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To: VSRT Group
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Subject: Modeling an atmospheric spectral line of ozone

1] Radiative transfer

When a radio wave travels through a medium some of the signal is lost due to absorption in the medium while some signal is generated in the medium. The amount of absorption is characterized by the "opacity". If the signal is measured in units of temperature the radiative transfer when the atoms or molecules producing the signal are in thermal equilibrium with the medium is given by

$$T_{out} = T_{in} e^{-\tau} + T_{medium} \left(1 - e^{-\tau}\right)$$

where T_{in} is the input brightness temperature

T_{out} is the output brightness temperature

τ is the opacity

T_{medium} is the temperature of the medium

In general the atoms or molecules responsible for the spectral line signal may not be in thermal equilibrium and T_{medium} become $T_{excitation}$. The "excitation" temperature can even be negative in which case the signal grows and we have Microwave Amplification by Stimulated Emission Radiation or a MASER.

For a small opacity signal grows by $T_{medium}\tau$

2] Path through the atmosphere

The path through the atmosphere to the antenna is effected by the curvature of the Earth so that a ray at low elevation passes through less atmosphere than it would if the Earth were flat. For a plane parallel atmosphere on a flat Earth the path through each layer of the atmosphere is increased by 1/sin (elevation) or a secant (elevation). Consider a layer 1 km thick at a height, h km, above the surface of the Earth. To estimate the path we need to solve for the difference between distance to the top of the layer, for which we have a triangle with sides of R and R+h+1, to the bottom of the layer for which we have a triangle with sides R and R+h-1, when R is the radius of the Earth. Both triangles have the angle of 90 + elevation where the ray reaches the antenna. This is illustrated in the figure 1. We can write a simple function, telev( ) to perform this calculation.

3] Adding up the layers

To calculate the spectrum of the atmospheric line we need to add up the layers since each layer will have a different medium, temperature and opacity. This is done by an integral which is approximated by a sum as follows:

$$T(\nu) = \sum_{h=10}^{h=100} T_{medium}(h)\tau(h,\nu)telev(h) \qquad (1)$$

where h is the layer height and ν is the frequency. Equation 1 is complicated by the fact that while the atmospheric temperature and path length through each layer are only a function of height whereas the opacity depends on both of height and the frequency.

4] Line shape

The frequency dependence of the signal is known as the line shape. Qualitatively the line shape is narrow and peaked as illustrated in figure 1 for the ozone molecules high in the atmosphere because there are fewer neighbors with which the ozone molecules collide. These collisions result in a "pressure" broadening of the line so that the layers lower down have a very broad spectrum compared with the narrow spectrum of ozone molecules which is only broadened by the Doppler shift due to the random thermal motions of the molecules. The spectrum for ozone above about 90 km has a line width of only about 18 kHz compared with 3 GHz for the ozone near the ground. Since the ozone spectrometer only analyzes a 1.25 MHz bandwidth we don't observe the lower ozone because the line is so broad. Within the 1.25 MHz the spectrometer is sensitive to ozone in the mesosphere with increasing sensitivity to the highest region of the mesosphere at the start of the thermosphere.

a) Temperature profile

For calculations of the ozone line profile it is assumed that the mesosphere temperature is 260 K for heights less than 80 km and decreases to 190 K for heights above 80 km.

b) Pressure Profile

The atmospheric pressure, p, is assumed to follow a power law in which the density decreases by a factor of 10 every 15.35 km increase in altitude so that

$p(h) = p(0)10^{-h/15.35}$

c) Detailed line shape

The line shape is assumed to be the combination of Doppler and pressure broadening. The Doppler width follows a Gaussian shape

$\exp\left(-0.693 f^2/w^2\right)$

w = half power half width = 9.193 kHz at 260 K given by

$w = fline * sqrt\left(2.0\ln(2.0)kT/m\right)/c$

where $fline$ = line frequency in MHz = 11.072×10^3

k = Boltzman's constant = 1.38×10^{-23} J/K

m = weight of ozone = $48.0 \times 1.67 \times 10^{-27}$ kgm

c = velocity of light = 3×10^{8} m/s

The pressure broadening is assumed to follow a Lorentz shape

$$\left(\frac{pw}{\pi}\right) \Big/ \left(f^2 + pw^2\right)$$

where pw = pressure width

$\simeq$ 1 GHz at 1 atmosphere (100 kPa)

and is proportional to the atmospheric pressure

d) Ozone concentration

The ozone concentration is assumed to be 1 part per million by volume or 1ppmV from which we can calculate the number of ozone molecules per cubic centimeter, *n*, from

$$n = 6.022 \times 10^{23} \times 1.293 \times 10^{-3} \times 273 \times p \times V \times 10^{-6} \Big/ \left(28.97 \times T\right)$$

Where

6.022×10^{23} is Avagadro's number of the number of elementary entities per mole

1.293×10^{-3} the weight of 1 cubic cm of air at 273 K and 1 atmosphere pressure

p is the pressure in atmospheres

V is the volume mixing ratio in ppmv

28.97 is the molecular mass of air

T is the temperature in Kelvin

e) Line intensityThe line intensity of the 11.072 GHz ozone (03) transition is taken to be

$10^{-6.99} \times 10^{-14} \times n$

from *//spec.jpl.nasa.gov/cgi-bin/catform*

f) Correcting the line strength for temperature

The line intensity in the JPL catalog is for a temperature of 300 K. This needs to be corrected for the temperature of the ozone in the mesosphere using the relation given in equation all of Rothman et al.

$$S(T) = S(300)\left[\frac{Q(300)}{Q(T)}\right]\left[\frac{e^{-c2E/T}}{e^{-c2E/300}}\right]\left[\frac{300}{T}\right]$$

Where we have used the low frequency approximation for the last factor of A11.

S= line intensity

Q = total internal partition function

C2 = 1.433 cm K

E = energy of lower state in cm^{-1}

= 8.02 from the JPL tables

The total partition function is approximately proportional to temperature but a more accurate ratio can be obtained from interpolation of the values given in the JPL tables. The correction for temperature had been ignored in the past and in addition there was an error in the conversion from ppmv to molecular concentration.

Putting it all together

$\tau(h,\nu) = shape(h,\nu) \times line\_strength$ where the shape is the "convolution" of the Doppler and pressure broadening.

g) Antenna beam efficiency

The antenna beam efficiency is reduced to about 75% owing to the LNBF spill-over. This loss is incorporated into the calculation at ozone ppmv.

The annotated C code for the line profile follows and a sample plot is shown in figure 2.

```
double to3(double freq, int mode, int regn, double oztem, double vel)
{
    double col, f, h, t, tt, p, m, sum, sum2, w, pw, n, i, shape, dshape,
elev, resl;
    double hstart, hstop, hpeak, ht, stren, q_300, q_190;
    int j;
    elev = 8;
    f = freq + vel * 11.072e03 / 3e08;
    hpeak=95;   // more consistent with SABER
    ht = 75;     // best fit 25 Feb 09
    q_300 = 3553.04; // total internal partition at 300 K
    q_190 = 2230.0 - (225.0-oztem)*(3553.04 - 1198.671)/150.0; //
interpolation from JPL tables
    sum = col = 0;
    j = 0;
    hstart = 50; hstop = 120;
    if(regn == 1) {hstart = ht; hstop = 120;}
    if(regn == 2) {hstart = 50; hstop = ht;}
    for (h = hstart; h <= hstop; h++) {
        if (h < ht)
            t = 260;
        else
            t = oztem;            // 190K temperature of Mesosphere above 80
km
        p = pow(10.0, -h / 15.35); // Smith 96 km
        m = 0;
        if(h>=50 && h<ht) m=1.17e-6; // region 1
```

```
        if(h>=ht) m=exp(-0.693*(h-hpeak)*(h-hpeak)/(5.0*5.0))*20e-6; //
region
2 for 20 ppmv
        n = p * (6.0221e23 * 1.293e-3 * 273.0 / (28.97 * t)) * m; // error
fixed
        i = -6.9997;
        stren = 0.74*pow(10.0,
i)*(exp(-1.4388*8.02/t)/exp(-1.4388*8.02/300.0))*(300.0/t)*(q_300/q_190);
//  8.02 is the lower level energy in cm^-1
// 0.74 for beam efficiency
// see A11  - c2=-1.4388, E=8.02, - assumes Q not dependent on t
// 6.0221e23 is Avogadro's number, 1.293e-3 is the weight of 1 cubic cm of
air
// at 1 atmosphere
// at 273K - n is the number of O3 molecules per cubic cm
        col += n * 1e05;        // add to get total ozone for debug
information only
        w = 11.072 * 1e3 * sqrt(2.0 * log(2.0) * 1.38e-23 * t / (48.0 *
1.67e-27)) / 3.0e8; // Doppler width
        resl = resol * 0.5 * 1e-6;  // resol
        w = sqrt(w * w + resl * resl) + 2.5e-3 * 0.5;  // + cal_err not in
quadrature
        shape = sum2 = 0;
//        pw = 2e3 * p;     // pressure width 2 MHz/torr   half-width half-
max
        pw=3.051e03*p*pow(296.0/t,0.676)/1.3157;  // Colmont 300 GHz lines
        for (tt = -0.05; tt <= 0.05; tt += 0.0005) { // perform convolution
to
get combined width
            if(mode) {
            dshape = exp(-0.693 * tt * tt / (w * w)); // Doppler line shape
            mcalc[j] = dshape;
            }
            else dshape = mcalc[j];
            j++;
//            shape += dshape * (1.0 / PI) * pw / ((f + tt) * (f + tt) + pw *
//            pw); // multiply by pressure shape
            shape += dshape / ((f + tt) * (f + tt) + pw * pw); // multiply by
pressure shape
            sum2 += dshape;     // sum
        }
//        shape = shape / sum2;   // normalize
        shape = shape * pw / (sum2 * PI);   // normalize
        sum += shape * stren * 1e-14 * n * 1e05 * t * telev(elev, h); // add
up the layers
    }
    return sum;
}

double telev(double elev, double h)
{
    double aa, bb, cc, aa1, bb1, cc1;
    aa = 6356.0;                // radius of earth
    bb = aa + h + 0.5;          // distance of upper edge of layer from
center
of earth
    aa1 = 1.0;
```

```
    bb1 = -2.0 * aa * cos((90.0 + elev) * PI / 180.0);
    cc1 = -bb * bb + aa * aa;
    cc = (-bb1 + sqrt(bb1 * bb1 - 4.0 * aa1 * cc1)) / 2.0; // solve for
distance from antenna
//  printf("el %f cc %f h %f\n",elev,cc,h);
    bb = aa + h - 0.5;          // distance of lower edge of layer from
center
of earth
    cc1 = -bb * bb + aa * aa;
    cc -= (-bb1 + sqrt(bb1 * bb1 - 4.0 * aa1 * cc1)) / 2.0;
//  printf("el %f cc %f h %f\n",elev,cc,h);
    return cc;
}
```

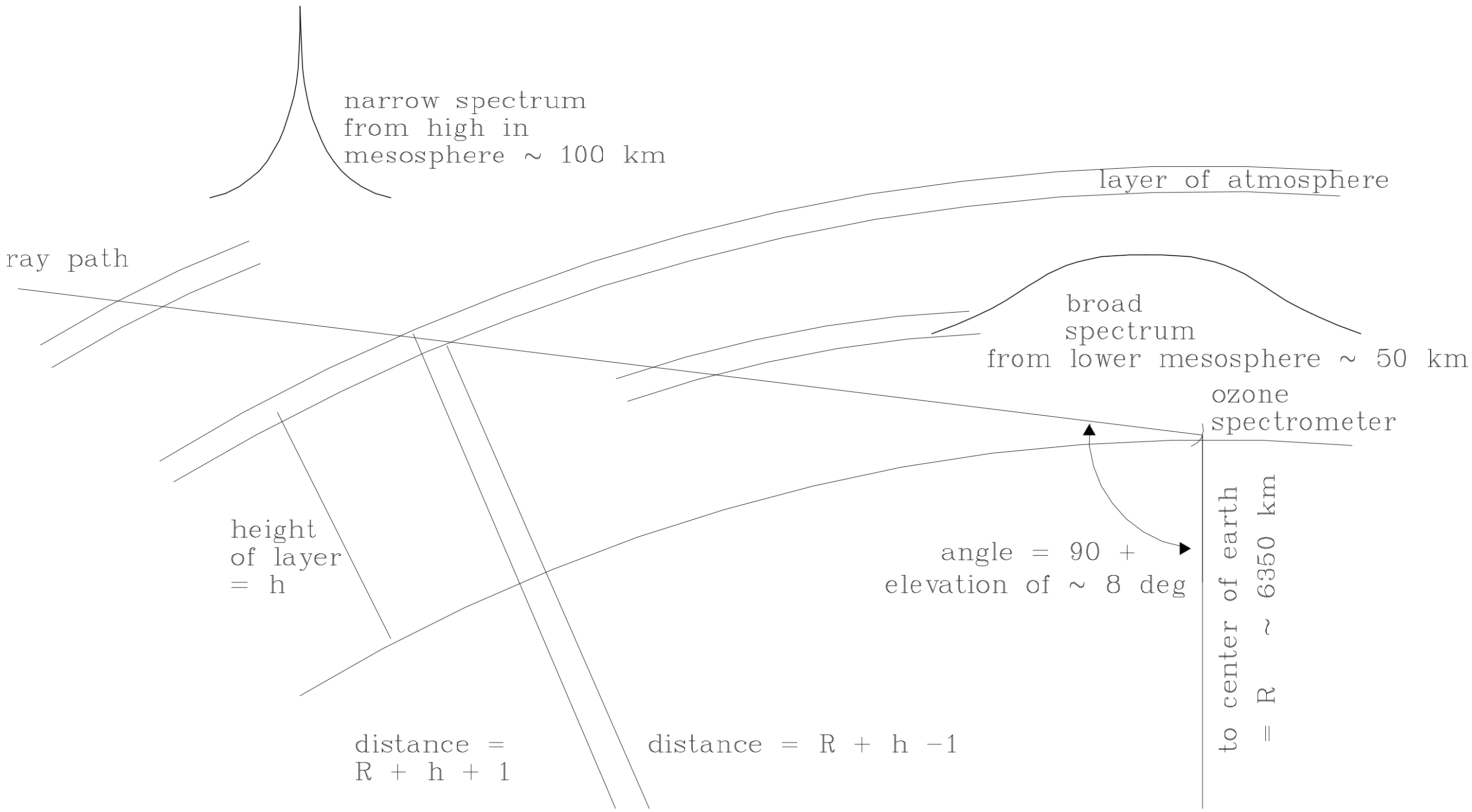

Figure 1. Geometry of emission from Ozone to spectrometer through the earth's atmosphere - (not to scale)

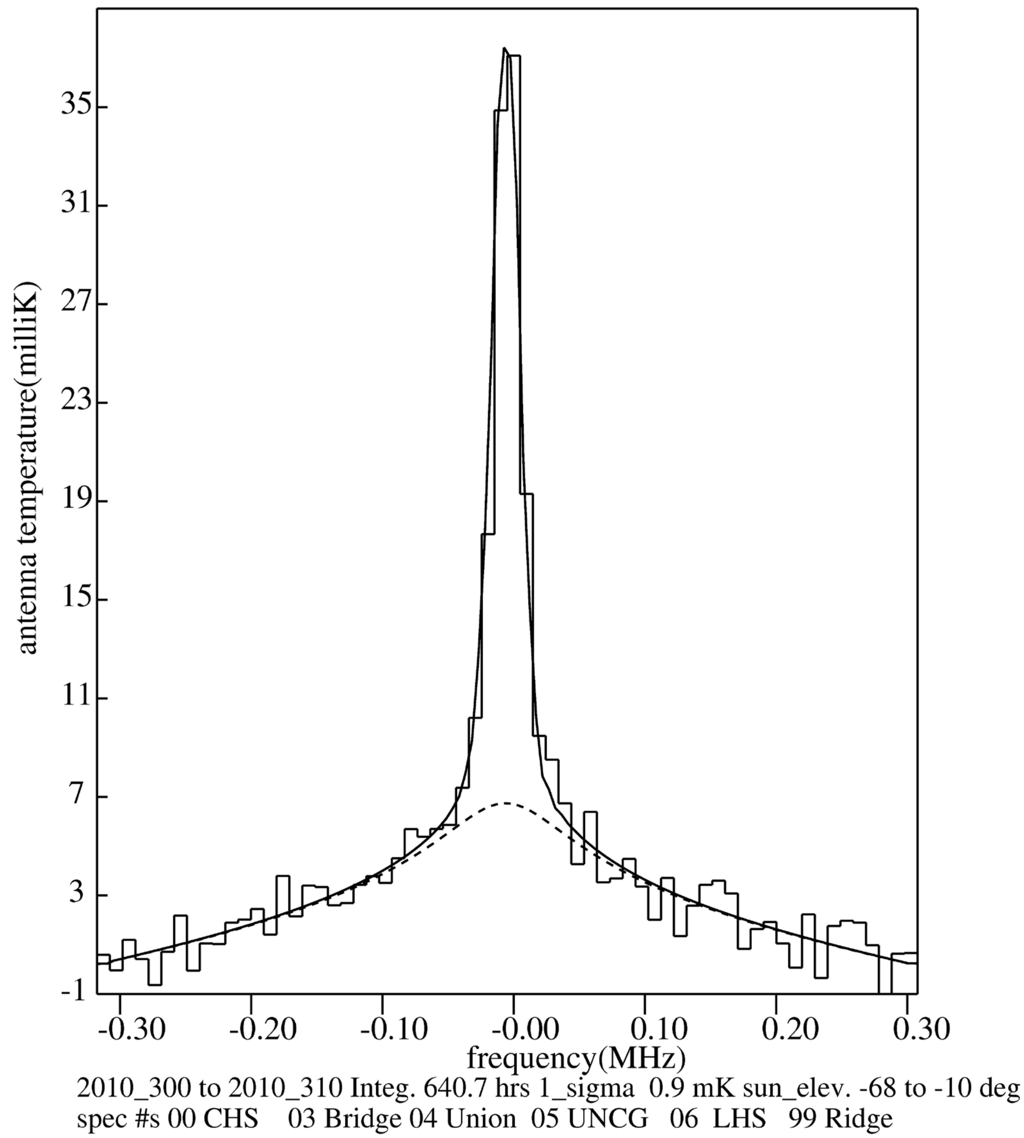

Figure 2. Sample spectrum of 10 day average. The difference between the solid line and the dashed lins is the best fit spectrum to the ozone above 80 km. It corresponds to a mixing ratio of a Gaussian of 10 km full-width at 95 km with 14 ppmv.