

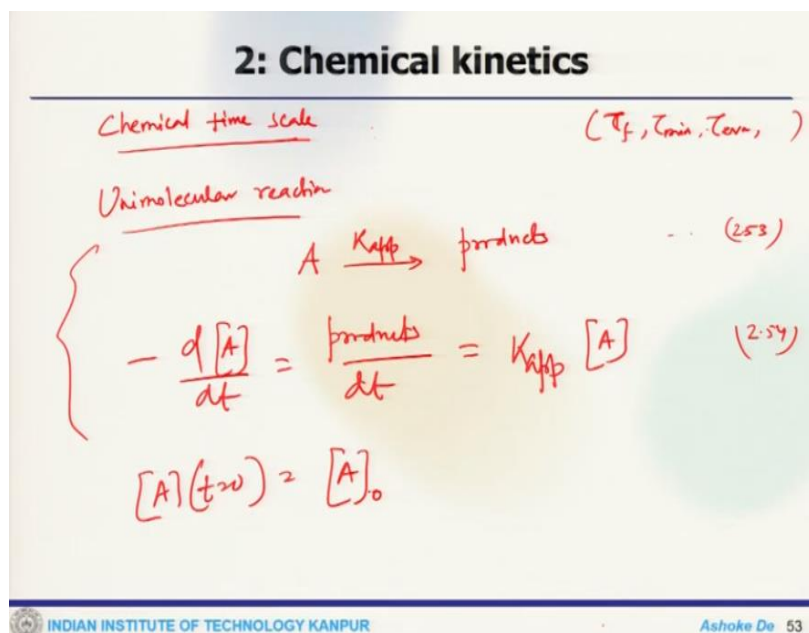
**Turbulent Combustion: Theory and Modelling**  
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**Lecture – 10**  
**Chemical Kinetics (Contd.,) and Combustion Chemistry**

Welcome back a let us continue the discussion on the chemical kinetics and here now we have looked at how the elementary reactions involved in the production of multiple species of the intermediate radicals. And intermediate radicals it is quite important to reaction to move forward and also while talking about the intermediate radical we have discussed about chain reactions where the chain initiation takes place.

Then there is chain propagation where the free radicals are produced and finally the chain termination process to get to the stable product. And using the concept of steady state approximation, we can find out the rate coefficients and the production rate and all this things are already to look at how we can now find out the chemical kinetics.

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So, let us see how we calculate the chemical time scale this is one of the important thing that requires because most of the reacting system they are exposed to free dynamical behaviour and flow scale time scale another phenomena. Also the magnitude of the time scale relative to the

convective or mixing time scale is of importance in combustion because these reactive systems are there are two time scale, like flow time scale there would be mixing timescale.

If it is multiphase flow, there will be evaporation time scale that would be other time scale if it is radiation effect on other things. So that is why the reaction time scale of really of important in that sense. Let us start with the simple one with Uni molecular reaction. If you start with uni molecular reaction that is A goes to stick to our nomenclature and continue the notation similar fashion. So, this is our; now this is what we already seen in 2.53 and this rate was:

$$\frac{\text{products}}{dt} = K_{app}[A]$$

This is what we have seen in 2.54. So these are already for unimolecular system who have seen this. Now what you can do you can integrate this for constant and for assume A at t=0 is  $[A]_0$ . Now we integrate to find out what happened.

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**2: Chemical kinetics**

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$[A](t) = [A]_0 \exp(-K_{app}t) \quad \dots (2.67)$

$\frac{[A](t_{char})}{[A]_0} = \frac{1}{e} \quad \dots (2.68)$

Combining eq. (2.67) & (2.68)

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So, then the concentration at any time t would be:

$$[A](t) = [A]_0 \exp(-K_{app}t)$$

Now the characteristic time scale can be defined as the time required for the concentration of A to fall from its initial value to a value equal to 1 by e times the initial value. So, that means what we say to A to by ratio will go when this is (1/e). So, this is what the characteristics time scale. Now only come this to 2.67 and 2.68 what we get is that, so you are now combining to equation 2.67 and 2.68.

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**2: Chemical kinetics**

$\frac{1}{e} = \exp(-K_{app}\tau_{chem}) \dots (2.69)$

or  $\tau_{chem} = \frac{1}{K_{app}} \dots (2.70)$

Bimolecular rx.

$A + B \xrightarrow{K_{bimol.}} C + D \dots (2.6)$

$\left\{ \frac{d[A]}{dt} = -K_{bimol.} [A][B] \dots (2.7) \right.$

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So what we get:

$$\frac{1}{e} = \exp(-K_{app}\tau_{chem})$$

Which is 2.69 or:

$$\tau_{chem} = \frac{1}{K_{app}}$$

Which is 2.70. So this is what one can estimate for Uni molecular reaction the chemical time scale for the Uni molecular reaction. Now you look at what happens for a bi molecular reaction. So, here we got an A + B forming C + D this is what we have taken earlier and that would be K bimolecular coefficient so if you try to find out the d[A]/dt, it will be:

$$\frac{d[A]}{dt} = -K_{bimol}[A][B]$$

This 2.9 this is already for a bimolecular reaction we have seen it.

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**2: Chemical kinetics**

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$$x \equiv [A]_0 - [A] = [B]_0 - [B] \quad \dots (2.71)$$

$$[B] = [A] + [B]_0 - [A]_0 \quad \dots (2.72)$$

Substitute eq 4.71 into 4.9, integrate them

$$\frac{[A](t)}{[B](t)} = \frac{[A]_0}{[B]_0} \exp\left\{([A]_0 - [B]_0) K_{bim} t\right\} \quad \dots (2.73)$$

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Now for this single reaction A and B are related to stoichiometry. So, any change in A has a corresponding change in B. Now you define that  $A_0$  that should be corresponding change in B. So, which will let you to have  $A + B_0 - A_0$ . Now you substitute equation 4.71 into 4.9 and integrate then we get concentration of A at time and B at time:

$$\frac{[A](t)}{[B](t)} = \frac{[A]_0}{[B]_0} \exp\{([A]_0 - [B]_0) K_{bim} t\}$$

So you get an exponential expression for the same thing including your A and B.

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**2: Chemical kinetics**

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Substitute 2.72 into 2.73

$$\frac{[A]}{[A]_0} = \frac{1}{2} \quad \text{when } t = \tau_{chem}$$

$$\tau_{chem} = \frac{\ln\left[e + (1-e)\left(\frac{[A]_0}{[B]_0}\right)\right]}{([B]_0 - [A]_0) K_{bim}} \quad \dots 2.74$$

if  $[B]_0 \gg [A]_0$

$$\tau_{chem} = \frac{1}{[B]_0 K_{bim}} \quad \dots (2.75)$$

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Now again, we do the same thing now we got 2.72 and 2.73, now we substitute 2.72 into 2.73  
So, what you get is:

$$\frac{[A]}{[A]_0} = 1/e$$

When:

$$t = \tau_{chem}$$

which means it will allow you to have:

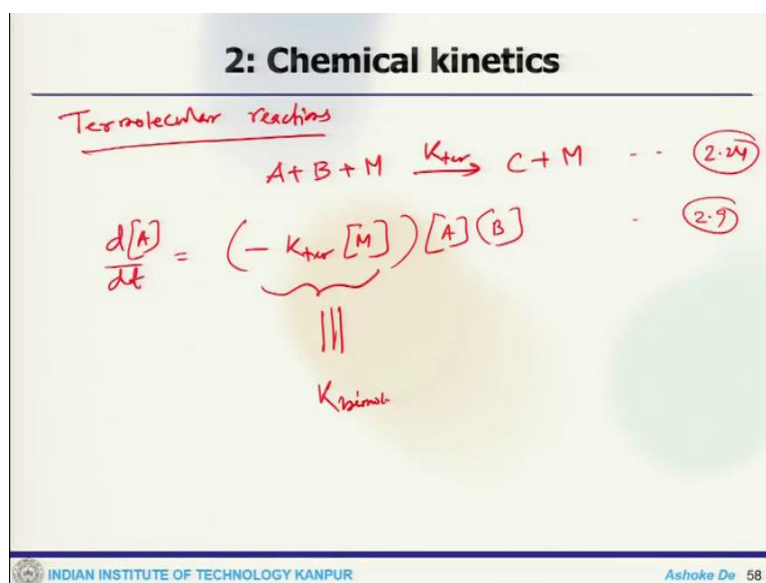
$$\tau_{chem} = \frac{\ln \left[ e + (1 - e) \left( \frac{[A]_0}{[B]_0} \right) \right]}{([B]_0 - [A]_0) K_{bi}}$$

So, for a bimolecular reaction, to get an expression for the chemical time scale. Now if the concentration is quite high for B then this is:

$$\tau_{chem} = \frac{1}{[B]_0 K_{bi}}$$

So, simplification if the concentration is too high then essentially this term goes to 0 1 by k bimolecular so this what you get a simplified expression for a particular system again bimolecular system.

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Now last one is the tri molecular system so that what happens to the trimolecular system. So, we have taken example  $A + B + M$  to  $C + M$  with  $K_{trimolar}$  which will be; so this is what we have previously defined. Now for simple system at constantly concentration of M is constant. So in that case we got:

$$\frac{d[A]}{dt} = (-K_{tri}[M])[A][B]$$

Now this term  $K$  plays the same role as  $K$  bimolecular here. So this is the term if you look at it carefully, this is the complete term plays an; for this sort of an equivalent see one can think about  $K$  bimolecular, so the effect is similar to that.

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### 2: Chemical kinetics


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$$\tau_{chem} = \frac{\ln [e + (1-e)([A]_0/[B]_0)]}{([B]_0 - [A]_0) K_{tri} [M]} \dots (2.77)$$

$\underbrace{K_{tri} [M]}_{\equiv K_{bim}}$

if  $[B]_0 \gg [A]_0$

$$\tau_{chem} = \frac{1}{[B]_0 (K_{tri} [M])} \dots 2.78$$


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So, then the characteristics time scale for the trimolecular system one can estimate as:

$$\tau_{chem} = \frac{\ln [e + (1 - e) ([A]_0/[B]_0)]}{([B]_0 - [A]_0) K_{tri} [M]}$$

This is exactly where the equivalency is the  $K_{bimolecular}$ . So, using the equivalency the bimolecular system we can find out that. And similarly if the concentration of B is quite high so, this time scale would be:

$$\tau_{chem} = \frac{1}{[B]_0 (K_{tri} [M])}$$

So, that is a simplified expression for that system.


Now this is what happens when basically you look at these different Kinetic and Whole idea is that you can find out these characteristics time scale with the chemical time scale.

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### 3: Combustion Chemistry

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- For many kinetically controlled systems, the number of elementary reaction steps is so large that simple analytical solutions are not possible.
- Most of the time, a large number of chemical species are involved.
- Even in combustion of simple hydrocarbons, number of species involved is quite high.
- To illustrate how the fundamental principles of chemical kinetics apply to real-world problems, we will consider some examples.

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Now we will move to an third one is the combustion chemistry. Now this is an important again aspect and what we are discussing now, these are all very, very important aspect of the fundamental of combustion process. Once we know this thing that will become the building block for turbulent combustion. Now for many kinetically control system, the number of elementary reaction state is quite high.

So, that means simple analytics that means when you look at even for example, the combustion of  $\text{CH}_4$ , it goes through few hundred elementary steps. If you are interested you can go to any website called GRIMECH which is made from the Barkley group University of Berkeley California you can see their different mechanism version. The latest one is GRI 3 which is for Methane combustion and you can see there are multiple reactions there.

So it becomes quite large number of steps where the analytical solution is not possible to find out chemical time scale. So top of that not only the elementary steps, we have large number of chemical species which are also involved. So that means one and you have large number of reactions step then you have large number of species so in totality that becomes quite combustion to find out the analytical expression for chemical time scale.

Even if it is for simple hydrocarbon as I mentioned that  $\text{CH}_4$  number species involved is quite high. So, how the fundamental principles of chemical kinetics apply to this will consider some example here.

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**3: Combustion Chemistry**

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**Hydrogen-Oxygen Reaction**

The reaction between hydrogen and oxygen is a good example of a multicomponent kinetic system. To describe the system properly, we should consider eight major species and at least 16 reactions.

- The overall reaction is:

$$2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$$

This reaction is exothermic; but mixtures of gaseous hydrogen and oxygen are quite stable at atmospheric conditions. Any conceivable direct reaction between the two gases is zero.

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Now, let us start with an example of the hydrogen oxygen reaction. This particular reaction is the global reaction on overall reaction. But if you look at the elementary step it could have multiple species major species and there would be some reaction state and overall this reaction is exothermic reaction where gaseous hydrogen and oxygen required stable at atmospheric condition. Now any conceivable direct reaction between two gases is not possible.

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**3: Combustion Chemistry**

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- The reaction half-time at atmospheric conditions has been estimated to be much larger than the age of the universe.
- If the reaction is initiated by some free-radical species, then the reaction proceeds very rapidly and violently.
- The radicals are typically H and O atoms produced from the dissociation of  $\text{H}_2$  and  $\text{O}_2$ , respectively.
- We will consider a simplified mechanism that represents the gross features of  $\text{H}_2 + \text{O}_2$  at low  $P$ .

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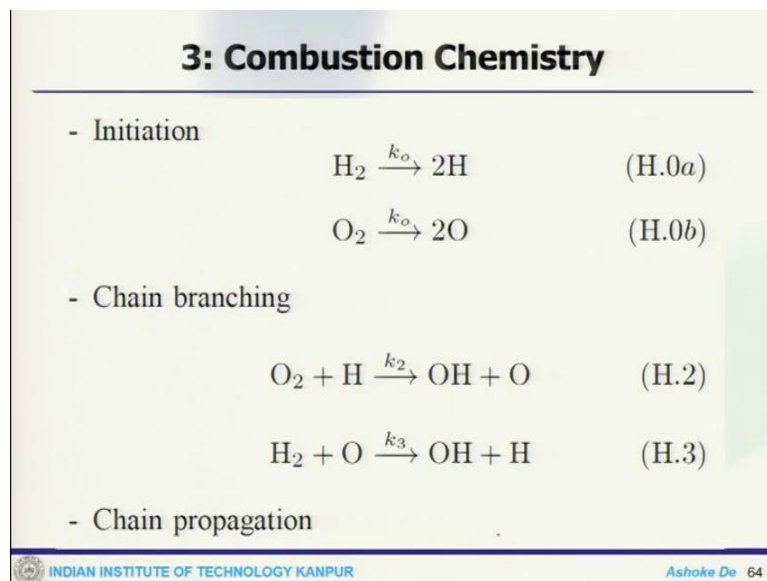
So, the reaction half time at atmospheric condition has been estimated to be much larger than the age of the universe. Which says that if the reaction is initiated by some free radical species in the reaction proceeds, very rapidly and violently. This is one of the important where these



elementary reactions become important so and when you get this free radical. Because any free radical they are quite reactive nature as soon as they are formed.

They would be having a tendency to go to some stable product and try to react with that and some more radicals or some other product. So that is where the elementary step reactions are important where the free radicals will form and they will allow the reaction to move further. And this particular hydrogen oxygen case there could be H, O, OH forms.

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Now we will consider the simplified mechanism that represents the hydrogen oxygen reaction at low pressure. So, the first steps of the reaction so there would these are step chain reaction. So, first step towards the reaction is the initiation. So what happens if the initiation step that hydrogen adjustable product it gets into H radicals and oxygen as a stable product it gets into OH radical. Now once that happens so this is the initiation of the process.

Now my chain branching starts to takes place, so then O<sub>2</sub> and H will combined to form OH and O so H<sub>2</sub> and O which are form at the initiation stage they will combine to form OH and H. Now, if you look at this process again, you get another free radical which is OH and this.

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**3: Combustion Chemistry**

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$$\text{H}_2 + \text{OH} \xrightarrow{k_1} \text{H}_2\text{O} + \text{H} \quad (\text{H.1})$$

- Chain termination

$$\text{H} + \text{wall} \xrightarrow{k_4} (1/2)\text{H}_2 \quad (\text{H.4})$$
$$\text{H} + \text{O}_2 + \text{M} \xrightarrow{k_5} \text{HO}_2 + \text{M} \quad (\text{H.5})$$

- Initiation step is the dissociation of some amount of molecular species by a spark, flame, electric discharge, or some other means.

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Now the propagation, now H<sub>2</sub> combined with OH to get H<sub>2</sub>O and H. So, these are the steps which will take place and then finally the termination comes into the picture where H to the wall it will terminate or H with the oxygen to form HO<sub>2</sub> and M. So, what happened that initiation step is the dissociation of some amount of molecular species by, so when you look at this initiation step to get this dissociation to take place there will be some amount of spark or flame or something has to be provided which will dissociate these things.

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**3: Combustion Chemistry**

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- Bond energies:

O = O : 5.1 eV  
H – H : 4.5 eV  
O – H : 4.4 eV

- Reaction (2) is endothermic by 0.7 eV (about 70 kJ/mol) and progresses slowly.

- Reactions (3) and (1) are endothermic by 0.1 eV, and these reactions are relatively fast.

- The OH and O radicals are therefore rapidly consumed, and the principal chain carrier is H atoms.

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Now what is that happens? When you get the free radicals then free radical start now, there are some other energy which are associated with different bonds of these molecule is like OO HH and they have different level of energies. Now in reaction 2 which we are talking here they are

endothermic reaction by some amount. Reaction 3 and 1 are endothermic by some amount on this reaction relatable fast. So you can also estimate from this bond energies and all this calculation that which reaction is quite fast and which is slow.

Therefore this H and O radicals are the rapidly consumed and the principal chain carriers remains as in each atom. So which will tell you out of this radicals what you get in this process which will be more reactive and which will stay there and allow to have.

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### 3: Combustion Chemistry

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$n^* \equiv H$

$$\frac{d[H]}{dt} = k_0[H_2] - k_2[H][O_2] + k_3[O][H_2] + k_1[OH][H_2] - k_4[H] - k_5[H][O_2][M] \quad \dots \quad 3.1$$

$$\frac{d[OH]}{dt} = k_2[H][O_2] + k_3[O][H_2] - k_1[OH][H_2]$$

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So, then you can find out the rate equation for this free radical  $n^*$  in H, which is taken as same as that H. So your  $n^*$  is here the H so that means you will find out:

$$\frac{d[H]}{dt} = k_0[H_2] - k_2[H][O_2] + k_3[O][H_2] + k_1[OH][H_2] - k_4[H] - k_5[H][O_2][M]$$

So that is your; so now other radical species like one can find out the OH also. Similarly this should be:

$$\frac{d[OH]}{dt} = k_2[H][O_2] + k_3[O][H_2] - k_4[OH][H_2]$$

Which is your second step of the reaction.

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**3: Combustion Chemistry**

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$$\frac{d[O]}{dt} = k_0[O_2] + k_2[H][O_2] - k_3[O][H_2] \quad \dots (3.3)$$

$[O] \text{ \& } [OH] \ll [H]$

$$\frac{d[O]}{dt} = \frac{d[OH]}{dt} = 0 \quad \dots (3.4)$$

$$[O]_{ss} = \frac{k_0[O_2] + k_2[H][O_2]}{k_3[H_2]} \quad \dots (3.5)$$

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And for O this will be:

$$\frac{d[O]}{dt} = k_0[O_2] - k_2[H][O_2] - k_3[O][H_2]$$

Which is 3.3. Since O and OH are both much lower than H that means both O and OH lower than H we can assume that both of the species at steady state. So,

$$\frac{d[O]}{dt} = \frac{d[OH]}{dt} = 0$$

O at steady state is:

$$[O]_{ss} = \frac{k_0[O_2] + k_2[H][O_2]}{k_3[H_2]}$$

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**3: Combustion Chemistry**

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$$[OH]_{ss} = \frac{k_2[H][O_2] + k_3[O][H_2]}{k_1[H_2]} \quad \dots (3.6)$$

$$[OH]_{ss} = \frac{2k_2[H][O_2] + k_0[O_2]}{k_1[H_2]} \quad \dots (3.7)$$

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And similarly for OH, OH at steady state is:

$$[OH]_{ss} = \frac{K_2[H][O_2] + K_3[O][H_2]}{K_1[H_2]}$$

Now substituting this for O steady state or we will use that O steady state that we got here, put there we get:

$$[OH]_{ss} = \frac{2K_2[H][O_2] + K_0[O_2]}{K_1[H_2]}$$

And substitute the steady state value of OH and O radicals in the rate equation of the free radical density.

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**3: Combustion Chemistry**

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$$\begin{aligned} \frac{dn^*}{dt} &= k_o[H_2] - k_2[H][O_2] + k_3 \frac{k_2[H][O_2] + k_o[O_2]}{k_3[H_2]} [H_2] \\ &+ k_1[H_2] \frac{2k_2[H][O_2] + k_o[O_2]}{k_1[H_2]} - k_4[H] - k_5[H][O_2][M] \\ &= \underbrace{k_o([H_2] + 2[O_2])}_{w_o} + \underbrace{(2k_2[O_2])}_f - \underbrace{(k_4 + k_5[O_2][M])}_g n^* \end{aligned} \quad (3.8)$$

so that

$$\frac{dn^*}{dt} = w_o + (f - g)n^* \quad (3.9)$$

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That means (dn\*/dt) which is essentially here is H which we have already look at it. This is the n\* here is, so free radical density if we write that we k<sub>0</sub>[H]<sub>2</sub> – k<sub>2</sub>[H][O<sub>2</sub>] and k<sub>3</sub> and all these things here. Basically it is and little bit of involved and nothing, but the algebraic expression. So, all your OH and O steady state that we got we put it back there. And finally you get in simplified state of the steady state:

$$\frac{dn^*}{dt} = \omega_0 + (f - g)n^*$$

But this expression which will involve hydrogen and oxygen, f is this and g is this. So, that is where you get the radicals.

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### 3: Combustion Chemistry

$f =$  chain branching  
 $g =$  chain termination

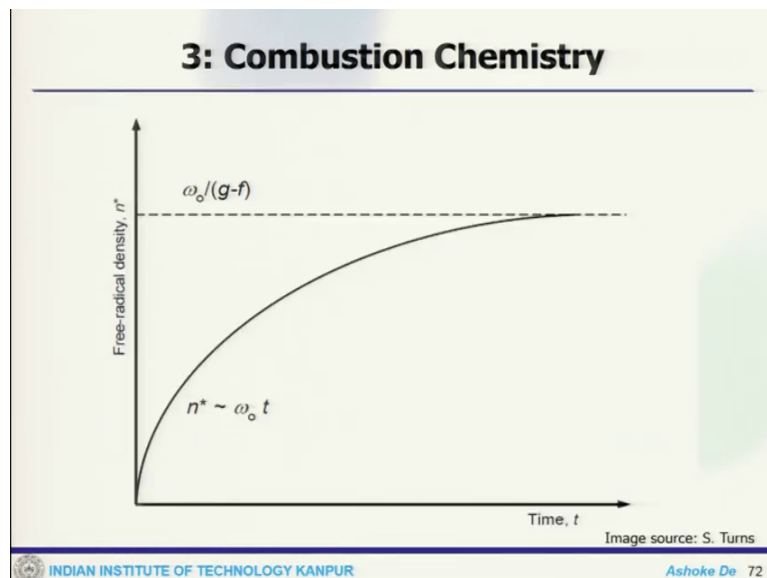
1:  $g > f$  : termination exceeds branching  
 2:  $g < f$  : branching " termination.

$k_4 > (2k_2 - k_5[M])[O_2]$  ... (3.10)

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Where  $f$ , if you look at here that will be the Chain branching one can identify that and  $g$  would be Chain termination. Now if that is the situation there will be two possibilities number 1  $g > f$ . So, that means termination exceeds branching or possibility 2  $g < f$  that means branching exceeds termination. So the solution one of the possibilities one implies that, so this imply that  $k_4 > (2k_2 - k_5 [M] [O_2])$ . So that  $g > f$  is assured sufficiently low  $O_2$  pressure.

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And if you got them with time, this is how your free radical density in this direction and this is the time. And this is how this evolve and this situation state.

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### 3: Combustion Chemistry

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$$n^* = \frac{\omega_0}{g-f} \{1 - e^{-(g-f)t}\} \quad \dots \quad (3.11)$$

slope  $\rightarrow \omega_0 t$        $n_{ss}^* = \omega_0 / (g-f) \quad \dots \quad (3.12)$

At higher  $O_2$  press.       $g < f$ , then

$$n^* = \frac{\omega_0}{f-g} \{e^{-(f-g)t} - 1\} \quad \dots \quad (3.13)$$

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Now solution will become then  $n^*$  is:

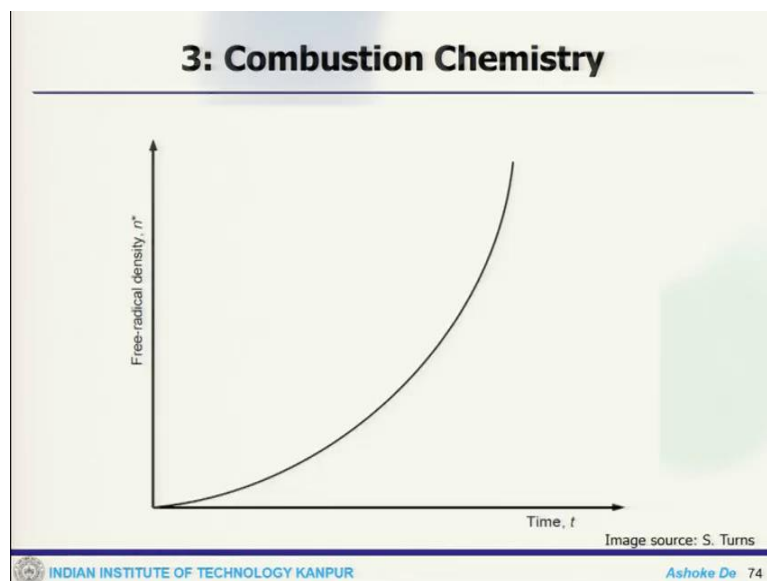
$$n^* = \frac{\omega_0}{g-f} \{1 - e^{-(g-f)t}\}$$

This is 3.11, now it is third time  $n^*$  increases almost linearly with flow. So, with the slope of  $\omega_0$  and which as a steady state value which is  $[\omega_0 / (g-f)]$ . At oxygen pressure at higher  $O_2$  pressure,  $g < f$  so then the solution remains  $n^*$  is:

$$n^* = \frac{\omega_0}{f-g} \{e^{-(f-g)t} - 1\}$$

Which is 3.13.

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And if you got that, this is how the free radical density that will evolve with the time. So, one case is higher pressure and another case is the lower pressure. So, we can see how that happens.

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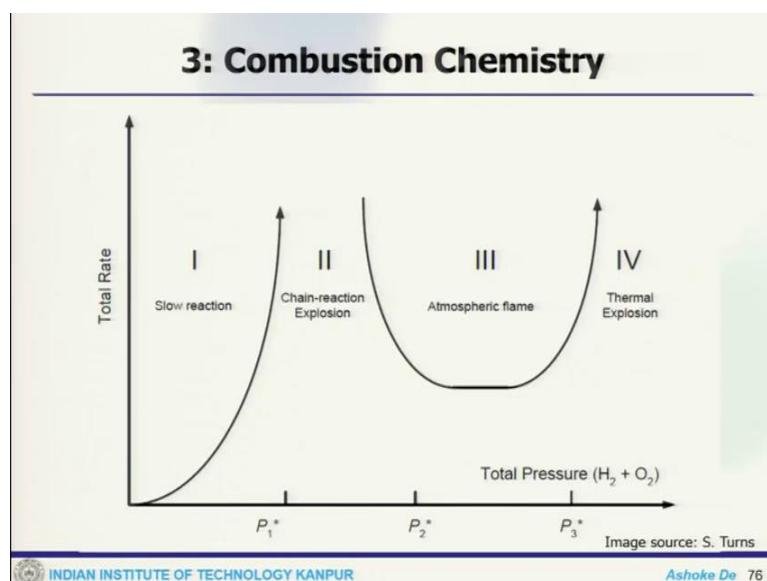
### 3: Combustion Chemistry

- In this case, the free-radical concentration increases exponentially, and, since the overall rate depends on the radical concentration, the reaction velocity increases rapidly. This is usually termed as an explosion.
- The hydrogen-oxygen reaction behaves quite differently in different pressure regimes.
- It is possible to construct an explosion boundary for the hydrogen-oxygen reaction as a function of temperature and pressure.

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Now this case, the free radical concentration increase exponentially and since the overall rate depends on the radical concentration the reaction velocity also increases rapidly. So, this kind of situation happens, this is usually termed as explosion. So, that means it is a balance between radical concentrations. Hydrogen-oxygen reaction behaves quite differently in different pressure regimes. So, that is there so you can possible to construct explosion boundary for hydrogen oxygen reaction.

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And if you look at the total rate, different pressure total rate different pressure, total pressure for hydrogen and oxygen first regime could be slow reaction second regime could be chain reaction explosion. Third would be atmospheric flame thermal expansion. So, in step 1 here the valve recombination is limited and proceeds to steady state. Second stage here  $f$  begins to exceed  $g$  so, the branched chain reaction.

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### 3: Combustion Chemistry

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- *Region I:* The reaction is wall-recombination limited, and proceeds to a steady-state.
- *Region II:*  $f$  begins to exceed  $g$ , the branched-chain reaction takes over and explosion ensues.
- *Region III:* As the pressure is further increased, the explosion is quenched and another regime of steady-state is encountered.

In III, kinetics are dominated by relatively unreactive  $\text{HO}_2$  (hydroperoxyl) radicals. Other reactions, in addition to those we considered above, are important and include the following:

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So, at region one that is the region to begin exceeds  $g$  and branched reaction takes over explosion ensues. So, now in the regime 3 where you come to here when the pressure is further increase the explosion is quenched. Another resumes of study, study occur, so at this state in the explosion quenched and another resume of steady state. So, free kinetics are dominated by relatively and reactive  $\text{H}_2\text{O}$  other reactants in addition be considered above are important and also can be included.

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**3: Combustion Chemistry**

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$$2\text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{O}_2 \quad (\text{H.6})$$
$$\text{H}_2 + \text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{H} \quad (\text{H.7})$$
$$\text{H} + \text{HO}_2 \longrightarrow 2\text{OH} \quad (\text{H.8})$$
$$\text{H} + \text{HO}_2 \longrightarrow \text{H}_2 + \text{O}_2 \quad (\text{H.9})$$
$$\text{H} + \text{HO}_2 \longrightarrow \text{H}_2\text{O} + \text{O} \quad (\text{H.10})$$
$$\text{H}_2\text{O}_2 + \text{M} \longrightarrow 2\text{OH} + \text{M} \quad (\text{H.11})$$
$$\text{H}_2\text{O}_2 + \text{H} \longrightarrow \text{H}_2\text{O} + \text{OH} \quad (\text{H.12})$$
$$\text{H}_2\text{O}_2 + \text{H} \longrightarrow \text{H}_2 + \text{O}_2 \quad (\text{H.13})$$
$$\text{H}_2\text{O}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{HO}_2 \quad (\text{H.14})$$
$$\text{H} + \text{OH} + \text{M} \longrightarrow \text{H}_2\text{O} + \text{M} \quad (\text{H.15})$$
$$\text{H} + \text{H} + \text{M} \longrightarrow \text{H}_2 + \text{M} \quad (\text{H.16})$$

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So, these are the, those steps which one can involve and see how many steps are there.

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**3: Combustion Chemistry**

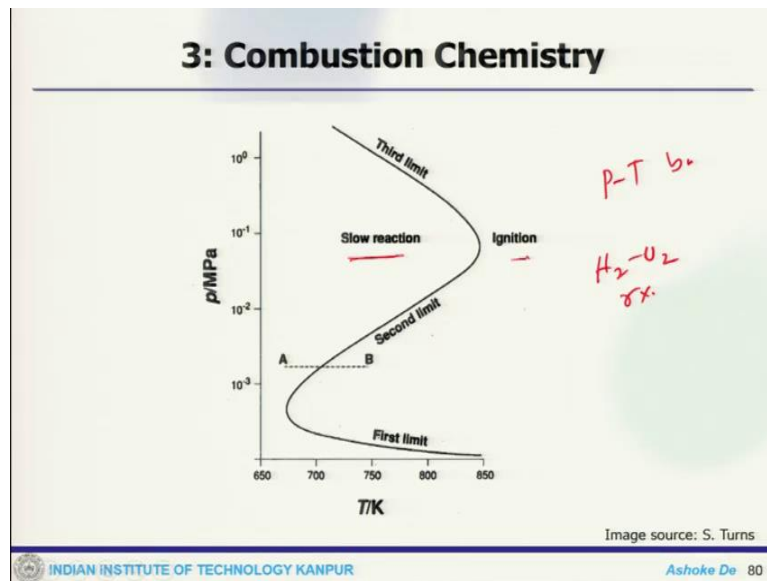
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- *Region IV*: At a still high pressure, the amount of heat liberated in the exothermic steps of the mechanism becomes larger than can be dissipated by conduction and other thermal transport processes, and the temperature rises. This, in turn increases the rates of initiation and provides heat for endothermic chain-branching reactions leading to more heat release, resulting in a thermal explosion.
- Experimentally observed ( $P - T$ ) boundaries of the  $\text{H}_2\text{-O}_2$  reaction in a closed vessel is shown below.

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Now regime 4 at little high pressure, so this is the regime 4 the amount of heat liberated in the exothermic steps of the mechanism becomes larger than can be dissipated by conduction and other transport processes at the temperature raises. So, this in turn increases the rate of initiation and provide heats of endothermic change branching reactions leading to the heat release which will lead to explosion. So, essentially this is the region where it becomes quite.

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So, one can show these boundaries in a pressure temperature curve where you have a slow reaction ignition. This is the; so this is your P - T boundary of  $H_2-O_2$  reaction. So that is P - T boundary. So, you can see different limits first limit, second limit and third limit and this side is slow reaction. This side is the ignition. So this is how hydrogen and oxygen reaction actually propagate so we will stop here and take it up in the next lecture.