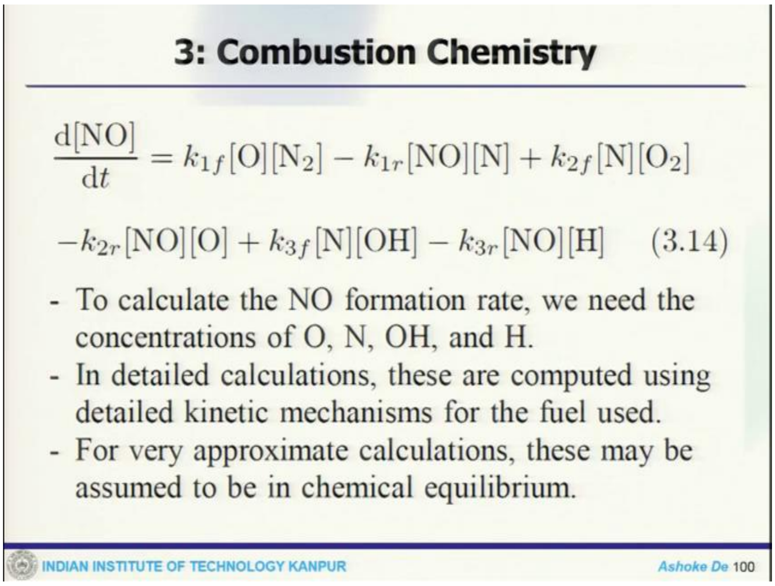

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$$\frac{\mathrm{d[NO]}}{\mathrm{d}t} = k_{1f}[\mathrm{O}][\mathrm{N_2}] - k_{1r}[\mathrm{NO}][\mathrm{N}] + k_{2f}[\mathrm{N}][\mathrm{O_2}]$$

$$-k_{2r}[\mathrm{NO}][\mathrm{O}] + k_{3f}[\mathrm{N}][\mathrm{OH}] - k_{3r}[\mathrm{NO}][\mathrm{H}] \qquad (3.14)$$

- To calculate the NO formation rate, we need the concentrations of O, N, OH, and H.
- In detailed calculations, these are computed using detailed kinetic mechanisms for the fuel used.
- For very approximate calculations, these may be assumed to be in chemical equilibrium.

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Now, one can estimate the concentration or the NO production rate from the six reactions. So, these are contribution of forward reaction, reverse reaction for the first second forward second. So, we need also the concentration of O which is present there we need OH, N and H. So, now when you go to detailed kinetic mechanisms and the fuel used you can calculate from those things.

But otherwise one may actually very crudely approximate them and to be assumed that in chemical equilibrium. And then you can calculate these things if you assume that in chemical equilibrium.

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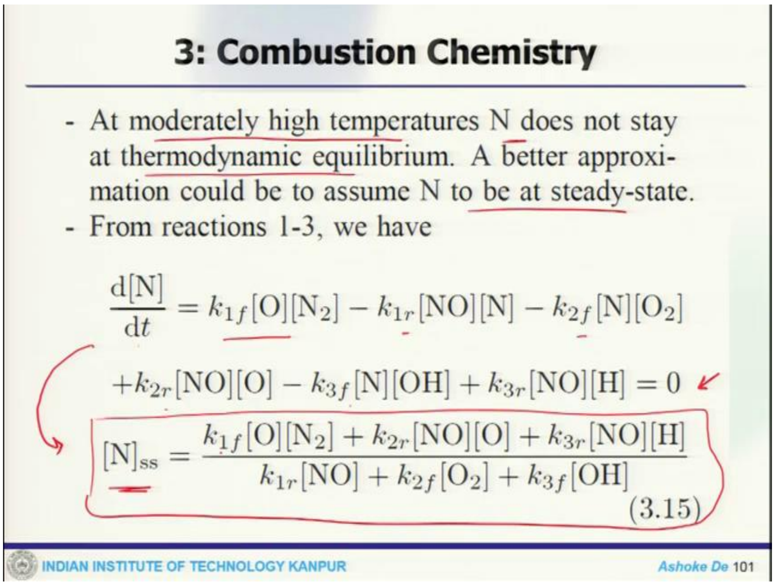

3: Combustion Chemistry

- At moderately high temperatures N does not stay at thermodynamic equilibrium. A better approximation could be to assume N to be at steady-state.
- From reactions 1-3, we have

$$\frac{d[N]}{dt} = k_{1f}[O][N_2] - k_{1r}[NO][N] - k_{2f}[N][O_2]$$

$$+k_{2r}[NO][O] - k_{3f}[N][OH] + k_{3r}[NO][H] = 0$$

$$\boxed{[N]_{ss} = \frac{k_{1f}[O][N_2] + k_{2r}[NO][O] + k_{3r}[NO][H]}{k_{1r}[NO] + k_{2f}[O_2] + k_{3f}[OH]} \quad (3.15)}$$

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Now moderately high temperature N does not stay at thermodynamic equilibrium. So, this is one of the important observations if we are moderately high temperature so N atom or that does not stay at the thermodynamic equilibrium. That means even to evaluate that if you use this Chemical equilibrium assumption so that may not be appropriate dependable operating condition.

In that case better approximation can be assumed to be at steady-state. Now, if that is the situation then you can write that (d[N]/dt) the production rate so this is coming from your forward reaction. And this is this is what we have get from these three reactions where now you are writing for N. Then this is forward, reverse and second forward and second reverse third forward and third reverse.

And to be in steady state this is equal to 0 and then if you do the algebra here which will be bit involve you can see the N at steady state and which will involve the different species concentration and reaction rate coefficients and everything. So, then you can find out at the steady-state what would be there.

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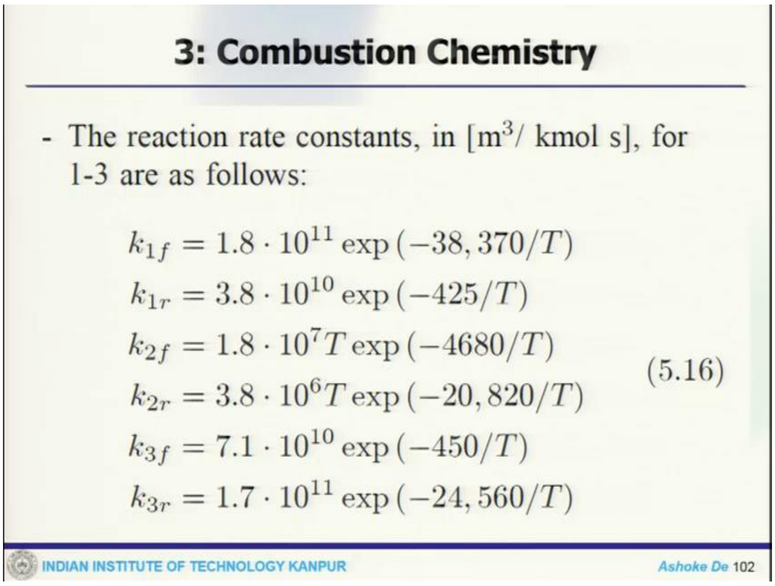

3: Combustion Chemistry

- The reaction rate constants, in [m^3/ kmol s], for 1-3 are as follows:

$$\begin{aligned} k_{1f} &= 1.8 \cdot 10^{11} \exp(-38,370/T) \\ k_{1r} &= 3.8 \cdot 10^{10} \exp(-425/T) \\ k_{2f} &= 1.8 \cdot 10^{7} T \exp(-4680/T) \\ k_{2r} &= 3.8 \cdot 10^{6} T \exp(-20,820/T) \\ k_{3f} &= 7.1 \cdot 10^{10} \exp(-450/T) \\ k_{3r} &= 1.7 \cdot 10^{11} \exp(-24,560/T) \end{aligned} \qquad (5.16)$$

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Now the reaction rate constant which are; because this is well established mechanism. So these are available readily in literature and one can actually look at that forward reaction rate coefficients. These are all in SI unit. So, this is your A and all these cases, this is your activation energy divided by R, this factor and this is your T. First reaction reverse is like that. Second reaction you have some T to the power one.

So that means in this particular case. You get some exponents one so that A is 1 here. So the second forward and reverse reaction contain some temperature dependent parameter. And these are the as usual (A/RT). So, this you can find out any standard literature if you look at it.

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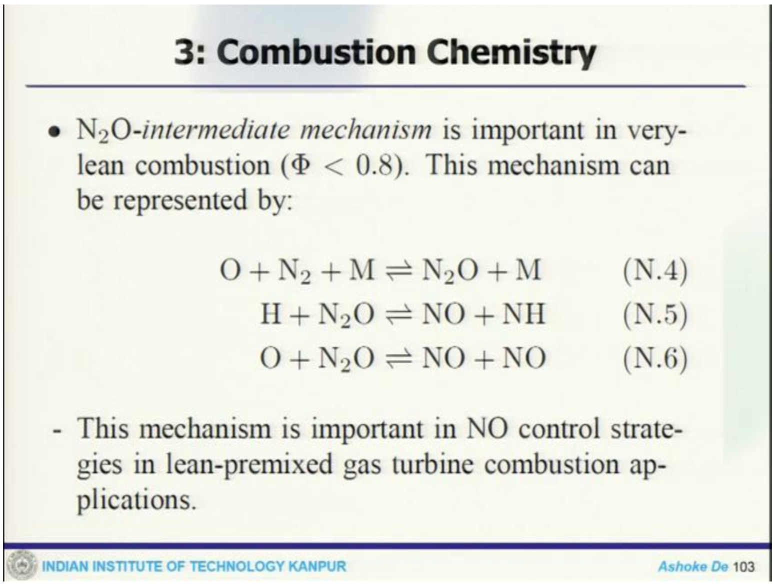

3: Combustion Chemistry

- N_2O-*intermediate mechanism* is important in very-lean combustion ($\Phi < 0.8$). This mechanism can be represented by:

$$O + N_2 + M \rightleftharpoons N_2O + M \qquad (N.4)$$
$$H + N_2O \rightleftharpoons NO + NH \qquad (N.5)$$
$$O + N_2O \rightleftharpoons NO + NO \qquad (N.6)$$

- This mechanism is important in NO control strategies in lean-premixed gas turbine combustion applications.

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Now we look at that let us talk about thermal N formation. Now, if you look into intermediate mechanism, this is also important in very lean combustion. So, when you talk about very lean combustion that means equivalence ratio less than 1. And now how you defined it into this intermediate mechanism, you have N_2 reacting with O and other molecules it will form N_2O and N_2 will react with NO finally NO.

So this mechanism is also important in NO control strategy is in lean premixed gas turbine combustion because one would like to avoid this N_2 intermediate mechanism so that you do not;

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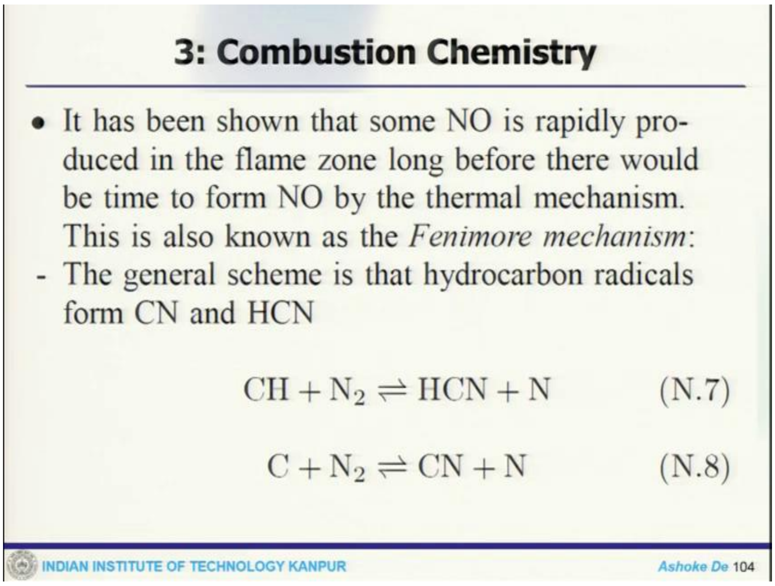

3: Combustion Chemistry

- It has been shown that some NO is rapidly produced in the flame zone long before there would be time to form NO by the thermal mechanism. This is also known as the *Fenimore mechanism*:
- The general scheme is that hydrocarbon radicals form CN and HCN

$$CH + N_2 \rightleftharpoons HCN + N \qquad (N.7)$$

$$C + N_2 \rightleftharpoons CN + N \qquad (N.8)$$

Now it is well known or shown that the, some NO is rapidly producing in flame zone obviously because if it is thermal NO then it would be in post flame zone before they come to NO by thermal mechanism. So this is known as Fenimore mechanism. So, general scheme for that in that case hydrocarbon radicals is H reacting with N_2O and to form HCN and CN and all these things.

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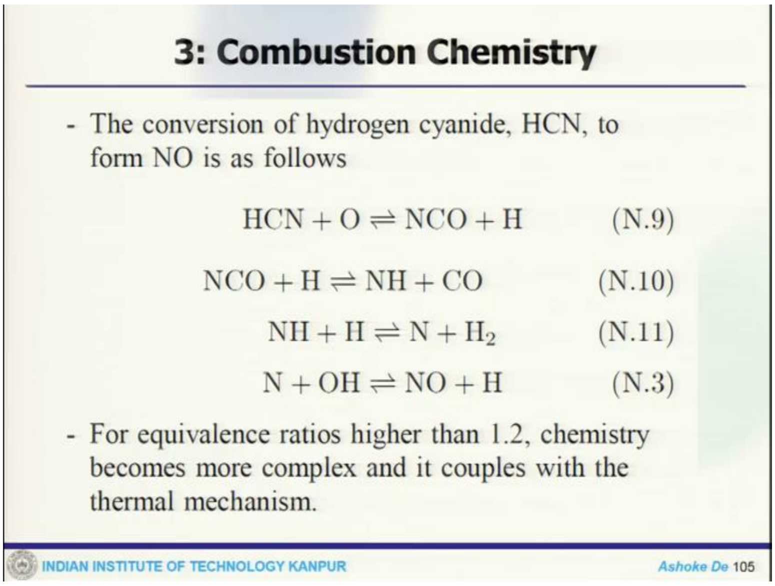

3: Combustion Chemistry

- The conversion of hydrogen cyanide, HCN, to form NO is as follows

$$\mathrm{HCN + O \rightleftharpoons NCO + H} \qquad (\mathrm{N.9})$$

$$\mathrm{NCO + H \rightleftharpoons NH + CO} \qquad (\mathrm{N.10})$$

$$\mathrm{NH + H \rightleftharpoons N + H_2} \qquad (\mathrm{N.11})$$

$$\mathrm{N + OH \rightleftharpoons NO + H} \qquad (\mathrm{N.3})$$

- For equivalence ratios higher than 1.2, chemistry becomes more complex and it couples with the thermal mechanism.

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Now, that is what you get and then the conversion of hydrogen cyanide HCN to form NO as follows. So that means if you form this and then you can from now hydrogen cyanide will react to oxygen to form NCO, now NCO form to NH and then finally you get NO and this happens where you are in the zone where intermediate radicals are formed. Now, if your equivalence ratio is higher than 1.2 then the chemistry becomes more complex and it couples with the thermal mechanism.

So that means what happens, so there are different situations for one can one is the; if we just to complete this NO business. This is where one could be thermal NO_x, which is actually in the active in the post in zone and that because the temperature is quite high. Then in flame zone you can have prompt NO and that also depends what kind of operating condition is this? I mean no matter what it is. All these things depend on the operating condition and then depending on the fuel or in N_2 intermediate mechanism, there could be some NO formation.

So that is why regular daily combustion system you may not see NO but in the large-scale applications you do see NO, so this is what we talked about different kinetics and then the mechanisms and how they impact the reacting system. So that is all about the combustion chemistry that we want to discuss. So we will stop here today and continue the discussion in the next lecture.