Problem 3
HW 6
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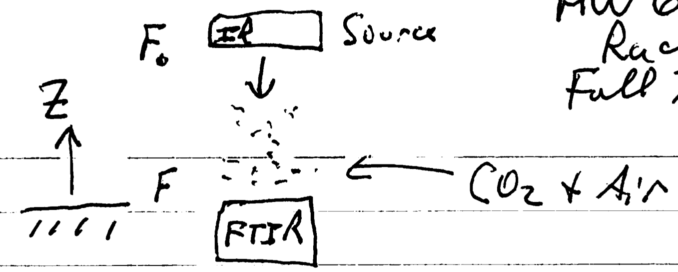
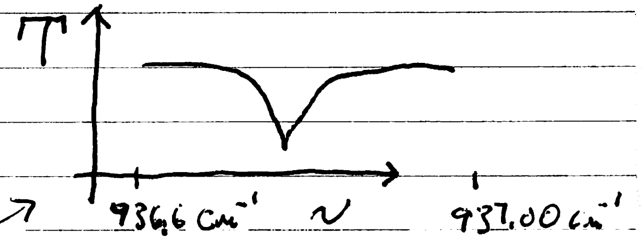
Problem 3

Given



Let $T = \frac{F(\nu)}{F_0(\nu)}$ = transmittance.



Single absorption line by CO_2.

Figure 4.5 of Stamnes + Thomas

Problem: Make a model for this observation.

Solution: Open-ended questions like this require a multi-faceted approach for a solution. Pressure broadening dominates line strength in the troposphere. Make that assumption.

(1) Beers Law: $$T = e^{-\int_0^\infty N\, k\, dz} = e^{-\tau}$$

Let τ be the total optical depth.

(2) $$\tau = \int_0^\infty N(z)\, k(\nu)\, dz$$ ← Path

CO_2 density with height, eg $\frac{\text{Molecules}}{m^3}(z)$

Absorption Cross section per molecule for CO_2, $\frac{m^2}{\text{molecule}}$

Note: Units in Eq (2) make sense.

Now we tackle each part in turn.

$N(z)$

Density of Molecules

Strategy ⇒ Use isothermal atmosphere approximation to get $\rho(z)$ density with height and convert to $N(z)$.

(3) $$dP = -\rho g\, dz \quad (\text{Hydrostatic Eq})$$

(4) $$P = \rho R T \quad (\text{I.G.L.}) \qquad R = R_0 / \mu_{mw}^{air} \qquad R_0 : \text{Univ. Gas Constant}$$

Combining (3) and (4), $\frac{dP}{P} = \frac{-g}{RT}\, dz \Rightarrow P = \tilde{P}_0 e^{-z/H}$,

(5) $H \equiv RT/g$, $\tilde{P}_0 \equiv$ surface Pressure,
Assumes T = constant !!

Density, $\rho(z) = \tilde{\rho}_0 e^{-z/H}$, $\tilde{\rho}_0 = \tilde{P}_0 / R\tilde{T}_0$,

So

$$\underbrace{N(z)}_{\frac{\text{molecules}}{m^3}} = \rho(z)\left[\frac{Kg}{m^3}\right] \frac{1}{\mu_{mw}^{air}}\left[\frac{\text{mole}}{Kg}\right] * N_a \frac{\text{molecules}}{\text{mole}} \cdot \underbrace{C}_{\text{Concentration in PPM of } CO_2} \underbrace{\times 10^{-6}}_{\text{Convert to fraction}}$$

∴ vertical distribution of CO_2 is

(6) $$N(z) = \frac{\tilde{P}_0}{R\tilde{T}_0} \frac{N_a}{\mu_{mw}^{air}}\, C \times 10^{-6}\, e^{-z/H},$$

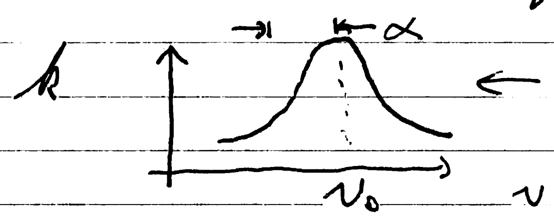
Absorption Cross Section per molecule: $k(\nu, P, T)$

(7) $$k(\nu, P, T) = \frac{S}{\pi} \frac{\alpha}{(\nu - \nu_0)^2 + \alpha^2}$$

Lorentzian Profile

S = line Strength

α = air broadened half width at half maximum.



← Line broadening due to Collisions, "Pressure broadening" of spectral line.

k depends on P and T through $\alpha(T, P)$.

(8) $$\alpha = \alpha(T, P) = \alpha_0 \frac{P}{P_0} \left(\frac{T_0}{T}\right)^n$$ where

$\alpha_0(T_0, P_0)$, n, ν_0 come from the Hitran database,

$T_0 = 296K$, $P_0 = 1$ atm Pressure.

From Hitran through spectral calc, get

(9) $$S = 1.38 \times 10^{-23} \left[\frac{cm^2}{\text{Molecule}} \, cm^{-1}\right]$$

$$\alpha_0 = 0.069 \; cm^{-1}$$

$$\nu_0 = 936.803747 \; cm^{-1}$$

$$n = 0.78$$.

h continued.

Note from Eq 5 we can write for α in Eq 8,

$$\alpha(z) \cong \alpha_0 \frac{\tilde{P}_0 e^{-z/H}}{P_0} \left(\frac{T_0}{\tilde{T}_0}\right)^n \quad \text{or}$$

(10) $$\alpha(z) = \tilde{\alpha}_0 \, e^{-z/H} \quad \text{where}$$

(11) $$\tilde{\alpha}_0 = \alpha_0 \frac{\tilde{P}_0}{P_0} \left(\frac{T_0}{\tilde{T}_0}\right)^n \quad \text{is}$$

the value of α_0 in Denver where the observation was obtained.

$P_0 = 1$ atm
$\tilde{P}_0 = 0.840$ atm (Denver)

$T_0 \cong 296\,K \approx \tilde{T}_0$
surface T in denver CO by assumption.

Note: Eq (10) and (11) are simple because we have assumed an isothermal atmosphere!

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All together now:

$$\tau = \int_0^\infty N(z)\, k(\nu, z)\, dz \qquad \text{Eq } 2$$

(12). $$\tau = \underbrace{\frac{\tilde{P}_0}{R\tilde{T}_0} \frac{N_a}{\mu_{mw}}}_{\text{Eq }(6)} C \times 10^{-6} \underbrace{\frac{S}{\pi}}_{\text{Eq }(7)} \tilde{\alpha}_0 \int_0^\infty \frac{e^{-z/H}\, e^{-z/H}\, dz}{(\nu-\nu_0)^2 + \tilde{\alpha}_0^2 e^{-2z/H}}$$

or

(13) $$\tau = \frac{\tilde{P}_0}{R\tilde{T}_0} \frac{N_a}{\mu_{mw}} C \times 10^{-6} \frac{S}{\pi \tilde{\alpha}_0} \overbrace{\int_0^\infty \frac{e^{-2z/H}\, dz}{x + e^{-2z/H}}}^{I},$$

(14) where $$x \equiv \left(\frac{\nu - \nu_0}{\tilde{\alpha}_0}\right)^2$$ ↑ Pole at ∞ when $x \to 0$

In (13), let $u = e^{-2z/H}$ $\quad du = -\frac{2}{H} e^{-2z/H} dz$.

Then

$$I = \frac{H}{2} \int_0^1 \frac{du}{x + u}.$$ Notice the pole when $u = 0$, $x = 0$.

Try $y = x + u$ $\quad dy = du$

(15) $$I = \frac{H}{2} \int_x^{1+x} \frac{dy}{y} = \frac{H}{2} \left\{ \ln(1+x) - \ln(x) \right\}$$
$$= \frac{H}{2} \ln\left[\frac{1+x}{x}\right]$$

There is an unavoidable pole due to $x = 0$, e.g. when $\nu = \nu_0$. Here is a fix, next page.

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In Eq (13), H is the scale height of the atmosphere. $H \approx 6$ km. By the height $Z = 3H$, $\frac{\rho(Z)}{\rho_0} \sim e^{-3}$ is small.

Atmosphere terminates at $Z = mH$ → so let us have $Z = mH$ be the upper limit of integration in Eq (13),

$$I \equiv \int_0^{mH} \frac{e^{-2Z/H}}{\chi + e^{-2Z/H}}\, dZ$$

$$u = e^{-2Z/H} \qquad du = -\frac{2}{H} e^{-2Z/H}\, dZ$$

$$I = \frac{H}{2} \int_{e^{-2m}}^{1} \frac{du}{\chi + u} \qquad y = \chi + u \quad dy = du$$

(16) $$I = \frac{H}{2} \int_{\chi + e^{-2m}}^{1+\chi} dy/y = \frac{H}{2} \left\{ \ln(1+\chi) - \ln(e^{-2m} + \chi) \right\}$$

(17) $$I = \frac{H}{2} \ln \left[\frac{1+\chi}{e^{-2m} + \chi} \right]$$

The final solution. Using (11) and (17) in (13),

$$\tau = \frac{\cancel{\tilde{P}_0}}{\cancel{R\tilde{T}_0}} \frac{N_a}{\mu_{mw}} C \times 10^{-6} \frac{S}{\pi} \frac{1}{\alpha_0} \frac{P_0}{\cancel{\tilde{P}_0}} \left(\frac{\tilde{T}_0}{T_0}\right)^n \frac{\cancel{R}\tilde{T}_0}{2g} \ln\left[\frac{1+x}{e^{-2\overbrace{m}^{H/2}}+x}\right]$$

$$(18) \qquad \tau(\nu) = \frac{N_a C \times 10^{-6}}{\mu^{air}_{mw}} \frac{S P_0}{2\pi \alpha_0 g} \left(\frac{\tilde{T}_0}{T_0}\right)^n \ln\left[\frac{1+x}{e^{-2m}+x}\right] \qquad \text{where}$$

$$x = \left(\frac{\nu - \nu_0}{\tilde{\alpha}_0}\right)^2$$

$$\tilde{\alpha}_0 = \alpha_0 \frac{\tilde{P}_0}{P_0} \left(\frac{T_0}{\tilde{T}_0}\right)^n$$

MKSA Units

$$S = 1.38 \times 10^{-23} \frac{cm^2}{molecule} cm^{-1} \ast 10^{-4} \frac{m^2}{cm^2}$$

$$\alpha_0 = 0.069 \ cm^{-1}$$

$$\nu_0 = 936.803747 \ cm^{-1}$$

$$n = 0.78$$

$$C = 385 \ PPM$$

$$g = 9.8 \ m/s^2$$

$$\frac{\tilde{P}_0}{P_0} \approx 0.84 \qquad P_0 = 10^5 \ PA \qquad \tilde{T}_0 \approx T_0$$

$$\boxed{\text{Choose } m = 2}$$