**Combustion in Air Breathing Aero Engines**
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Lecture - 54
**Flame Stabilization and Blow off-II**

Hello. Just give you a very brief recap. We were discussing about laser induced fluorescence and in few seconds I will just show you what we were discussing. So, we have this we have this energy nuclear coordinate diagram, where essentially the OH was So residing in the ground state and the incident laser comes and it is each molecule it gets promoted to a higher electronic state undergoes into system crossing gets down to the lower electronic state.

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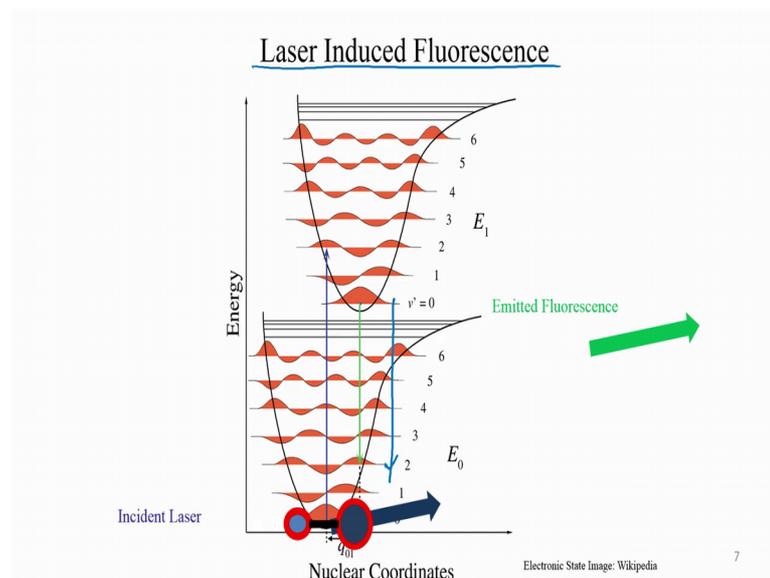
And then goes back to the ground state the original vibrational state, because of inter system crossing in the lower electronic state. But while crossing this while going down from the higher electronic state to the lower electronic state it essentially emitted the photon because of the energy difference and this photon is emitted is essentially the fluorescence that we can collect. And using that that we can the number of photons collected we can correlate it essentially to the mole fraction of OH radicals that are represent in the in the original state before the light hit the OH molecule.

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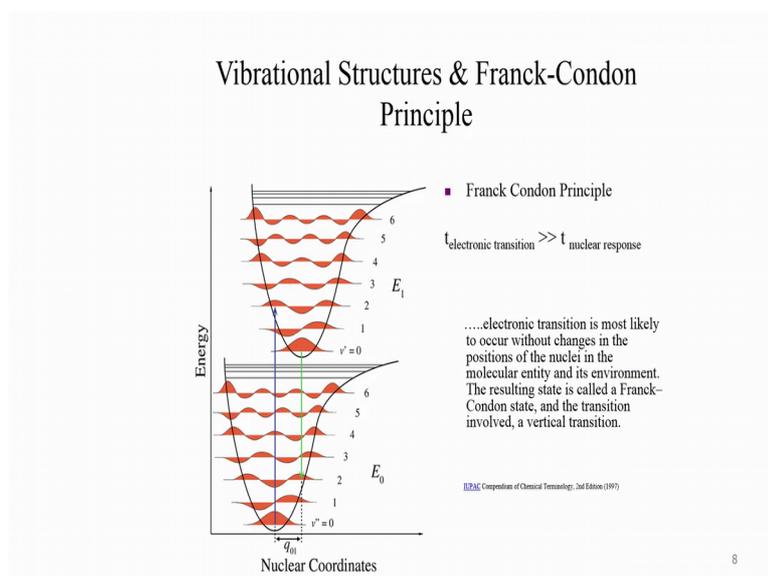
So, this is the essentially the thing that and that we have this ground state. So, the laser which absorbs it is promoted to the higher states and then here some inter system crossing and then it goes down to fluorescence.

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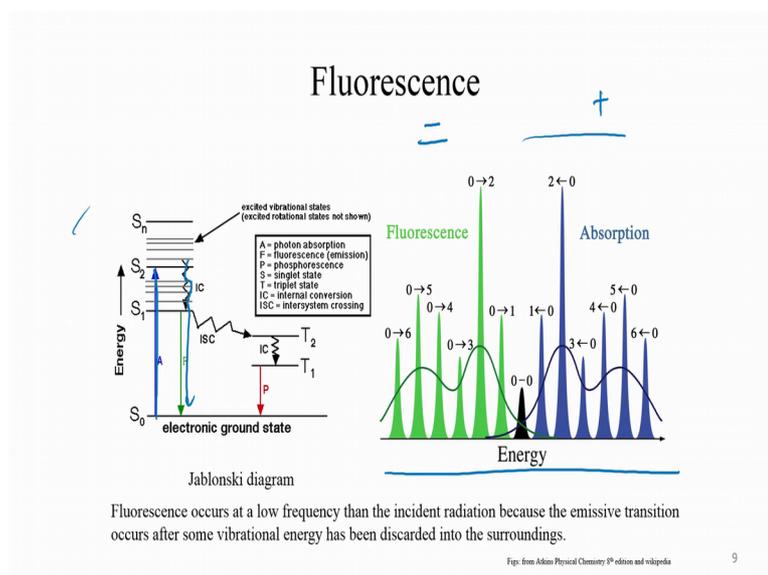
And there can be another thing called phosphorescence, but fluorescence happens much faster fluorescence or phosphorescence happens at much slower rate and that it takes more time. So, it can be easily distinguished. And as such in the energy level you see this is the absorbed energy is always higher then the then the then the fluorescence energy

and as a result if this is blue in color this is the fluorescence can is essentially green in color. But it does not happen typically wavelengths like if you wanted to watch laser induced fluorescence the absorption wavelength is about 283.6 nanometers. And the emission of the fluorescence wavelength is essentially 310 nanometers.

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Here we will address two fundamental questions.

- What governs whether the transition will take place ?
  Based on this we choose the laser wavelength.

- How do we model the emitted fluorescence signal ? $I \propto X_{OH}$
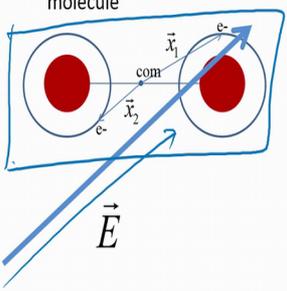 Based on this we interpret the results.

So, it is not that big of a difference it is not like blue and green, but it is slightly higher than the emitted wavelength ok.

Now, here we need to address 2 questions that is what governs whether the transition will take place or not that is how do we choose the laser wavelength. As I said that we if we just shine any light into it we cannot have the fluorescence. And that the second thing is that how do we model the emitted fluorescence signal that is how do we correlate this the intensity of the light to the number density of the mole fraction of OH. So, that is into these things because these are the 2 most important thing considerations and we will take it up in a little bit fundamental manner. So, what essentially happens? So, what is light metal interaction, what happens when a laser light comes and hit is the molecule?
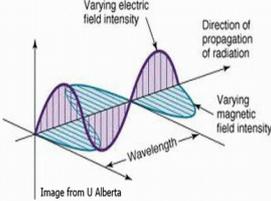
So, suppose this is molecule this is the center of mass these are the is a diatomic molecule.

So, and then a light which is essentially an electromagnetic wave comes and hit is the molecule. So, this electromagnetic wave has a dipole moment associated with it. And that is given by this thing that is a position vector times the charge. And now we since this is the dipole moment of this of the molecule, this is the dipole moment which is an intrinsic property of this molecule. So, that is given by mu is equal to the position vector of the 2 of the 2 atoms, but the center of mass of this where this center of this the electronic clouds around it, and the charge of these this electron clouds. So, that is given by that is the dipole moment. And now consider an electric field which is comes and hit is this molecule and the electric field is given by E vector.

So, the additional potential energy that this molecule gets because of the interaction with the electric field is essentially this guy that is the dot product of this dipole moment vector times the electric field ok.

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Now the electric field of course, as you know is essentially the electromagnetic field has a perpendicularly oscillating magnetic field. And it can be resolved into this. Now what this electronic electromagnetic field does is that it essentially introduces your perturbation on the Schrodinger wave equation that governs this molecule. We will not go into this just to show you briefly that if this is the Schrodinger the time dependent Schrodinger wave equation.

So, it introduces a perturbation on this H 0 which is the normal state and this is H prime is a part of your part of state. And then what we can essentially show that is that there are the wave function thus, thus formed out of this perturbed Schrodinger wave equation ok.

When is the light absorbed and transition to higher electronic state occurs ?

- When the laser photon energy is resonant with the optically allowed transition.

- Solving the previous equation it can be shown that the probability of the transition is given by the transition dipole moment:
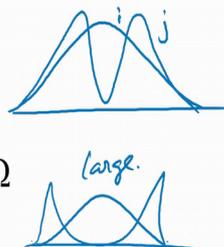
$$\mu_{TR} = \int \psi_i^* \mu \psi_j d\Omega$$

And we can essentially we can do some analysis, and it can be shown that that this light can be absorbed by this molecule when it satisfied certain criteria. So, the whether this light we will be absorbed by this molecule or not that is given by this transitional dipole moment, which is essentially this integral that is given by this complex conjugate of this wave function the dipole moment and then this the wave function integrate over the entire volume of the molecule. And this essentially gives you the probability of the transition.

So, essentially it boils down because this is as i and i j where as this is say for the lower state and this is for the higher state. So, essentially it boils down that if the wave function of the lower state is like this. Then the wave function of the higher state is like this. And if these 2 and they say this is i and this is j and if these 2 wave functions have sufficient overlap then this becomes large. Then this becomes large, but as if this wave functions are like that that if there is a wave function which is like this. So, then the overlap is small then this quantity becomes small and then as a result of that the mu TR that is a transition dipole moment becomes small. So, essentially the transition dipole moment is the probability that are whether the transition can happen.

So, when the wave functions of the ground state of the lower state and the upper state are matching, I can overlap and significantly then this transition dipole moment is a large value. And that tells that the absorption can happen. So, essentially it depends. So, that

that essentially governs whether the whether the light we will be absorbed by the OH molecule not.

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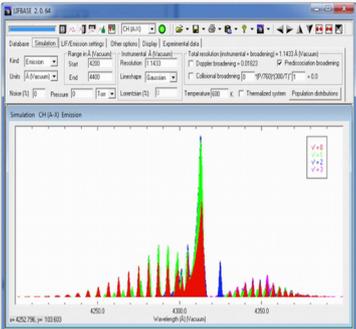
So, but essentially we do not when we do experiments we do not need to calculate this transitions dipole moment anytime or every time. We have the software is called lifbase etcetera, from which we can see that where the laser light can be absorbed and emitted. So, from that we essentially get the reference that for use a (Refer Time: 07:04) from that for OH LIF laser induced fluorescence you select, you need to select laser wavelength of say 283.6 nanometers.

So, this is typically that the idea whether a reasons why this wavelengths are chosen there can be other wavelengths also which can be chosen around this. And there are typically other considerations that this wavelength should not be temperature sensitive if you are only interested in measuring the concentration or if you want to use temperature to temperature measurements using LIF OH LIF, techniques then you have to do some other wavelength so on and so forth. We will not go into that the next question is that, but essentially what I want to tell you is that that way that the light we will be absorbed by OH is a very important thing. Because if there is no absorption then there is no fluorescence, in fundamentally the absorption is essentially guided by this quantity that is a transition dipole moment.

How do we model the emitted
fluorescence signal ?
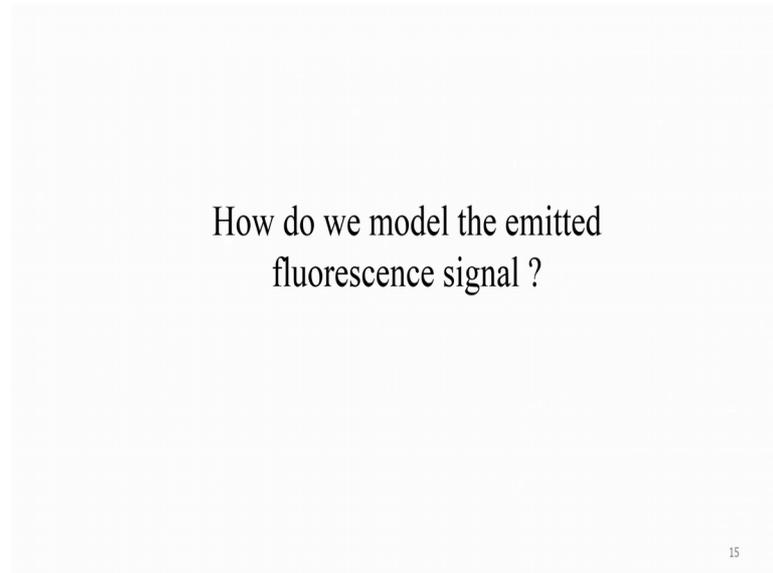
But in practice we find out that particular wavelength from the different softwares which is already contains this analysis is documented.

Then the question is that suppose we now are in a position to choose a particular laser and a particular wavelength of that light, but now then after we get the signal suppose we get a strong signal in some region suppose we get a weak signal in some region. Now using that is the strength of the signal that suppose here we get an intensity of like 200 counts in some place we get the intensity of like 210 counts by using the 200 count how I you can we tell what is the mole fraction. How can we tell that the 200 counts comes constant to a mole fraction of point 2? Or corresponds to a mole fraction of 0.6? So, that is a essentially we need to model the emitted fluorescence signal.

So, single photon laser induced fluorescence once again is a simplified model.

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Single photon laser induced fluorescence species concentration detection: model

Formal rate equation governing the time dependent population: $n_j(t)$ [cm^{-3}] of a specific energy level among a set of levels i, is given by

$$\frac{dn_j(t)}{dt} = \sum_{i \neq j} n_i(t) R_{ij} - \sum_{i \neq j} n_j(t) R_{ji}$$
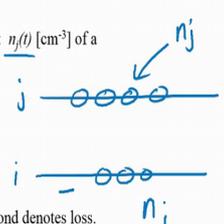
First summation denotes events which populate j while the second denotes loss.

The total rate coefficient for all events transferring molecules from level i to j is R_{ij} [s^{-1}]

Hanson, Seitzman, Paul, APL B 1990

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This is done by this considering this too this small this by this formal rate equation governing the time dependent population that is this n j is essentially the population density of this number of molecules. At the among a set of levels i, it is a essentially the population at this level j. We among a given this is the essentially the this essentially the of the species j among a different levels i. So, the number of population density of the species j and i given level is sorry, this is n j is essentially the population of given species in the level j among different levels i. So, I is essentially the counter which goes I goes from 1 to n. So, can also j.

So, this is the population so this is j and this is i. So, we have several populations of j here and several pollutions of i here. So, this is essentially n j and this is essentially n i. And this there can be like multiple sub search so the rate of change of population of this OH. So, this is the higher state this is the lower state. So, the rate of change of population of this number density of molecules in the level j is essentially given by the number of the by the by the addition into that level. By the by the addition in the level which populate j, and this is the by the last which basically d popular j ok.

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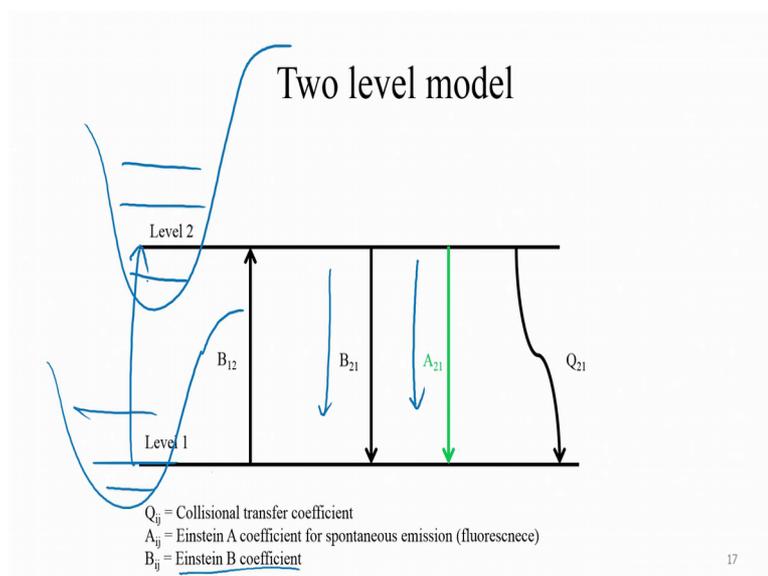
And these are essentially the rate concepts by which this molecule from i to j is transferred in a. So, this is a complicated model, but in a just in a 2 level model, we can show that this is this is the one level this is 2 level. So, and these are the different constants whereas, this B constants B 1 2 is essentially in Einstein B constant is the is the absorption coefficient, this is the emission coefficient and this is the spontaneous emission coefficient which is corresponds to the fluorescence A 2 1 ok.

1 2 means the absorption coefficient for going from state one to state 2. And so, this is this is can be corresponds to this level that we had shown before right that these are the different states like this. So, this is the lower level this is the higher level. So, the OH essentially is going from this level to this level and it is essentially coming down. So, that is what is what you want to show here briefly. And you can also I mean if you are interested you should look into this paper by Hanson Saltzman Paul, who essentially brought made the first a planar laser induced fluorescence measurements. So, this is this in this 2 level model we have from level 1 to level 2 B 1 2 is the Einstein B coefficient A 2 1 is the Einstein a coefficient for spontaneous emission and q are 2 1 i j or q 2 1 is the collision transfer coefficient.

Now, as you see that in OH when it goes to excited state it has a lot of energy kinetic energy. It is can collide with surrounding molecules like nitrogen molecules oxygen molecules and it can lose some energy also. So, that also needs to be quantified and

assess this collision becomes very, very important in high pressure environments collision loss So that essentially changes the wavelength because you see. If you come down to because if you collide very heavily in a higher energy state you we will essentially lose a lot of energy and it you will come down to a lower vibrational state. So, the since a wavelength the emission wavelength etcetera or the intensity can also change because of that.

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$$\frac{dn_2(t)}{dt} = n_1(t)[Q_{12} + B_{12}I_\nu] - n_2(t)[Q_{21} + B_{21}I_\nu + A_{21}]$$

I_ν is the laser spectral intensity: W cm^{-2} Hz^{-1}

Before the laser pulse level 2 has negligible population hence $n_2(t=0) = 0$

Note: Total population is conserved. Hence,

$$n_1(t) + n_2(t) = \text{constant} = n_1^0 = n_1(t=0)$$

$$I \sim f(n_1^0)$$

We can solve these two equations to get:

So, now this can be simplified into this that you can find out what is the rate of change of the population density in the second state. And that is given by this supply from the first state this is and this is the reduction from the second state.

So, it is like a like this that like this control volume analysis. So, rate of change of mass inside the control volume is equal to the influx minus out flux. So, that is equal to the number the rate of change and the rate of change of the mass in the in the control volume is equal to the influx minus out flux. So, exactly this is the same that is the rate of change of the number density of particles at the level 2 is essentially the influx from state 1 and out flux from state 2.

Now, before the laser we can say that that before the laser pulse that is before the laser pulse, I said this OH molecules. The level 2 has a negligible population and n 2 at t equal to 0 is 0. So, that is fine and also the number of because the number of particles or the numbers of molecules are conserved just like mass. So, the n 1 plus n 2 is equal to

constant and that is equal to n 1/ 0 which is equal to n 1 at time t equal to 0. So, n 1 0 means this thing n 1 at time t equal to 0 that is. So, n 1 essentially means that if this was the ground state and this is the upper excited state. So, n 1 is the number of populations at equal to 0. And this is a very important thing because this is what we want to measure, we are not interested in measuring n 2 or n 1 at other times. We want to measure what is the concentration by collecting the light we want to measure what is the concentration or the number density of molecules, before the laser hit the molecular.

So, this is what we want to measure. And so it can be like this. So, because of the overlap suppose this goes into this state. And this OH goes into this state, and then it will by crossing it will come to this state and it will go to this. So, this is my fluorescence. So, then we need to essentially find out the intensity of the light collected as a function we want to find intensity as a function of n 1 0, that is this guy which is equal to n 1 at time t equal to 0. So, how do we do that?

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$$n_2(t) = n_1^0(t)\left[Q_{12} + B_{12}I_\nu\right]\tau\left[1 - e^{-t/\tau}\right]$$

$$\tau = \left[Q_{12} + B_{12}I_\nu + (g_1/g_2)B_{12}I_\nu + Q_{21} + A_{21}\right]^{-1}$$

when laser pulse width $\gg \tau$

Steady state fluorescnece rate R_p (nos. of photons/cm^3/s]

$$R_p = A_{21}n_0^{ss} = A_{21}n_1^0\left[B_{12}I_\nu + Q_{12}\right]\tau$$

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So, we can essentially i tend 2 in terms of n 1 by using this if we integrate it we can write it like this, in terms of our time constant which is this. And then we can find out ultimately that the steady state fluorescence rate that is the number of photons emitted due to fluorescence per unit volume per unit time is essentially given by this quantity.

So, this is r p is essentially at n 1 0 a to 1 times n 1 times n 1 0 at steady state and this is the thing.

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Hence we get:

$$R_p = n_1^0 B_{12} I_\nu \frac{A_{21}}{A_{21} + Q_{21}} \frac{1}{1 + I_\nu / I_\nu^{sat}}$$

I_ν^{sat} : saturation intensity defined as

$$I_\nu^{sat} = \frac{Q_{12} + A_{21}}{B_{12}(1 + g_1/g_2)}$$

When $I_\nu \ll I_\nu^{sat}$

$$R_p = n_1^0 B_{12} I_\nu \frac{A_{21}}{A_{21} + Q_{21}}$$

$\Rightarrow$ Fluorescence signal is proportional to laser intensity

When $I_\nu \gg I_\nu^{sat}$

$$R_p = n_1^0 \frac{A_{21}}{1 + g_1/g_2}$$

So, what do you see now here we give n 1 0. So, that is what we want. So, then finally, what we can do is that we can do all these things that there can be different situations when we can have saturated fluorescence we can have unsaturated fluorescence. So, anyway saturated fluorescents means when the even after putting light you do not have you have basically saturated the upper state. So, then you do not have any molecules coming into that. So, then the essentially the intensity of light becomes cannot be any proportional to the number of cannot be it is always solution to the number of molecules, but it is a it is a different state it does not corresponds to quenching it is a it is a different set, but affairs, but when what we have is that when the intensity of light is less than the threshold for saturation. We have the rate of fluorescence to be given by this ok.

We have the rate of fluorescence is essentially directly proportional to the number density of particles before it hit the before it hit the laser light before the laser light hit the molecules. This Einstein B coefficient I mu is the laser intensity. So, larger the laser intensity larger is a rate of fluorescence. And then this Einstein a coefficient and this quenching factor. But when I nu is greater than I nu sat that is then you see that it does not depend on the laser light anymore. So, putting in more laser light does not change your fluorescence output and it is given by this thing. Also you see that there is no quenching.

So, finally, what we can find is that that the number of photons hitting the photo detector that is what is of most importance. So, that is a little bit a of a complicated there is a little bit of a complicated formula that we get so, but this is if you do the entire analysis this is what we find that the number of photons number of fluorescence photon hitting the photo detector. Because that we will corresponds to my intensity count in my camera. There is a transmission efficiency there is a collection solid angle, there is a fractional population of the lower laser couple state, and then this is the most important thing.

Let me highlight this in red. This is what we are after that is you see that N p there is a number of photons is directly proportional to the mole fraction of the absorbing species. Of course, it depends on the gas number density volume Einstein B coefficient and spectral fluence of the laser etcetera, and these other coefficients you see quenching is also important quenching is also present, but ultimately when all the other factors are constant which we need to somehow calibrate. So, calibration in to create quantitative fluorescence calibration is a very important exercise. But the thing is that at the end if we do that your N p that is the number of photons number of fluorescence photons hitting the photo detector is proportional to the mole fraction of the absorbing species.

So, if you are doing OH belief then the number of photons hitting it is essentially proportional to x mole fraction for OH. And as you see the mole fraction is extremely important we can convert to instructions or etcetera also, but mole fraction is a very, very

important measurement that we need to do in combustion. So, that will tell you where the reaction is proceeding in what to what degree. So, using this we see that we can essentially find out that using laser induced fluorescence the number of photons fluorescence photons that are hitting the photo detectors. So, which we will appear as a strong intensity or low weak intensity is directly proportional to the mole fraction of ox. So, this is the bottom line from this exercise.

So, on one hand we choose the wavelength by using by fundamentally depends on the transition dipole moment, but as such it depends on the it depends on the we can find that out from the LIF base, but essentially you see that the number of photons or the fluorescence intensity that we collect in the camera is essentially proportion of the mole fraction of OH.

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Quenching

Consider $A_{21}/(A_{21}+Q_{21})$: Fluorescence Efficiency, $\sim A_{21}/Q_{21} \ll 1$

1. By diminishing the fluorescence signal Q affects species detectivity
2. Any ambiguity of the precise magnitude of Q is carried over linearly and directly affects the accuracy of measurement.

One approach to calculate quenching rate is

Where n = total number density of mixture $\quad Q_{21} = n\sigma\langle v \rangle$
$\quad\quad\quad\sigma$ = mixture averaged quenching cross section
$\quad\quad\quad$<v> = mean molecular speed.

So, quenching directions is to be done when the pressure is high, but I will not go into that anyways.

Simplifying

If σ = constant

$$Q_{21} = n\sigma\langle v \rangle \sim nT^{1/2}$$

Fluorescence signal (photons/pixel) N_p is given by

$$N_p = const. f_1(T)\chi_m n\left[1/\left(nT^{1/2}\right)\right]$$

$$\Rightarrow N_p = const.\chi_m\left[f_1(T)/T^{1/2}\right]$$

An appropriate transition could be chosen such that the temperature dependence of N_p is minimized then:

$$N_p = const.\chi_m$$

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And So, what we find here is that this N p there is a number of photons hitting the it detector is proportional to mole fraction as such the stronger the intensity the stronger in the population of the absorbing species.

So, this is very important because you see that that OH absorbs 283 nanometers. So, you see you have we have not talked about one point, one beauty about this method is that, that in combustion reactions when you have you can have thousands and thousands of species. So, we want to measure one particular species out of the thousand OH, because of this very beautiful fact that only OH absorbs at 283 nanometers. OH molecule and this the lays and this light has a such a beautiful coupling of 283 nanometers that out of the thousand we can only absorb only ensure that OH is being is absorbing this light and nothing else, and from that if we can find out the number of fluorescence photons and that is by correcting the light from a camera we can find out the concentration of OH.

So, even in this soup of species we can find out the color OH this thing of OH. Of course, it is not that simple it depends this light depends on other factors and population of other molecules also, but to the most extent to the to the to the order one it depends on the population of OH if you choose 283 nanometers, and essentially we can find out the concentration of OH in a soup of other molecules. But if you want to do quantitative floral laser in this row since then it is not straightforward one needs to be one needs do series of calibrations and needs to have a idea about what kind of other molecules are

present. But typically qualitatively we can find out that the higher the fluorescence intensity higher is the mole fraction of that molecule at that region.

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You will you will even be able to appreciate this when we give you examples, and using this laser induced fluorescence we will try to see how we can solve phenomena of practical interest. So, how what do we need to do what do we need for doing PLIF or this laser induced this is this stands for planar laser. So, for that we first need Nd-YAG glazier which is a pump laser and then we did a doubling crystal dye laser with the doubling crystal.

So, the Nd-YAG glazier essentially pumps this dye laser and this bad dye laser gives a wavelength that say 2 which you can be tuned to 283 nanometers you need a camera to detect the photon. And you need an intensifier because in density it is too small and also you need to get it So that you can you do not collect other emissions you only collect the fluorescence emission in a very short amount of time. And of course, you need optics and calibration necessaries and you need some image frozen also.
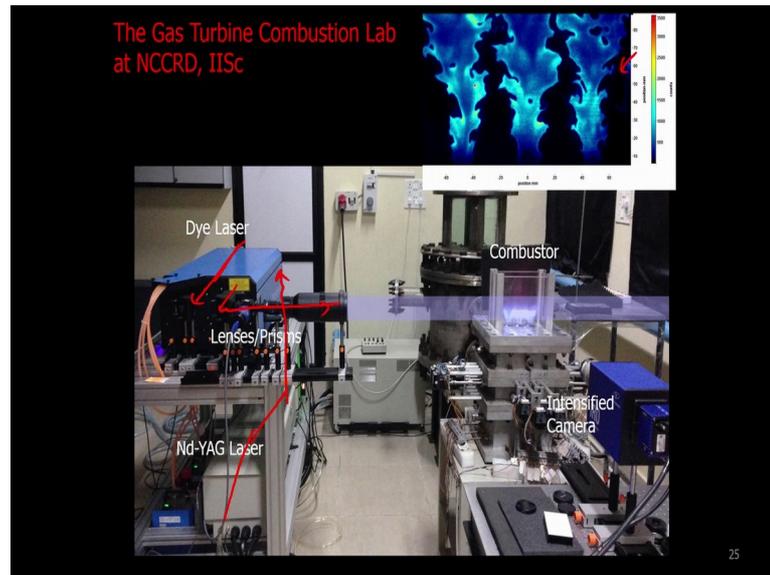
So, this is the facility that we have at ISC at the gas turbine combustion lab. So, this is our dye laser. And so, this is our Nd-YAG laser which pumps that dye laser through this fiber optics and mirrors and then this dye laser sends out this light. So, dye laser light comes out here and then this passes to the sheet making optics which makes a sheet, and we have essentially a model gas turbine combustor here and we shine light on that and what we get is something like this. So, you see that you see this we will see this is a turbulent flame. So, that is why you have a distorted frame structure it is essentially this setup represents a sector of a of a gas turbine combustor, but at lower pressure. So, you see clearly that by this laser induced fluorescence we are clearly able to find out which are the flame locations.

So, for example, we can easily find out using image processing these the flame locations is something like this, because that is where OH goes rises up sharply. So, and also we can find out that why you we can find try to find out why this reaction is happening at a at a first at a at a at a why the reaction is why OH production is strong at certain regions and the OH production is less than certain regions. So, this is the typical PLIF signal that you get. Of course, here we combine with something like was called particle image velocimetry of velocimetry also, because as I said that in combustion 2 things are important kinetics and fluid mechanics. So, from this everybody PLIF you can quantify the intermediate concentrations to first order.

Now we need to understand the flow field, and for that we need to do the particle image velocimetry, which we will be taken up in the next class.

Thank you.