

## 2. Modeling Atmospheric Transmission and Emission

Let us examine the low spectral resolution structure of atmospheric absorption (1-transmission) as indicated in Fig. 1. The absorption path here is the entire atmosphere looking vertically from the ground and from the 11 km altitude level respectively. Notice how the absorption properties change with altitude.

During our discussion of the Radiative Transfer Equation, we found it necessary to define a volume extinction coefficient that is the sum of four terms:

$$\alpha_v = k_v (\text{gases}) + k_v (\text{aerosols}) + \sigma_v (\text{gases}) + \sigma_v (\text{aerosols}) \quad (1)$$

These 4 terms include an absorption coefficient and a scattering coefficient for the gas molecules in the path and separately for the aerosols (particles) in the path. In general, the coefficients associated with aerosols and the scattering coefficient associated with molecules are relatively slowly varying functions of frequency (or wavelength) when compared with molecular absorption coefficients. In this segment of our course, we'll focus our attention on the molecular absorption coefficients and examine methods that have been used to determine the related transmission functions along atmospheric paths over which pressure, temperature and molecular mixing ratios are changing.

Fig. 2 compares measurements and models of transmission as a function of frequency (wavenumber) over a horizontal sea level path 5.12 km long. Most of the actual molecular absorption structure can be seen in these plots. (Compare Fig. 2 with Fig. 1).

### a. HITRAN (HIgh resolution atmospheric TRANsmission)

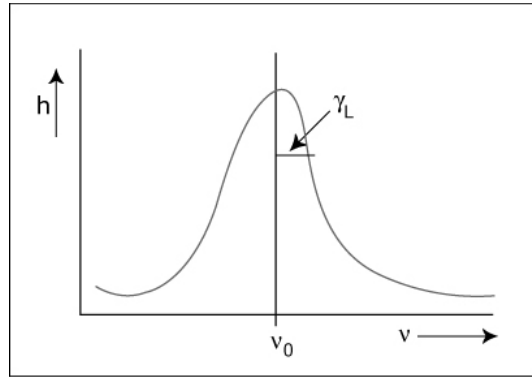
Vibration-rotation transitions (and pure rotational transitions) of molecules will lead to absorption "lines" associated with transitions between specific energy levels of the molecule (See Fig. 3). Collisions modify the energy levels of individual molecules so that there is a distribution of energy levels, effectively smearing out the "line" structure of absorption as shown in Fig. 3. We will refer to these features as "lines", however.

Let us consider an individual spectral line associated with molecules located in the lower portion of the atmosphere (pressures higher than about 10 mb). The Lorentz, pressure-broadened line shape is given by:

$$k_v^i = \frac{S^i(T) \gamma_L^i(P, T)}{\pi \left[ (v^i - v_0^i)^2 + \gamma^{iL}(P, T) \right]} \quad (2)$$

where  $S^i(T)$  = Line Strength,  $\gamma_L^i$  = Line half-width  
 $v^i$  = Line center frequency

$$\text{and } S^i = \int_0^\infty k_v^i dv$$



We also have that the line strength is given by:

$$S(T) = S(T_0) \left( \frac{T_0}{T} \right)^n \exp \left[ - \frac{hcE''}{k} \left( \frac{T_0 - T}{T_0 T} \right) \right] \quad (3)$$

Rotational partition function:  $n = 1$  for linear molecules

$n = 3/2$  for tri-atomic non-linear molecules

where  $E''$  = Energy of the lower state of the transition and  $T_0$  is a standard temperature at which  $S(T_0)$  is measured and

$$\gamma_L^i = \gamma_{L0}^i \frac{P}{P_0} \sqrt{\frac{T_0}{T}}$$

We have used the Boltzmann relation to describe the number of molecules in the lower state of the transition.

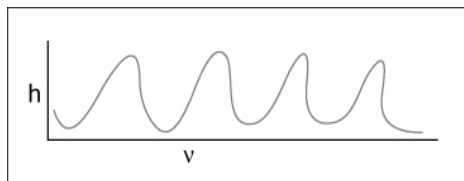
$$N_i = \frac{N e^{-hcE''/kT}}{Q_v Q_r}$$

And the line strength is proportional to this number density.

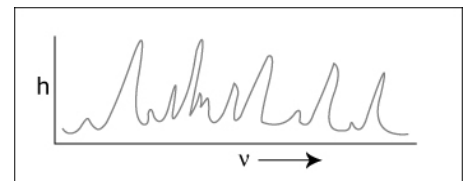
$$S \propto N_i$$

Prior to about 1970, it was recognized that the important atmospheric gases (e.g.,  $H_2O$ ,  $CO_2$ ,  $O_3$ ) had several series of spectral lines that could be modeled as being

either regular



or random



over appropriate spectral intervals. Furthermore, most field instruments for radiation measurements were inadequate to measure the actual spectral structure anyway.

Therefore, "band models" were developed to represent the average transmission (and absorption) over limited spectral regions. This led to the development of LOWTRAN and MODTRAN which we'll discuss later.

By 1970, experimental spectroscopy was improving and it was recognized that a combination of theory and experiment provided the opportunity to identify the spectral parameters of atmospheric molecules and molecules and thereby simplify the computation of atmospheric transmission. Improvement in the speed and memory of computers also encouraged such a concept.

From Eqs. 2 & 3, we can see that if we define the  $\nu^i, S^i, \gamma^i, E''^i$  for each of several spectral lines in the interval,  $\Delta\nu$ , we can compute the average transmission (or absorption) over the interval without the need for a spectral model. (However, we do also require a knowledge of the atmospheric temperature, pressure and molecular abundance.) We then have:

$$\tau_\nu = \exp\left[-k_\nu^i m_j\right] \text{ for a single line of molecule (j) at frequency } \nu.$$

$$\tau_\nu = \exp\left[-\sum_j \sum_i k_\nu^{ji} m_j\right]$$

$$\tau_\nu = \exp\left[-\sum_j \left[\int \sum_i k_\nu^{ji} dm_j\right]\right]$$

and, finally:

$$\bar{t}_{Av} = \frac{\int_{\Delta\nu} t_{\nu_0} g(\nu - \nu_0) d\nu}{\int_{\Delta\nu} g(\nu - \nu_0) d\nu}, \text{ where } g \text{ is an instrument shape function.}$$

### **Summary of HITRAN**

1. HITRAN 2000 – over 705,000 lines of 38 gases covering the spectral range:

$$0, z < \lambda < \infty \text{ } \mu\text{m} \quad 0 < \nu < 50,000 \text{ cm}^{-1}$$

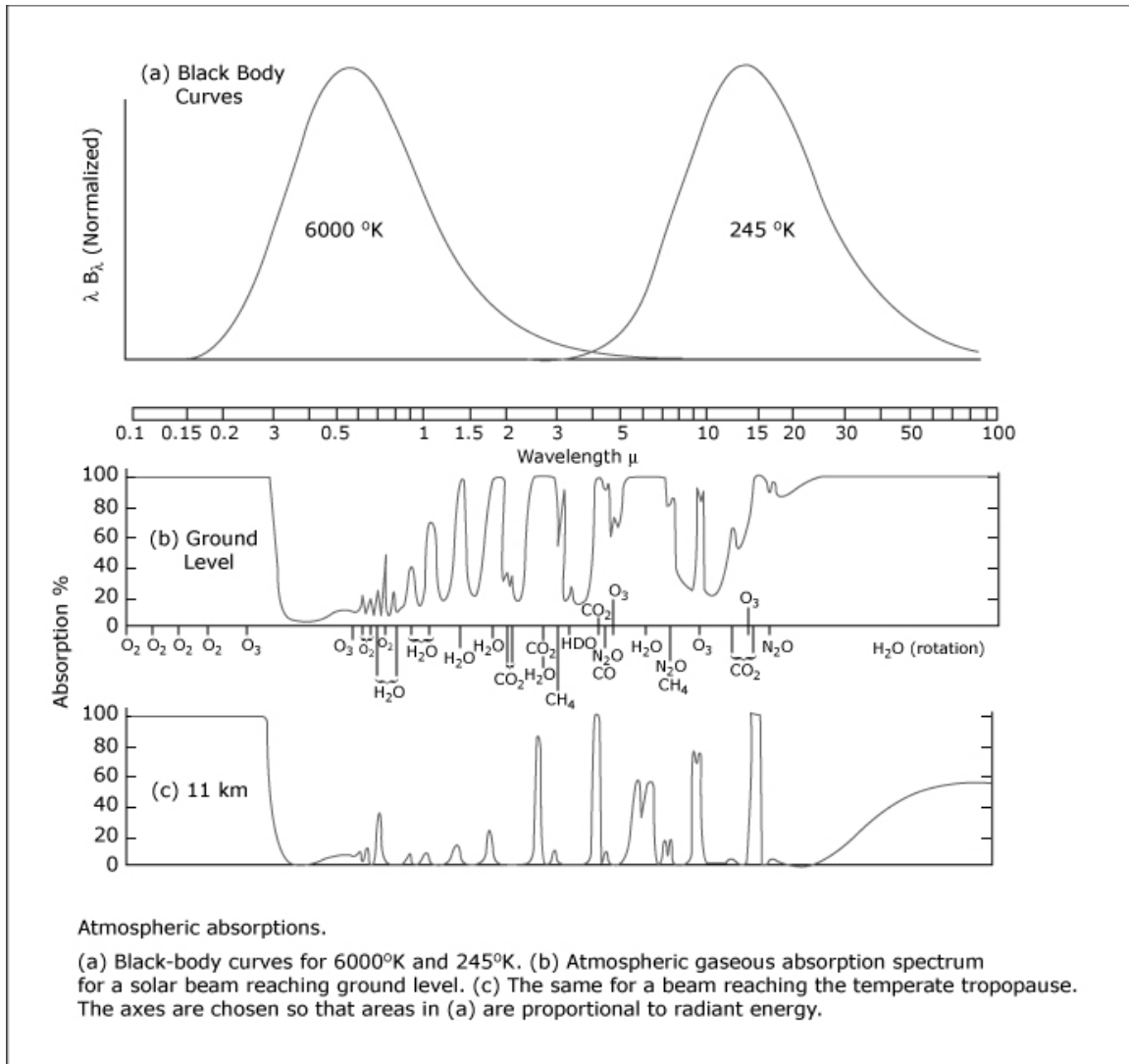
H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, N<sub>2</sub>O, CO, CH<sub>4</sub>O<sub>2</sub>, NO, SO<sub>2</sub>, NO<sub>2</sub>, NH<sub>3</sub>, HNO<sub>3</sub>, OH, HF, HCl, HBr, HI, ClO, OCS, H<sub>2</sub>CO, HOCl, N<sub>2</sub>, HCN, CH<sub>3</sub>Cl, H<sub>2</sub>O<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, PH<sub>3</sub>, COF<sub>2</sub>, SF<sub>6</sub>, H<sub>2</sub>S, HCOOH, HO<sub>2</sub>, O, ClONO<sub>2</sub>, NO<sup>+</sup>, HOBr.

2. HITRAN 2004 contains an even larger number of species and line parameters.
3. Line strengths are proportional to isotopic abundances.
4. Line overlap from individual molecular species.
5. Line overlap from different molecular species.

### **HITRAN Complications**

1. Line wings from outside.
2. Line shape.
3. "Continuum" absorption.
4. Pollutant lines.

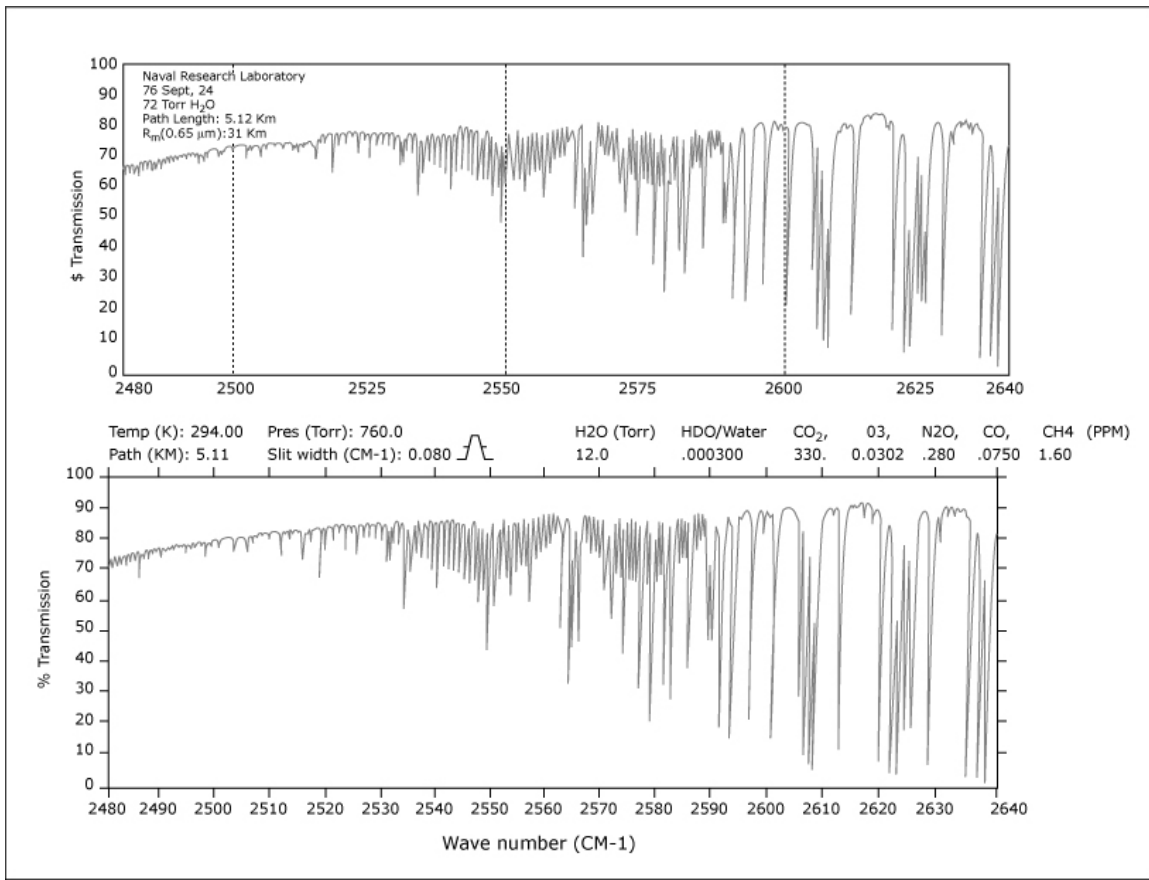
We're now ready to examine the HITRAN exercise labeled "Exercise 2: HITRAN-PC".



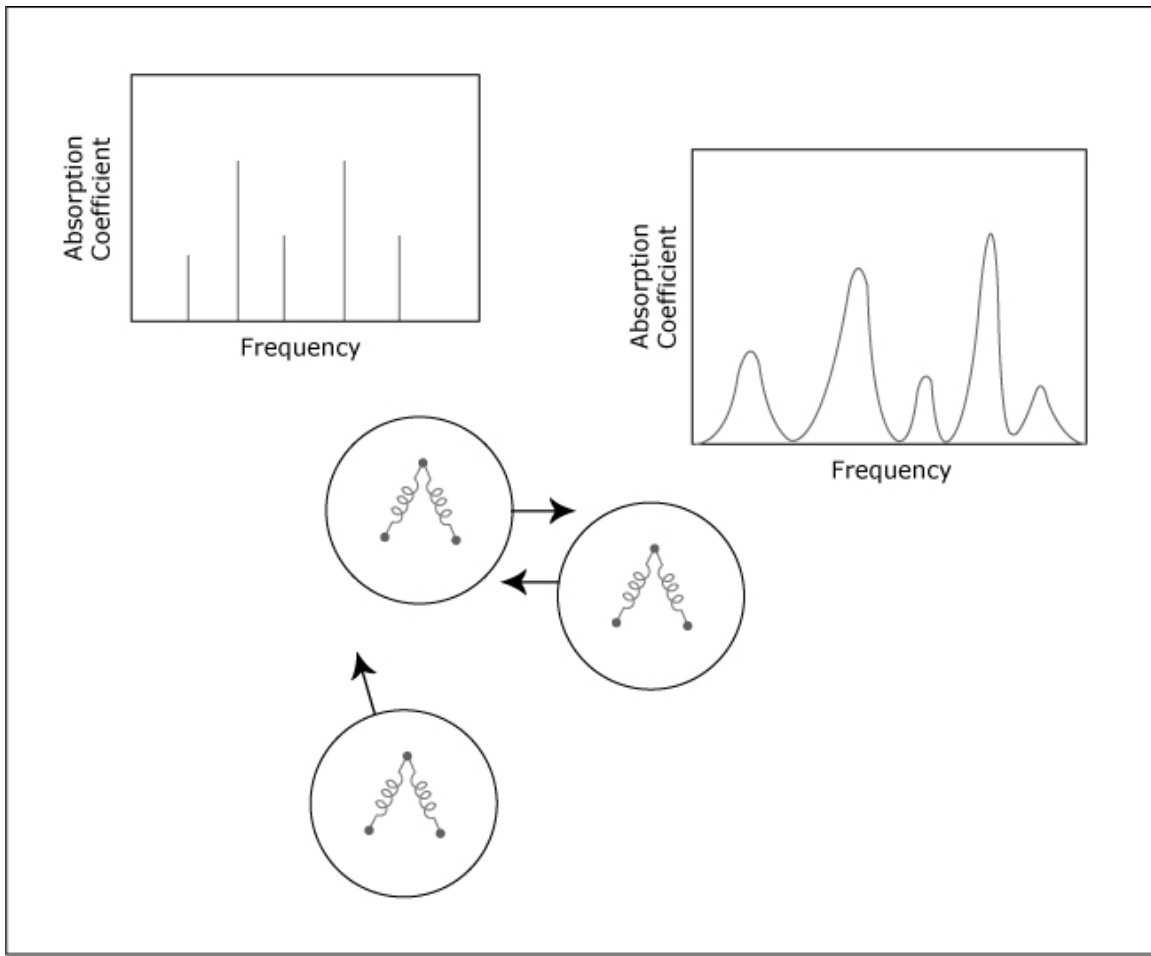
Reference: R.M. Goody, Atmospheric Radiation, Oxford Clarendon Press, 1964, Fig.

1.1

**Fig. 1**



**Fig. 2**



**Fig. 3**

## Atmospheric Radiation (12.815)

### Band Models

#### Scales of frequency

1. Planck function – slow variation with frequency for both Planck function and its derivative.
2. Unresolved band contour – Planck function can be considered constant over most individual absorption/emission bands.
3. Spacing between rotational lines ( $1 - 5 \text{ cm}^{-1}$ ).
4. Monochromatic scale where absorption coefficient can be considered constant ( $2 \times 10^{-2} \text{ cm}^{-1}$  for 1 atmosphere pressure decreasing  $2 \times 10^{-4} \text{ cm}^{-1}$  for Doppler lines above about 30 km).

Line-by-line (or convolved monochromatic) calculations can be done, but remains formidable for practical applications – except for a few reference cases.

Generally we still need to make averages over many spectral lines. Thus, we develop a variety of “band models”.

So – we need to deal with average transmission (and average absorption).

$$\bar{T}_i = \frac{1}{\Delta v_i} \int_i T_v dv \quad (1)$$

where  $\Delta v_i = \int_i dv$  is the width of the  $i^{\text{th}}$  frequency interval and

$T_v = \exp(-\tau_v)$  is the monochromatic transmission.

Because of the slow variation of the Planck function with frequency, we can write the thermal emission in terms of mean transmission as follows:

$$\begin{aligned} I &= \int_0^{\infty} I_v dv = \int_0^{\infty} dv \int_0^{\infty} B_v e^{-\tau} d\tau = \int_0^{\infty} dv \int_0^1 B_v dT_v \\ &\approx \sum \Delta v_i \int_0^1 B_i dT_i \end{aligned} \quad (2)$$

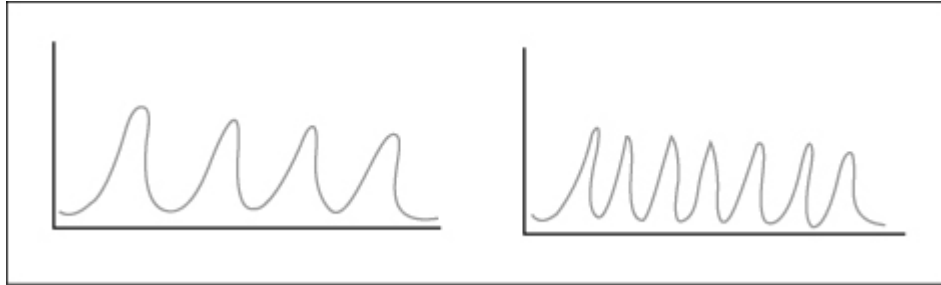
where  $B_i$  is the (almost constant) value of the source function in the  $i^{\text{th}}$  interval.

#### Multiplication Property of Transmission:

If we have 2 sets of un-correlated spectra in a given spectral interval and if the lines of either array are randomly arranged in the interval, the net transmission in the interval can be written as:

$$\bar{T}_v(1,2) = \bar{T}_v(1) \times \bar{T}_v(2) \quad (3)$$

This same property arises for 2 regularly spaced sets of lines in the spectral interval,  $\Delta v_i$ , where the line spacing of the 2 sets of lines are different.



This condition cannot be exact as the spectral interval gets sufficiently small so that it contains too few lines. But, for reasonable-size intervals containing several lines, Eq. 3 is a very good approximation. The physics of molecular spectroscopy suggests that this will be so for any conceivable set of conditions that may occur for atmospheric molecules.

### **Single (Isolated) Line of Lorentz Shape**

Here we will limit the discussion to homogeneous paths (where  $T$ ,  $p$ , and gas mixing ratios are constant along the path).

Monochromatic Absorption:  $A_v = 1 - T_v = 1 - \exp(-k_v m)$  (4)

Integrating over all frequency space, we have:

$$A_v = \frac{1}{\Delta v} \int_{-\infty}^{+\infty} [1 - \exp(-k_v m)] dv \quad (5)$$

where we also define the Equivalent Width as

$$W = A_v Dv = \int_{-\infty}^{+\infty} [1 - \exp(-k_v m)] dv \quad (6)$$

This term refers to the width of a rectangular line whose center is completely absorbed, having the same absorption as the single line under consideration.



Using the Lorentz line profile of Eq. 7 and defining variables,  $x$  &  $y$ :

$$x = S m / 2 \pi \alpha_L \qquad \tan \frac{y}{2} = \frac{(v - v_0)}{\alpha_L}$$

$$k_{\nu_i} = \frac{S \alpha_L}{\pi \left[ (v - \nu_i)^2 + \alpha_L^2 \right]} \qquad (7)$$

$$A_{\nu} = \frac{\alpha_L}{\Delta \nu} \int_{-\pi}^{\pi} \left\{ 1 - \exp \left[ -x (1 + \cos y) \right] \right\} d \left( \tan \frac{y}{2} \right) \qquad (8)$$

Integrating by parts yields:

$$A_{\nu} = \frac{2 \pi \alpha_L}{\Delta \nu} L(x) \qquad (9)$$

with  $L(x) = x e^{-x} \left[ I_0(x) + I_1(x) \right]$  (10)

This function is known as the Ladenburg and Reiche function where  $I_0(x)$  and  $I_1(x)$  are modified Bessel functions defined as follows:

$$I_n(x) = i^{-n} J_n(ix) \text{ and } J_n(x) = \frac{i^{-n}}{\pi} \int_0^{\pi} e^{ix \cos \theta} \cos n\theta \, d\theta \qquad (11)$$

For small  $x$ , the following series expansion is valid:

$$L(x) = x \left[ 1 - \sum_{n=1}^{\infty} (-1)^{n+1} (2n-1)(2n-3) \dots 5.3.1 \cdot \frac{x^n}{n!} (n+1)! \right] \qquad (12)$$

For large  $x$ , there is an asymptotic expansion:

$$L(x) = \left( \frac{2x}{\pi} \right)^{1/2} \left[ 1 - \sum_{n=1}^{\infty} (2x-1)^2 (2n-3)^2 (2n-5)^2 \dots \frac{3^2 \cdot 1^2}{n!} (8x^n) \right] \qquad (13)$$

So – for small  $x$  we have

$$A_{\nu} \approx \frac{2 \pi \alpha_L x}{\Delta \nu} = \frac{S m}{\Delta \nu} \qquad (14)$$

We could have obtained this result directly from Eq. 5 by expanding the exponential:

$$A_{\nu} = \frac{1}{\Delta\nu} \int_{-\infty}^{\infty} k_{\nu} m d\nu = \frac{m}{\Delta\nu} \int_{-\infty}^{\infty} k_{\nu} d\nu = \frac{Sm}{\Delta\nu}$$

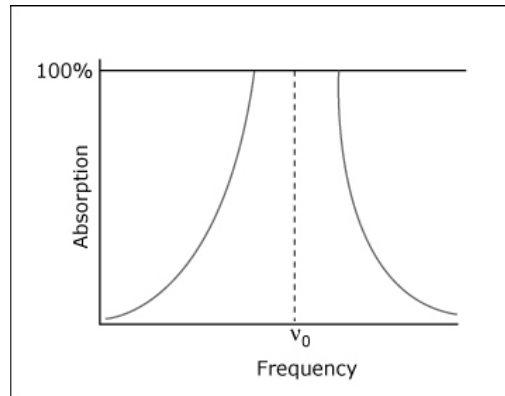
We can see the conditions that need to apply --  $h_{\nu}m \ll 1$  at all frequencies (in particular, at the line center).

For large  $x$ , we have:

$$A_{\nu} = \frac{2\pi\alpha_L}{\Delta\nu} \left(\frac{2x}{\pi}\right)^{1/2} = \frac{2}{\Delta\nu} \sqrt{Sm\alpha_L} \quad (15)$$

Significance of the Strong Line Limit:

The center of the line cannot be further absorbed after 100%, so its only the line wings that can increase the absorption.

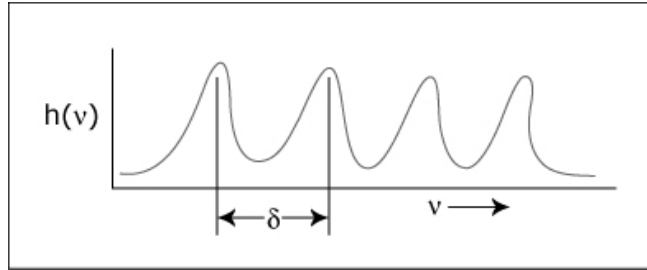


These 2 limits (Eqs. 14 & 15) are useful in the development of approximations for infrared radiative transfer calculations.

### **Regular Band Model (Elsasser Model):**

Several atmospheric molecules demonstrate approximate regular spacing of vibration-rotation absorption lines: e.g. – CO<sub>2</sub>, N<sub>2</sub>O, CO. Let us consider that all line intensities are the same over a limited spectral range. Then, the appropriate absorption coefficient will be:

$$k_{\nu} = \sum_{-\infty}^{\infty} \frac{S \alpha_L / \pi}{(\nu - i\delta)^2 + \alpha_L^2} \quad \text{where } \delta \text{ is the line spacing} \quad (16)$$



Application of Eq. 5 to this absorption coefficient leads to:

$$A_{\nu} = \operatorname{erf}\left(\frac{\sqrt{\pi S \alpha_m}}{\delta}\right) \quad \text{where } \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2} dx \quad (17)$$

$$\text{For small } x, \text{ we have } A_{\nu} = \frac{2x}{\sqrt{\pi}} = \frac{2\sqrt{S \alpha_m}}{\delta} \quad (18)$$

which is similar to the individual, isolated line in the strong line limit. The weak-line limit will be  $A_{\nu} = \frac{S m}{\delta}$

**Random Band Model** (with constant line intensity):

Consider an array of  $N$  identical lines of the same molecular species distributed randomly in frequency between  $-N\delta/2$  and  $+N\delta/2$ . The absorption coefficient is  $\sum_{i=1}^N k_i$  and the resulting transmission is:

$$T = \exp\left(-m \sum_{i=1}^N k_i\right) = \prod_{i=1}^N \exp(-m k_i) \quad (19)$$

The probability that a line lies in  $dv_i$  is  $dv_i/\delta$  and the joint probability that there are lines between  $v_1$  and  $v_1 + dv_1$ ,  $v_2$  and  $v_2 + dv_2$ ,.....  $v_n$  and  $v_n + dv_n$  is  $\prod_{i=1}^N \frac{dv_i}{\delta}$

Considering all possible arrangements of lines, allowing each line to lie anywhere in the range  $\frac{-N\delta}{2}$  to  $\frac{+N\delta}{2}$ , the appropriate average is:

$$\bar{T} = \frac{\prod_{i=1}^N \int_{-N\delta/2}^{+N\delta/2} \frac{dv_i}{\delta} \exp(-m k_i)}{\prod_{i=1}^N \int_{-N\delta/2}^{+N\delta/2} \frac{dv_i}{\delta}} \quad (20)$$

$$\bar{T} = \left[ \frac{1}{N} \int_{-N\delta/2}^{+N\delta/2} \exp(-mk_v) \frac{dv}{\delta} \right]^N = \left( 1 - \frac{1}{N} \right)^{+N\delta/2} \left[ 1 - \exp(-mk_v) \frac{dv}{\delta} \right]^N \quad (21)$$

as  $N \rightarrow \infty$ , we have

$$\bar{T} \rightarrow \exp \left\{ -\frac{1}{\delta} \int_{-\infty}^{+\infty} [1 - \exp(-mk_v)] dv \right\} = \exp \left( -\frac{W}{\delta} \right) \quad (22)$$

or  $\bar{A} = 1 - \exp[-\bar{A}(\text{isolated line})]$  (23)

### **The General Random Model:**

A frequency range contains  $N$  lines, each a single member of a different infinite, random array with equal line intensity and line spacing  $N\delta$ . From Eq. 22, the mean transmission of one of the  $N$  array is:

$$\bar{T}_i = \exp(-W_i/N\delta) \quad (24)$$

The conditions for the multiplication property are met for random arrays so we have the average transmission for all  $N$  arrays as:

$$\bar{T} = \prod_{i=1}^N \bar{T}_i = \exp \left[ -(N\delta)^{-1} \sum_{i=1}^N W_i \right] \quad (25)$$

$$= \exp \left( -\frac{\bar{W}}{\delta} \right) \quad (26)$$

where  $\bar{W}$  is the average equivalent width for the  $N$  lines in the frequency interval.

If we have a list of line intensities, we can compute  $\bar{W}$  for a given spectral interval.

### **The Correlated K-Distribution:**

For a spectral interval containing several spectral lines, the average transmission is independent of the spectral location of the lines, but depends on the absorption coefficients (or line intensities, half-widths) of the lines. The Correlated K-Distribution method for computing radiative transfer takes advantage of this situation by grouping lines according to the absorption coefficient  $k_v$ . This enables us to replace the usual frequency (or wavenumber) integration for the average transmission by an integration over  $k$ -space. If the normalized probability distribution function for  $k_v$  in the interval  $\Delta v$  is given by  $f(k)$  and its minimum and maximum values are  $k_{\min}$  and  $k_{\max}$ , respectively, then the spectral transmission can be expressed by Eq. 27:

$$T_v(m) = \int_{\Delta v} e^{-k_v m} \frac{dv}{\Delta v} = \int_0^{\infty} e^{-km} f(k) dk \quad (27)$$

where we have set  $k_{\min} \rightarrow 0$  and  $k_{\max} \rightarrow \infty$ , for mathematical convenience and where

$$\int_0^{\infty} f(k) dk = 1$$

From Eq. 27, the probability distribution function is the inverse Laplace transform,  $L^{-1}$ , of the spectral transmission such that

$$f(k) = L^{-1}(T_v(m)) \quad (28)$$

If the spectral transmission can be expressed in terms of an analytic exponential function and if the inverse Laplace transform can be performed, then an analytic expression can be derived for the probability distribution function.

We can also define a cumulative probability function as follows:

$$g(k) = \int_0^k f(k) dk \quad (29)$$

where  $g(0) = 0$ ,  $g(k \rightarrow \infty) = 1$  and  $dg(k) = f(k) dk$ . By definition,  $g(k)$  is a monotonically increasing and smooth function in  $k$  space. The spectral transmission can now be written as:

$$T_v(m) = \int_0^1 e^{-k(g)} dg \cong \sum_{j=1}^M e^{-k(g_j)m} \Delta g_j \quad (30)$$

From Eq. 29, since  $g(k)$  is a smooth function in  $k$  space, the inverse will also be true here; that is,  $k(g)$  is a smooth function in  $g$  space. Consequently, the integration in  $g$  space, which replaces the tedious wavenumber integration, can be evaluated by a finite sum of exponential terms as shown in Eq. 30.

### **Non-homogeneous Atmospheres:**

So far, all our band model analyses have homogeneous paths over which temperature, pressure and molecular mixing ratio are constant. In the real world, the decrease of pressure with height, atmospheric temperature profiles and profiles of molecular mixing ratios (such as water vapor) lead to substantial non-uniformity in the vertical and to a lesser extent also in the horizontal.

### **Scaling approximations**

We pose the question: How well can the transmission of a variable atmospheric path be represented by the transmission of a path at constant temperature and pressure?

Since temperature is less important in determining atmospheric transmission than pressure and molecular concentration, it is customary to fix  $T$  by setting it equal to

the average value for the path of integration. If frequency can be separated from pressure and temperature in the monochromatic absorption coefficient, we can define an exact scaling approximation:

$$k_v(P, T) = \Phi(P, T) \eta(v) \quad (31)$$

The optical path then is

$$\begin{aligned} t_v &= \eta(v) \int_{\text{path}} F_v(P, t) dm = F(\bar{P}, \bar{t}) \int_{\text{path}} \frac{\Phi(P, t)}{\Phi(\bar{P}, \bar{t})} dm \\ &= F_v(\bar{P}, \bar{t}) \bar{m} \end{aligned} \quad (32)$$

where  $\bar{m} = \int_{\text{path}} \left[ \Phi(P, t) / \Phi(\bar{P}, \bar{t}) \right] dm$

This would enable us to scale the amount of absorbing gas,  $\mathbf{m}$ , and then calculate the absorption coefficient for the non-homogeneous path as if it were a homogeneous path of absorber amount,  $\bar{m}$ . Unfortunately, the Lorentz profile doesn't even approximately fit the form of Eq. 31 except for strong lines.

However, we have shown that specific expressions are obtained from weak line and strong line absorption (See Eqs. 14 & 15). These same 2 equations can be written for an optical path in a non-homogeneous atmosphere. For weak lines, we obtain:

$$\sum_{i=1}^N S_i(\bar{T}) \bar{m} = \sum_{i=1}^N \int_{\text{path}} S_i(T) dm \quad (34)$$

and if we omit the temperature dependence, we obtain

$$m = \int_{\text{path}} dm \quad (35)$$

For strong lines, we have:

$$\sum_{i=1}^N \left\{ S_i(\bar{T}) \alpha_{L,i}(\bar{T}) (\bar{P}/P_0) m \right\}^{1/2} = \sum_{i=1}^N \left\{ \int_{\text{path}} S_i(T) \alpha_{L,i}(T) (P/P_0) dm \right\}^{1/2} \quad (36)$$

If we omit the temperature dependence, we obtain:  $\bar{m} = \int_{\text{path}} \left( \frac{P}{P_0} \right) dm \quad (37)$

We can write both Eqs. 35 & 36 in the form,

$$\bar{m} = \int_{\text{path}} \left( \frac{P}{P_0} \right)^\beta dm$$

where  $\beta = 0$  for weak lines and  $\beta = 1$  for strong lines.

This is the procedure that was used in the LOWTRAN model in which the parameter,  $\beta$ , was determined empirically from laboratory measurements covering a range of homogeneous conditions covering all atmospheric conditions of interest.

Returning to Eq. 33, we can take both pressure and temperature distributions into account and obtain:

$$\bar{m} = \int_N \frac{\Phi(T)}{\Phi(\bar{T})} dm \quad (38)$$

where  $\Phi(T) = \sum_{i=1}^N S_i(T)$

and we have a 2-parameter scaling law:

$$\bar{m} = \int_{\text{path}} dm \quad (39)$$

$$\bar{P} = \int_{\text{path}} P dm / \bar{m}$$

This is the so-called Curtis-Godson approximation.

### **Non-homogeneous paths and the Correlated-k Technique**

Our correlated-k distribution method has been developed for homogeneous paths. Its application to non-homogeneous paths requires that we evaluate its applicability under conditions where the scaling approximations are valid (and for any other conditions that might be representative of the real atmosphere).

The circumstances under which the Correlated-k technique gives exact results are:

- 1) Whenever the condition identified in Eq. 31 is valid (for Strong Lorentz lines and Doppler lines);
- 2) For weak absorption, regardless of the line shape;
- 3) For an isolated line, for an Elsasser band (regardless of line shape) and certain other line shapes.

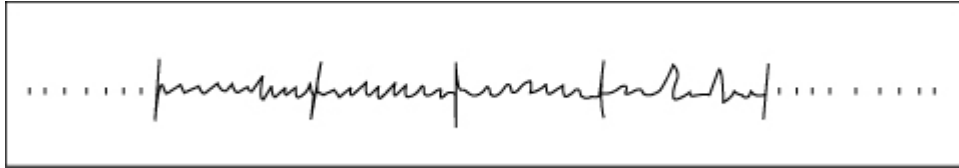
**MODTRAN**

- 3-parameter model.
- Based on HITRAN data.
- Average transmission down to  $2 \text{ cm}^{-1}$  (uses a  $1 \text{ cm}^{-1}$  bin).
- Frequency step =  $1 \text{ cm}^{-1}$

1. Narrow-band models

a) Random Model (Statistical Band Model) – Infinite array of spectral lines with Uniform Statistical Properties.

Statistically similar intervals flank interval of interest.



b) Regular Model (Elsasser Band Model) – An almost regular array of lines overlapped by un-correlated regular arrays.



2. Equivalent Width

a) Single line:  $\bar{A}_{\Delta\nu} = \frac{1}{\Delta\nu} \int_{\Delta\nu} [1 - e^{-k_\nu m}] d\nu$

b) Array of lines:  $\bar{A}_{\Delta\nu} = \frac{1}{\delta} \int_{-\infty}^{+\infty} [1 - e^{-k_\nu m}] d\nu$  where  $\delta$  = mean line spacing

Lets look at Random model in some detail:

Consider array of identical lines with shapes described by absorption coefficient,

Let N lines be distributed randomly between  $\frac{-N\delta}{2}$  and  $\frac{+N\delta}{2}$ . The absorption

coefficient at the center of array is:  $\sum_{i=1}^N k_i$



The transmission is:

$$t_v = \exp\left(-m \sum_{i=1}^N k_i\right) = \prod_{i=1}^N \exp(-mk_i)$$

The probability that a line lies in the interval  $dv_i$  is  $\frac{dv_i}{\delta}$  and the joint probability that there are lines between

$v_1$  and  $v_1 + dv_1$ ,  $v_2$  and  $v_2 + dv_2$ .....and  $v_N$  and  $v_N + dv_N$  is  $\prod_{i=1}^N \frac{dv_i}{\delta}$

Considering all possible arrangements of lines in the range  $\frac{-N\delta}{2}$  to  $\frac{+N\delta}{2}$

the average transmission is:

$$\bar{t} = \frac{\prod_{i=1}^N \int_{-N\delta/2}^{+N\delta/2} \left(\frac{dv_i}{\delta}\right) \exp(-mk_i)}{\prod_{i=1}^N \int_{-N\delta/2}^{+N\delta/2} \left(\frac{dv_i}{\delta}\right)}$$

As integrations are all identical, we have:

$$\begin{aligned} \bar{t} &= \left[ \left(\frac{1}{N}\right) \int_{-N\delta/2}^{+N\delta/2} \exp(-mk_v) \frac{dv}{\delta} \right]^N \\ &= \left\{ 1 - \frac{1}{N} \int_{-N\delta/2}^{+N\delta/2} [1 - \exp(-mk_v)] \frac{dv}{\delta} \right\}^N \end{aligned}$$

as  $N \rightarrow \infty$ , we obtain:

$$\bar{t} \rightarrow \exp\left\{-\frac{1}{\delta} \int_{-\infty}^{+\infty} [1 - \exp(-mk_v)] dv\right\} = \exp\left(\frac{-W}{\delta}\right)$$

$$\text{or } \bar{A} = \exp[-\bar{A}(\text{isolated line})]$$

Now – consider a frequency range containing N lines, each a single member of a different infinite array of random lines of equal intensity and line spacing,  $N\delta$ .

The mean transmission of one of the N array is:  $t_i = \exp(-W_i/N\delta)$

where  $W_i$  is the equivalent width of one line in the array under consideration.

The conditions for multiplication property are met for random arrays and the N arrays can be combined by multiplication:

$$\bar{t} = \prod_{i=1}^N \bar{t}_i = \exp\left[-(N\delta)^{-1} \sum_{i=1}^N W_i\right] = \exp\left(-\frac{\bar{W}}{\delta}\right)$$

where W is the average equivalent width for the N lines in the selected frequency range.

Note that this expression was derived without reference to the line profile and is not even restricted to a single profile for all of the lines. The only limitation is that the frequency interval should be large enough for the multiplication property to be valid.

Based on statistical band model for a finite number of lines in a spectral interval,

$$\bar{t} = \left(1 - \frac{\bar{W}}{\Delta\nu}\right)^{\bar{n}} \quad \text{where } \bar{W} = \text{Mean Equivalent Width}$$

$$\bar{W} = \sum_{i=1}^N \frac{\left[\int_{\nu} (1 - e^{-k_i, m}) d\nu\right]_i}{N} \quad (6)$$

and where  $\bar{n}$  is the effective number of lines in the bin,  $\Delta\nu$ .

$$\bar{n} = \Delta\nu\delta \quad \text{where } \delta = \text{average line spacing}$$

For large  $\bar{n}$ , the transmission simplifies to:

$$\bar{t} = \exp(-\bar{W}/\delta) \quad (7)$$

However, in this  $1 \text{ cm}^{-1}$  bin of MODTRAN, we cannot generally assume that  $\bar{n}$  is large, so we must stick with Eq. 6.

Our problem then is to compute  $\bar{W}$  and  $\bar{n}$  for all spectral bins across the spectral range of interest (visible to microwave region).

Lets consider that lines don't overlap and again we're assuming a Lorentz line shape. We then have:

$$\bar{W} = \int_{\nu} (1 - e^{-k_i, m}) d\nu = 2\pi\gamma L(u)$$

where  $y = \frac{\gamma_L}{\delta}$  and  $u = \frac{\delta m}{2\pi\gamma_L}$   $\delta = \text{ave. spacing}$  (8)

and  $L(\mu) = \mu e^{-\mu} \{I_0(\mu) + I_1(\mu)\}$

where  $I_0(\mu)$  and  $I_1(\mu)$  are Bessel Functions of the first kind.

For small  $\mu$ , we have that  $L(\mu) = \mu$  and for large  $\mu$ , we have that  $L(\mu) = \sqrt{\frac{2\mu}{\pi}}$ . These limiting cases lead to the following:

for small  $\mu$ :  $\bar{W} = \frac{m}{\delta} \sum_i S^i$

for large  $\mu$ :  $\bar{W} = \frac{2}{\delta} \sum_i (S^i \gamma_L^i)^{1/2}$

Thus, there are three parameters necessary to define the absorption:

$$\delta, \sum_i S^i \text{ and } \sum_i (S^i \gamma_L^i)^{1/2}$$

In the real world, finite spectral bins and overlapping lines modify these parameters somewhat. The resulting MODTRAN parameters are:

1. absorption coefficient =  $\frac{1}{\Delta v} \sum_i S^i(T)$  at several temperatures

2. line density =  $\frac{1}{\Delta v} \left( \sum_i S^i \right)^2 / \sum_i S^{i^2}$  at several temperatures

3. average line width =  $\sum_i \gamma_L^i S^i / \sum_i S^i$  at a standard temperature

These quantities are easily calculated from the HITRAN data base.

A Curtis Godson-type of approximation is applied to develop path weighted parameters for the usual in-homogeneous atmospheric paths over which we wish to perform radiative transfer calculations.

**Benefits of MODTRAN**

- More accurate
- Covers wider range of atmospheric conditions
- Useful at high altitude.

Liability of MODTRAN – Complexity of calculation requires computer.

Lets now turn to the PCModWin Exercise.