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Lecture - 21 Band models

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In the last lecture we were talking about concept of band absorptance. We defined band absorptance A B as integral over the band of the absorptivity within the band and this has to be integral over the band. We pointed out, that the band absorptance is a function of the partial pressure of the absorbing gas times the, length scale, line section parameter and the gas temperature. This is called the pressure path length. This is the line width by line spacing, this is called the line structure parameter and is gas temperature.

This quantity the band absorptance data is available for many important gases of relevance to engineering like carbon dioxide, water vapor, carbon monoxide and so on. The information for this, as value over each band of a gas, if we take carbon dioxide, we will have data for the 4.3 micron band the 2.7 micron band and so on.

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In the last class, in the last lecture we had shown how we can evaluate emissivity in absorbed gas based on the absorption, we define emissivity, the traditional definition which we were already used for solid surfaces. We said that we integrate over all the bands, of the gas and, so this will be nothing but, the value of the black body emissive power, at the center of the band, band center divided by, the temperature, and then in the height band property depending, on the path length of the gas, the line structure parameter or the ith band and temperature.

This quantity is what is available for gases like carbon dioxide, water vapor and so on. We also argued that for absorptivity the same definition would valid, but the different between absorptivity and emissivity will be really, in how do you weighting. We weight with the bands center again, but we weight with the temperature of the source from where the radiation is coming for example, the source is sun, we will have to look at suns black body temperature and then, this part is same this part is a gas property.

The key point we made was that, emissivity was a function of path length, beta i and temperature, while absorptivity was a function of path length, lines as a parameter, gas temperature and the source temperature. It is similar to what we discussed in the case of solid surfaces, that the emissivity depends on the temperature surface, well absorbed depends both on the surface temperature and the temperature of radiation from where, the source of radiation coming.

The same thing is valid for gases, flexible gases are two additional parameter defined the gas, one is the amount gas along the path and the nature of the structure of this quantity, called the lines structure parameter whether, the lines in the where the been rotation band of the gas, are very, very closely spaced and there are overlapping so that it doesn't play any role or the lines are very far apart and they can be treated independently. Now, it will be good to know how, we deal with this situation, in limiting cases to understand the nature of the band absorptance.

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For example, we defined the band absorptance, as integral over the band or 1 minus e to the power of minus a omega 1 d omega. Let us consider simple case, where a omega 1 is much, much less than 1 what we would call as, optically thin because there is very little gas and the absorption is very small. We approximate e to the power of minus omega 1 as 1 minus a omega 1 because, the value is small.

This becomes nothing, but delta omega a omega d omega into l and normally, the way this has written down in terms of length scale, the gas but, now practices to define an absorption coefficient. This quantity omega l d omega can be written in terms of integral a omega by rho, the density of the absorbing gas into rho a L into d omega. This is the mass absorption coefficient which define earlier, this is called the path length. Now, this path length will have units of kg per square meter.

The amount of matter along a path called u. We can be either rho a L or sometimes this also terms of path length p a L and related through the ideal gas law. Finally, we write A B has rho

I we call it has u, take it out it's not a function omega and then we write integral over of a omega d omega This is strength, we can call it as the band intensity called S. In the simple limit, in the linear limit, we can see that the band absorptance is nothing, but band intensity multiplied by the path length and, so this is the useful result.

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The next thing we can will take an example, in which for simplicity let's assume the band consists of one line for time being and we know that, the absorption coefficient of that line can be written in terms of intensity of jth line, times the b which is the line with. This is the Lorentz line. So, imagine we have single, Lorentz line we want to integral find out what is the absorptance single Lorentz line.

Then A B for a single Lorentz line, we call it a write down this is not the band. This is only a line, absorbed in single line it will be nothing, but this over omega 1 minus e to the power of minus s for time being because, pi b omega minus omega 0 square plus b square into u where we use the path length. Now, suppose line width is very small, the line width of this line happens to be very, very small that is in the most of the integration, we believe that this must be greater than b square.

Then we neglect this term, it does not contribute much then this integration can be performed very easily. We get a following result which is A is equal to 2 square root of b u. This is known as the, square root limit. The single line in the band and the line which is very, very

small, then we get a result, which shows that, so the condition for this is s u by b pi b is much, much greater than 1.

Under the this condition, we have the square root limit and, so this is the user information to have, that it can be in the linear limit if the path length is very, very small or if the line with is very small, then it can be in the square root limit and water vapor typically, shows the behavior which is equivalent to a square root limit. This information is useful, to determine how you will pick data from experimental they are available, how they can be fitted for the actual situation. Now, the next step we want to do is to go a little more ambitious and look at more than one line.

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This is called Elsasser band model. In Elsasser band model the aim was to ask, if there are large number of identical lines.

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In the spectral just show an example of an. Let us go back to our basics now, we saw that absorption gases is individual lines in the wave rotation band, by this lines can be broadened because, of collusions or because, of Doppler broadening. Hence, the calculation of absorption in gases is very much in demand that we should know the nature of the line structure, we need to know whether the lines are very far apart or the lines are strongly overlapping. These things play a very important role, in the calculation of the absorption of the gases.

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Now, we just considered a single line which because, of the collusions, underwent broadening and the width was here, alpha 1 to nu 0, the center of the line. This with the line, depends linearly, linearly on the pressure, total pressure the gas which determines, how many collusions there are. It also depends on temperature because, that determines in some sense the density of the gas also.

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It depends inversely on the square temperature. We can see that, when you deal with gases in very high temperature, the line width can be quite small and when we are dealing with gases at very high total pressure, like inside the diesel engine, then we can have very large line width. The line width can vary a lot depending on whether we are dealing with high pressure radiation transfer or a low pressure, high temperature, radiant transfer.



Now, here we show the difference in the line width and the structure of the line, the difference between this one, which is the Doppler broadening which is exponentially decaying which we saw along with Lorentz broadening which is here, which goes downwards one over one plus nu squared, V is a void function, which is a combination of Doppler and Lorentz. void follows essentially the shape of the Doppler broadening in the centre, but as the Doppler broadening effects go down, it takes over and follows the Lorentz broadening shape.

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The simplest module that Elsasser proposed, is having the series of line of identical height, identical spacing. This of course, is somewhat ideal, no real absorption band or gas show this kind of structure, but it is very, very useful and very eliminating to do this analysis because, there is simple and analytical experiment can be obtained.

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We will see later, we will look at lines which are equally spaced, but real world will of course, is somewhat different real world we will have, line spacing and height varying a lot. In many complex gases, like water vapor this almost looks random and, so we will use random as statistical models, but the simpler model is usually one using the Elsasser idea because, that mainly illustrates the basic features.

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$$k_{\nu,E} = \sum_{n=-\infty}^{\infty} \frac{S}{\pi} \frac{\alpha_{L}}{(\nu - n\delta)^{2} + \alpha_{L}^{2}}$$
$$k(s) = \frac{S}{\delta} \frac{\sinh \beta}{\cosh \beta - \cos s}$$
where $s = 2\pi \nu/\delta$ and $\beta = 2\pi \alpha_{L}/\delta$

We, look at the absorption coefficient, which is a function of the line intensity, line with and here line spacing is equal, there are end lines along this one and the line width. We are going to vary the line spacing here, this delta is spacing in two lines.

When we integrate this equation, over all n we get this result and the result what is seen is that, the absorption coefficient is function of the line intensity This integrates to sin and cosh functions, hyperbolic and hyperbolic cos and where the function beta is the line structure parameter which is nothing, but line, width by line spacing and of course, the frequency which is now represented in terms of the line spacing. Now, we have to intricate this further, so we will do that part now. (Refer Slide Time: 19:00)



We saw that result which is right now, suppose we want to go further in the derivation We actually want to derive the emissivity of the gas, in Elsasser band, then you have to write this has 1 per pi minus pie to plus pi of one of these lines, e to the power of minus 2 beta x sin hyperbolic and cosh, cos hyperbolic cosh minus cosz d z where, x is nothing but, s into frequency or this case omega by 2 pi line with and beta is nothing, by 2 pi b d this is a line structure parameter, this is a non dimensional frequency this is this is z here.

We have to integrate over frequency. This integration can be done. One can show that from the integration that the, emissivity of the Elsasser band and that is error function, times root pi by 2 s by d. Let me go back this is x this is the path length, this is the line structure, the frequency integration his already done. This in terms of the, length x and in terms of Bessel functions I 0 x and I 1 x. Now, this result is very useful because, we can we can now, although this expression really very complicated and all though this is in many books, it is to look at limiting cases and let us look at what limiting case of the Elsasser.

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The so called weak line that is when the line absorption's path length is very small, than we show that mean emissivity of the gas is 1 minus is minus s x by d or more. This is very simple result very, very close to what you might get for a gray gas. So, they must have 1 minus epsilon d and in the case of strong lines, that is when x is much, much greater than 1 essentially, similar to the optical method we had discussed earlier, this will be simplified to the other function square root of line spacing into and finally, if you have non over lapping line.

These things we can see them in this limit, in thin limit, weak line limit, notice is that, line structure plays no role, but in the strong line limit line structure is very much there, cause we can see b by d is playing role. This can be compared with the result we obtained earlier, the square root function involved here, but has some similarities to square root limit.

Now, if we look at more general analysis, this is the similar analysis in which we use the simple Elsasser band model, but we do a more complicated analyses we look at the conditions of various, situation let us now look at empirical expressions.

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So, empirical expressions for absorptance. Lot of laboratory measures have taken place for gases and band absorptance has been measured in various situations. In the limit when the line width by line spacing, is much greater than 1 and nu is small, as we can expect band absorptance because, linearly as the path length. This is the weak limit for obtain thin limit. On the other hand line with the line spacing so, over lapping lines and path length is much greater than 1 then A by B goes as log u.

These are the two very important limits that are available, in the literature based on actual measurements of band absorption from various gases. In thin limit they behave like, to be product in a graph of A B with u we will find a linear variation at low and are logarithmical. But the main issue is what is happening here, when the u is neither too large or too small. and so, the condition that has been arrived if we define data, as pi b d lines structure per parameter.

Than if u is in a certain limit, between greater than beta and less than 1 over beta, than lot of books suggested that A or B then should vary as the radius 2 root u beta minus beta, this is square root limit, that would typically be somewhere in this region, u is not too small and u is not too large and that is condition by this condition that is given here, where in u is greater than beta, but less than 1 over beta. U is some value that is too large and then the square root limit operates in this case.

Generally people fit the band absorptance with this limit. This is can be widely used and an example now, suppose we want an expression for absorptance which combines both linear and the log.

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View Insert Actions Tools Help H & P / D D 9 C ... 7-1-2-9-" O . Q $A_{B} = A_{0} \ln(1+u)$ $\mu(<1) \quad A_{B} = A_{0} \ln(1+u)$ $\mu(<1) \quad A_{B} = A_{0} \ln(1+u)$ $\ln e \text{ Structure Parameter plays no vice}$ $A_{B} = A_{0} \left[2 \sqrt{u\beta - \beta} \right]$ Combining liken & log Po 6 12 1 1

Combining linear log limit, we can write A B is equal to A 0 to log 1 plus u. Advantage of this expression is for small u, it will go as this and for large u, will go has log u. This quite convenient expression that has been used, but note that line structure parameter plays no role. This may not be that useful in situations where, the line structure is important.

We want to examine cases where, the line structure is important. Then we need to look at examples where, we have to fit the effect of line structure into expression and one example of that, can be provided is there are various complicated models available, but let us just give simple expression for A of B which will take into account the, lines parameter. We saw one example of that already, which is A B. Actually A B is equal to A 0 into this is different from these, there beta play no role. Essentially one must assume that beta is very, very large so that the lines are so over lapping, that the line structure gets smeared out.

But, if we counter gases in line structure is important, than you have to look at expression of this kind and we will consider what are these examples in our attempt to use band absorptance of gases and examples here in this situation. Now, how do we use this concept of band absorptance in real examples. We will take an example now, of radiative equilibrium in which, we consider a gas, which as single vibration rotation band and then, we would like to

be able to, rewrite the radiative heat transfer equation that, we had obtained. We will take an example, that is relevant to combustion application and, so let us see how we rewrite our expression, for radiative flux.

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The basic philosophy of this model is that if A is delta integral over all omega e to the power of a omega L d omega 1 minus e to the power of q r. We can see that d A d u is nothing, but delta omega a omega e minus a omega u d u. If we look at our equation for q r integrate over the entire band, we will have, e b 1 minus e b 2 black body emissive power that is standard.

Then we have used Kernel approximation like we did, in the example for Gaussian gray model same law, but we use, integration 0 to some distance y and we have e to the power of b omega and e to the power of b 1 omega, this is the gas radiation and the radiation of the wall and then integral over the wave number, a omega e to the power of minus 3 by 2 a omega into y minus and by beta 30 by tilde the d by delta can come out here and d omega can be there.

This quantity should be recognize nothing, but d A d u or d A d y in this case. So, with these definition and defining a non dimensional length scale as y by l and non dimensional path a nu s into p maximum path of this s into the length scale by the band with and non dimensional, when absorb this, if use this three definition.

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S P 1 S C C P S C 645 $\begin{aligned} \mathcal{Q}_{\mathbf{R}} &\simeq \left[\mathcal{Q}_{b1} - \mathcal{Q}_{b2} \right] + \frac{3}{2} A_{i} u_{o} \left\{ \int_{b} \left[\mathcal{Q}_{bu}(\vec{s}) - \mathcal{Q}_{bio} \right] \right. \\ &\left. \vec{A}' \left[\frac{3}{2} u_{o}(\vec{s} - \vec{s}) \right] d\vec{s} \right. \\ &\left. - \int_{\vec{s}} \left[\mathcal{Q}_{bo}(\vec{s}) - \mathcal{Q}_{b2b} \right] \vec{A}' \left[\frac{3}{2} u_{o}(\vec{s} - \vec{s}) \right] d\vec{s} \end{aligned}$

Than we can rewrite our expression for q R as e b 1 minus e b 2 plus 3 by 2 A 0 u 0 and to if we put bracket 0 to psi e b omega of psi tilde minus e b 1 omega, than the derivative of the band absorptance prime 3 by 2 u by psi d psi tilde minus derivative from psi to 1 of e b omega of pi tilde minus e b 2 which is a constant and the function of scale and derivative of the band absorptance of psi tilde minus psi is as tilde, which standard integral equation, that we obtain in this case. Now, let us see how this equation can be solved. Now, if we want to solve this equation, let us take it very, very simple example just to illustrate. Suppose, we have a heat source which we have done earlier.

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View Insert Actions Iools Help P 1 0 0 9 C 64% Z-1 000 $-\frac{d^2k}{dy} + \frac{s}{1} = 0$ $\frac{d^2y}{heat} \quad veleased by$ $U_0 >>1 \quad A = A_0 \ln u$ combustP

So minus d q R d y plus the heat source have to be 0. This is heat released by combustion. Then we can rewrite this whole equation, in the last part of that is for u 0 much, much greater than 1 pi minus half if 0 to 1 phi of psi tilde d psi tilde psi minus psi tilde where phi is a non dimensional temperature coefficient. This is very increasing limit for the different large parts of limits, where in we do not see any line structure parameter in your expression. We are merely only seeing the role of the logarithmic log limit because, in the limit as this we know that, the band of the absorbent coefficient as A to the power of 0 log u. So, derivative of the band format is 1 over u and that is what we are essentially getting hear and the solution to this equation, in this limit is a very elegant one which is the only solution which we have which is an analytical.

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Z-1-9-9-» 0 Q Q $\varphi(\xi) = \frac{1}{\pi} \left[\left\{ \left(l + \xi \right) \right\}^{1/2} \right]$ Large 12th leigh limit is not firmular to optically Thick limit P 4.

For non dimensional temperature profile will come out has, 1 upon pi psi into 1 minus psi into square root of that. This is the unusual result, the result where in you got and an analytical solution, to the temperature profile in a gas, having a vibrate rotation band and the limit where the path length is very large, but it is important recognize the large path length limit is not similar to optically thick limit.

Now, this is because, in a non gray gas, even if the path length is very, very large there will always be wave length regions, in which the gas is not going to absorb much radiation. So, radiation will just get through the gas. To illustrate this point we will take one example here, which is that, in this large path length limit, the gas will not completely absorb all the radiation.

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P 1 9 0 1 9 6 000 Prin = 1602 20%. 602 80% NZ Tg = 1500 K TW = 600 K $d_{g} = 0.41 \quad e_{g} = 0.18$ $q_{rag} = 0.41 \quad e_{g} = 0.18$ $q_{rag} = 1 - e^{-\frac{Q_{1}}{Q_{2}}}$ $d_{g} = 1 - e^{-\frac{Q_{1}}{Q_{2}}}$ $d_{g} = 1 - e^{-\frac{Q_{1}}{Q_{2}}}$

From the example we had last class in which we looked at the emissivity and absorptivity carbon dioxide and the good example of the gas, with the total pressure of 1 bar typical of 1 band situation, that is 20 percent carbon dioxide, 80 percent nitrogen, length scale of the order of 5 meters, gas temperature of 1500 Kelvin and the wall temperature of 600 Kelvin and when we did it at the last time, we saw that the absorptivity of the gas was around 0.41 while the emissivity was 0.18.

We can see that, in spite of fairly high temperature and fairly larger scale alpha g epsilon g do not approach one, there are quite small. Hence, neither of this can be thought of us the optical thick limit, in which we saw that in case of gray gas, it implied essentially, the emissivity and absorptivity approaching one. For example if we take gray gas, the emissivity of a gray gas will be 1 minus e to the power of minus a l.

In the thick limit, both alpha g and epsilon g will approach 1. But in real gases, that does not happen and, so that is an example that is, worth remembering. Real gases behave substantially different, from gray gas which is a notion which is, used in our example, but it is worth remembering that, this is not good in the thick limit because, thick limit the grey gas behavior, will not be same as real gases because, real gases to allow variation to be

transmitted. Now, in all the examples done, so far we had relied on empirical data, for band absorptance.

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Now to illustrate that, let us go and look at the problem here. Here we have shown the typical variation of the absorption coefficient in the range 150 to 1510 to 1520 centimeter to the power minus 1 and if highly high pressure, for a carbon dioxide band here we can see that, there are large number of lines here. This is a logarithmic scale. That the absorb coefficient vary anywhere from around 10 to the power of minus 3.001 to 100.

We have huge variation from 0.001 to 100 almost 100,000 is ration between this point and this point. Hence we can see, then when we do those integrals, for radiant calculation, one each extremely high resolutions in the wave number axis, to able to really capture this peak because, we use a very cruder step size here, you will not capture these peaks.

This is a major challenge we face in calculating absorption coefficient of gases, which is that there are large number of lines 100 of them and they go from almost 0 absorption to very high large absorption, varying apart 100,000 in a very short example short scale here and, so in order really capture the absorption lines here, we need extremely high resolution. This is what makes the computation of absorption coefficient or computations in radiative transfer, very complicated because, of this very large fluctuation in absorption coefficient. One way to get around this complexity, is to recognize the fact, that although there is very large fluctuation in absorption coefficient with, frequency of wave number, the actual frequency in which, that line lies is not that critical.

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In order to understand why let us now, go back and illustrate this with our example. We saw that epsilon g it is integral over the frequency of 1 minus e to the power of minus a omega l d omega This a omega is fluctuating by factors of 100,000 and it is multiplied by e b omega at the gas temperature. So, the key thing to understand is, this is slowly varying as function of omega, when compare to this, this function is varying, so we are going to take this, at the center of the line, out of the band and do only the integration and, some over all the band.

We will write this as ith band i equals to 1 n, N band of the gas, if we doing this integration now, it does not matter, where your absorption band is because, this is not varying much we have taken it out therefore, in this integration, the exact location of omega in a wave number place is irrelevant.

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We can go back this one and rearrange this graph.

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$$\mathcal{T}_{\Delta \nu}(u) = \frac{1}{\Delta \nu} \int_{\Delta \nu} \exp(-k_{\nu}u) d\nu = \int_{0}^{\infty} f(k) \exp(-ku) dk$$
$$\mathcal{B}(\mathcal{K}) = \int_{0}^{\mathcal{K}} \mathcal{F}(\mathcal{K}') d\mathcal{K}'$$
$$\mathcal{T}_{\Delta \nu}(u) = \int_{\Delta \nu} \exp(-k_{\nu}u) \frac{d\nu}{\Delta \nu} = \int_{0}^{1} \exp[-k(g)u] dg$$

This is the expression we want to calculate and integrate it in the frequency domain, and integrate over the absorption co efficient domain.

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In present we take one in line and here, ask all this locations where after 10 was round 100 around 10. Then locate bearing is around 1 find the probability in this band, that the absorption coefficient was 20 or 50 or 1 or 10 and once you know that probability.

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$$\mathcal{T}_{\Delta\nu}(u) = \frac{1}{\Delta\nu} \int_{\Delta\nu} \exp(-k_{\nu}u) d\nu = \int_{0}^{\infty} f(k) \exp(-ku) dk$$
$$\mathcal{B}(\mathcal{K}) = \int_{0}^{\mathcal{K}} f(\mathcal{K}') d\mathcal{K}'$$
$$\mathcal{T}_{\Delta\nu}(u) = \int_{\Delta\nu} \exp(-k_{\nu}u) \frac{d\nu}{\Delta\nu} = \int_{0}^{1} \exp[-k(g)u] dg$$

That is the f of k probability. f of k probability that, absorbed 1 is equal to k and use the path length.

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We will show how it looks like this is now, the same data that we saw earlier, written not in the frequency space, but in the probability of accuracy of that frequency with absorption coefficient equation. In absorption all the wave from 0.001 to 100 years is taken and determined what is the probability that is occurring. What we must notice clearly that, the highest probability is for very low absorption co efficient. So, there are the lot of transparent region in the gas between the lines, and then gradually it comes down to high absorption, but low probability. Notice that this result is very different from this graph.

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This graph was very, noisy things going up and down.

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On the other hand, this integration is very simple to do because, this quantity is very, very smooth except for little thing there.

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But, we can make it look better, if we plot the absorption coefficient as a function of the cumulative probability which is defined.

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$$\mathcal{T}_{\Delta \nu}(u) = \frac{1}{\Delta \nu} \int_{\Delta \nu} \exp(-k_{\nu}u) d\nu = \int_{0}^{\infty} f(k) \exp(-ku) dk$$
$$g(k) = \int_{0}^{k} f(k') dk'$$
$$\mathcal{T}_{\Delta \nu}(u) = \int_{\Delta \nu} \exp(-k_{\nu}u) \frac{d\nu}{\Delta \nu} = \int_{0}^{1} \exp[-k(g)u] dg$$

We can think, but 0 to k f of k d k this is the probability that absorption coefficient lies between 0 and k g of k cumulatively probability.

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So, ultimately what we see is that, all though the real absorption coefficient is very, very complex and, but weighting function of the frequency of wave number, if we do not integrate in the a n number of space, but desirability in the absorption coefficient space which we can do because, in the calculation the emissivity the absorptivity the black body function does not

very much in the within the absorption band, in comparison to the way the absorption coefficient varies.

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If we take out the black body function out of the integral, the remaining integration can be performed in the space of absorption coefficient and even better in terms of the cumulative coefficient. This is the very smooth function. This smooth function is so on for two different pressures low pressure and high pressure. We can see at high pressure absorption is larger to be to be expected.

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$$\mathcal{I}_{\Delta \nu}(u) = \frac{1}{\Delta \nu} \int_{\Delta \nu} \exp\left(-k_{\nu} u\right) d\nu = \int_{0}^{\infty} f(k) \exp\left(-k u\right) dk$$
$$\mathcal{B}(\mathcal{K}) = \int_{0}^{\mathcal{K}} f(\mathcal{K}') d\mathcal{K}'$$
$$\mathcal{I}_{\Delta \nu}(u) = \int_{\Delta \nu} \exp\left(-k_{\nu} u\right) \frac{d\nu}{\Delta \nu} = \int_{0}^{1} \exp\left[-k(g)u\right] dg$$

Now this integration is very trivial to do and that what it is finally done to get the transmittance, you merely integrated the countdown in the space of cumulative absorption coefficient function rather than frequency. This is called the correlated k method.



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This shows, how the real function ultimately is made to look both are low pressure and high pressure, as a very smooth function. This is what has made the computation of absorptivity emissivity very simple and today most of the calculations are done by this method.

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This method is called the correlated k method. So, the correlated k essentially indicates you that, we are collecting to their observation co efficient same value together and re mapping, the absorption coefficient which was originally a function frequency. Now, it is better function absorb coefficient itself and that functions much, much smoother and much easy to calculate and accuracy of this calculation has been compared, with the best calculated in detail line by line, which is very expensive in tedious and they have shown that this method is quite accurate.

So, most of the data available today is in terms of correlated k method. That method is much easy to compute than line by line. But line by line is still reference data because, that is the exact accurate method that we have, but most of the time we are going to use that data obtain to the correlated k method and, so most of the data available to us will be from the correlated k method. We will continue this discussion in the next lecture.