Spectral Modelling

Goal – to evaluate the transmission or absorption of (a section of) the atmosphere using knowledge of line data.

Problems
- the line data are not known for all cases and measurements are only available at coarse resolution
- even with the correct line data, the calculation is non-trivial (computationally expensive)

∴ Often use approximations involving line strength distribution or other parameters.

Simplest case: independent lines
i.e. lines that are sufficiently far apart that the absorption profiles do not overlap.

For this case, the equivalent width can be calculated for each line, and the total equivalent width is then just the sum:

$$\Delta W_{band} = \sum_i \Delta W_i$$ "line-by-line modelling"

Calculation of ΔW for a line usually requires parameters

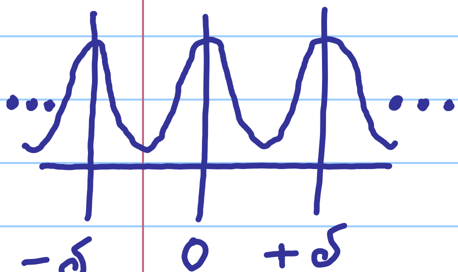
$$\underbrace{S\,(STP),\ \bar{\nu}_0,\ \alpha^L\,(STP),\ \alpha^D\,(STP)}_{\text{characteristic of the line}},\ \underbrace{T, p, u}_{\text{depend on gas path}}$$

However

- ΔW generally doesn't depend on $\bar{\nu}_0$
- many lines in a band have similar values of $\alpha^L\,(STP)$ and $\alpha^D\,(STP)$.

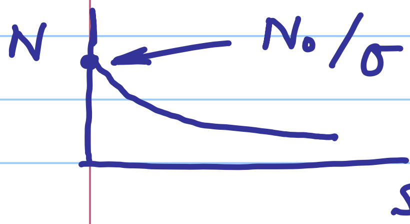
∴ Can produce a histogram of S and convert the sum $\Sigma \Delta W_i$ over all lines to a smaller sum of ΔW of the representative lines × the interval weightings (typically 4 intervals/decade on a log scale)

This leads to the idea of using analytic expressions for the line strength distribution. Four such distributions have been found to be useful.



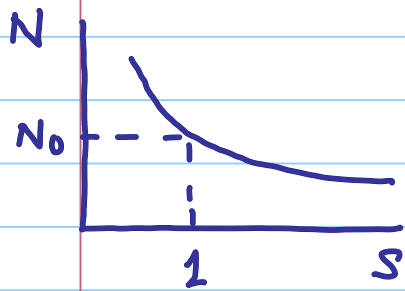
Elsasser $\quad N(S) = N_0\, \delta(\sigma)$

an array of equally spaced lines of the same shape and strength



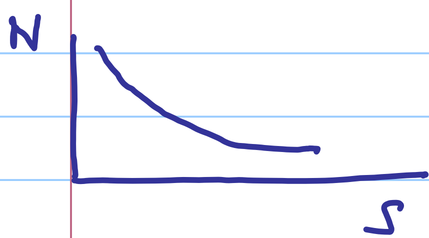
Goody $N(S) = \frac{N_0}{\sigma} \exp\left(-\frac{S}{\sigma}\right)$

lines are spaced randomly with statistical distribution of S. N_0 lines of average $S = \sigma$.



Godson $N(S) = \frac{N_0}{S}$

infinite number of lines. N_0 lines for each factor of e in strength S.



Malkmus $N(S) = \frac{N_0}{S} \exp\left(-\frac{S}{\sigma}\right)$

similar to Goody but increases the number of weak lines

where
$N(S)$ = number of lines of strength S
N_0, σ = parameters of the band
δ = line spacing

The analytic functions (band models) are useful because they give an analytic form for $\Sigma \Delta W$.
e.g., for Malkmus model with Lorentz line shape

$$\Sigma \Delta W = 2\pi N_0 \alpha_L \left[\sqrt{1 + \frac{\sigma u}{\pi \alpha_L}} - 1\right]$$

Then the analytic form for $\Sigma \Delta W$ can be used in other equations.

Evaluation of these expressions requires knowledge of the band parameters. These can be derived from the line data (long) but are often obtained by examining the behaviour at the ends - the weak and strong limits.

Curves of Growth

We showed that $\Delta W = S\rho x = Su$ for a weak line, so for a weak band, the equivalent width is $\sum_i S_i u$.

What about the equivalent width of a strong line?

$$\Delta W = \int_{-\infty}^{\infty} \left[1 - \tau_{\bar{\nu}} \right] d\bar{\nu}$$

$$= \int_{-\infty}^{\infty} \left[1 - \exp\left(-k_{\bar{\nu}} \rho x\right) \right] d\bar{\nu}$$

$$= \int_{-\infty}^{\infty} \left[1 - \exp\left(- S f_{\bar{\nu}} u\right) \right] d\bar{\nu}$$

for a Lorentz line

$$= \int_{-\infty}^{\infty} \left[1 - \exp\left(\frac{- S u \alpha_L / \pi}{(\bar{\nu} - \bar{\nu}_0)^2 + \alpha_L^2} \right) \right] d\bar{\nu}$$

Now, for a strong line, exp( ) ≈ 0 until $\Delta\bar{\nu} = \bar{\nu} - \bar{\nu}_0 \gg \alpha_L$

$\therefore$ Can replace $\Delta\bar{\nu}^2 + \alpha_L^2$ by $\Delta\bar{\nu}^2$.

Let $y^2 = \dfrac{Su\alpha_L/\pi}{\Delta\bar{\nu}^2} \Rightarrow d\bar{\nu} = \sqrt{\dfrac{Su\alpha_L}{\pi}}\left(\dfrac{-dy}{y^2}\right)$

$$\Delta W = \int_{-\infty}^{\infty}\left[1 - e^{-y^2}\right] d\bar{\nu}$$

$$= \int_{-\infty}^{\infty}\left[1 - e^{-y^2}\right]\sqrt{\frac{Su\alpha_L}{\pi}}\left(\frac{-dy}{y^2}\right)$$

$$= 2\sqrt{\frac{Su\alpha_L}{\pi}}\int_{0}^{\infty}\left[1 - e^{-y^2}\right]\frac{dy}{y^2}$$ even integral

This can be integrated by setting the lower limit to δ and allowing $\delta \to 0$.
Result is $\sqrt{\pi}$.

Thus the equivalent width of a strong Lorentz line is

$\Delta W = 2\sqrt{Su\alpha_L}$ vs. $\Delta W = Su$ for a weak line

So for the Malkmus - Lorentz case:

$$\Sigma \Delta W = 2\pi N_0 \alpha_L\left[\sqrt{1 + \frac{\sigma u}{\pi\alpha_L}} - 1\right]$$

$$= 2\pi N_0 \alpha_L\left[\sqrt{\frac{\pi\alpha_L + \sigma u}{\pi\alpha_L}} - 1\right]$$

$$\Sigma \Delta W = \frac{2 N_0 \sigma u}{1 + \sqrt{1 + \frac{\sigma u}{\pi \alpha_L}}}$$

avoids problems as $\frac{\sigma u}{\pi \alpha_L} \to 0$

Take the limits as $u \to 0$ and $u \to \infty$ and equate the expressions for the sum of equivalent widths and the model results.

Weak limit: $u \to 0$, $\frac{\sigma u}{\pi \alpha_L} \to 0$

$$\Sigma \Delta W = N_0 \sigma u = \sum_i S_i u$$

$$\therefore N_0 \sigma = \sum_i S_i$$

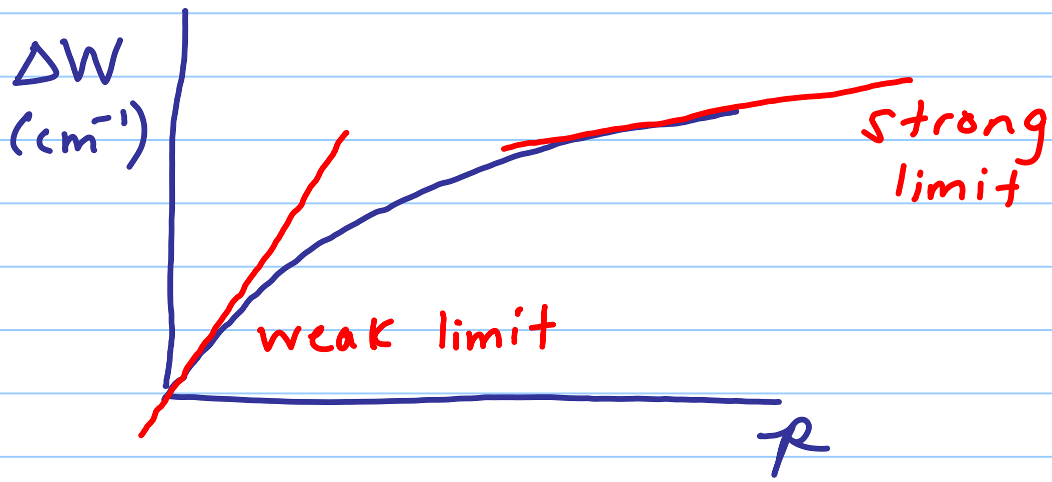
Strong limit: $u \to \infty$, $\frac{\sigma u}{\pi \alpha_L} \to \infty$

$$\Sigma \Delta W = 2 \pi N_0 \alpha_L \sqrt{\sigma \pi \alpha_L} = 2 \sum_i \sqrt{S_i \alpha_L u}$$

From these expressions, the model parameters N_0 and σ / α_L can be determined.

If there are no model parameters, we can use a <u>curve of growth</u>, which is a plot of equivalent width vs. abundance or pressure. Can then fit the weak and strong limiting slopes.

Since α_L and u are proportional to pressure p, ΔW is proportional to p in both the weak and strong limits but with different constants of proportionality.



Overlapping Lines

So far, we have been dealing with independent lines. When lines overlap, the total equivalent width is smaller than the sum of the individual equivalent widths (except for very weak lines).

e.g., two lines independent $\sum \Delta W = 2\int \left[1 - e^{-k_\nu u}\right] d\nu$

$$\geq$$

two lines superposed $\sum \Delta W = \int \left[1 - e^{-2 k_\nu u}\right] d\nu$

It can be shown that when lines overlap, randomly, the equivalent width is

$$\Delta W_{total} = 1 - \exp\left(-\sum_i \frac{\Delta W_i}{\delta}\right)$$ where δ = mean line spacing.

Inhomogeneous Paths and the Curtis - Godson Approximation

We have been assuming a homogeneous path (constant p, T, u). However, this is not valid for the atmosphere.

$\Rightarrow$ Want to find a homogeneous path that approximates the properties of an inhomogeneous path.

The difference between the homogeneous and inhomogeneous paths is the calculation of the optical depth for which the term $S f_{\tilde{\nu}} u$ must be replaced by the integral $\int S f_{\tilde{\nu}} u$.

To start, consider the weak limit, for which

$$\Delta W = \int_{-\infty}^{\infty} \left[1 - \exp\left(- \int_{u} S f_{\tilde{\nu}} \, du \right) \right] d\tilde{\nu}$$

Expanding exponential and reversing the order of integration gives

$$\Delta W = \int_{-\infty}^{\infty} \left[1 - \left(1 - \int_{u} S f_{\tilde{\nu}} \, du \right) \right] d\tilde{\nu}$$

$$= \int_{u} \int_{-\infty}^{\infty} S f_{\tilde{\nu}} \, d\tilde{\nu} \, du = \int_{u} S \, du = \underline{\underline{\bar{S} u}}$$

where $\bar{S} \equiv \int_0^u S(T)\,du \Big/ \int_0^u du$

$=$ mass-weighted average line strength

So for weak lines, we can use $\bar{S}$ and u, and treat the path as homogeneous!

For strong lines, we can show that the equivalent width is given by

$$\Delta W = 2\int_u \sqrt{S\alpha_L\,du}$$
$$= 2\sqrt{\bar{S}\,\bar{\alpha}_L\,u}$$

where $\bar{\alpha}_L = \int_0^u S(T)\,\alpha_L(p,T)\,du \Big/ \bar{S}u$

and $\bar{S}$ is as above.

These equations for $\bar{S}$ and $\bar{\alpha}_L$ are the <u>Curtis-Godson approximation</u> for an inhomogeneous path.

The τ of an inhomogeneous path is approximately equal to the τ of a homogeneous path (at constant p, T) whose integrated absorber amount is u with mean half-width $\bar{\alpha}_L$ and mean strength $\bar{S}$.

If T variations are ignored (slower than p variations), then we get the isothermal <u>Curtis-Godson approximation</u> for which the inhomogeneous path is equivalent to a homogeneous path of the same mass and T, with mass-weighted pressure

$$\bar{p} = \int p\, du \Big/ \int du .$$

The C-G approx. is useful in many atmospheric problems, especially in calculating heating rates.

It does not work if there is strong T structure or if the mass distribution varies inversely with pressure

e.g. u for O_3 increasing with z in the lower stratosphere.

<u>Infrared Cooling Rates</u>

We can now compute IR heating/cooling rates from the band parameters.

Recall the integral monochromatic form of Schwarzchild's Equation for LTE in a vertical path:

$$I(z) = B(T(0))\,\tau(z,0) + \int_{\tau(z,0)}^{1} B(T(z'))\, d\tau(z,z')$$

where z = vertical coordinate
and the eqn has been written for
upwards intensity.

Integrate this over a finite number of
bands such that B is constant in each band:

$$I(z) = \sum_i B_i(T(0))\, \tau_i(z,0) + \sum_i \int_{\tau_i(z,0)}^{1} B_i(T(z'))\, d\tau_i(z,z')$$

where
τ_i = average transmission over interval i.

Now integrate over angle using diffusivity
factors to get:
upward flux density

$$F^{\uparrow}(z) = \sum_i \pi B_i(T(0))\, \tau_i^*(z,0) + \sum_i \int_{\tau_i(z,0)}^{1} B_i(T(z'))\, d\tau_i^*(z,z')$$

and
downward flux density

$$F^{\downarrow}(z) = 0 + \sum_i \int_{\tau_i(z,\infty)}^{1} B_i(T(z'))\, d\tau_i^*(z,z')$$

where τ^* = modified transmission (like χ^*)

Net flux: $F(z) = F^{\uparrow}(z) - F^{\downarrow}(z)$

Heating rate:

$$\left(\frac{\partial T}{\partial t}\right)_{IR} = -\frac{1}{c_p \rho}\frac{\Delta F}{\Delta z} = \frac{g}{c_p}\frac{\Delta F}{\Delta p} = -\frac{q}{c_p}\frac{\Delta F}{\Delta u}$$

Can thus calculate the heating and cooling rates in the atmosphere.

e.g. Liou (p. 108) shows partial and total IR cooling rates in a clear tropical atmosphere.
→ calculated using Goody random band model parameters for IR H_2O, O_3, and CO_2, and the Curtis-Godson approx., as well as H_2O continuum absorption.
→ see slide.