Vertical path calculation on the Spectral Calculator

The transmittance through a uniform layer of absorbing gas is given by the Beer-Lambert law:

$$\tau = \exp\left(-kLq\,P/T\right) \qquad (1)$$

where k is the absorption cross section, L is the layer thickness, q is the concentration of the absorbing gas, P is the pressure and T is the temperature. To simulate the transmittance of a vertical path through the atmosphere, we simply divide the path into layers, and compute the product of the individual layers' transmittances. Almost all the effort in computing Eq. (1) lies in computing the cross section, k. This is accomplished efficiently and accurately with the *LinePak*™ radiative transfer library, but still represents a very intensive calculation, so we would like to use as few layers as possible.

The *Vertical Path* option of the *Atmospheric Path* tool uses a maximum of 8 layers. This gives good results for most cases, but certain situations may require more layers for high accuracy. In such cases, the path should be broken into smaller pieces, and simulations performed on each section. Save the spectrum from each piece, and finally compute their product using the *My Spectra* tool. Simple testing is the best way to determine whether this approach is needed for a given case.

For all but very thin layers, P, T and q can vary considerably from top to bottom. Modeling the layer using the conditions at either boundary, or their average, can result in biased transmittance values. Below we discuss how to best model a varying layer as a uniform layer of the same thickness.

Effective conditions for a layer

If the cross section, k, in Eq. (1) has only negligible dependence on q, P and T, the transmittance of a uniform layer with mixing ratio $\tilde{q}$, temperature $\tilde{T}$ and pressure $\tilde{P}$ will be the same as a layer with varying conditions if

$$\frac{\tilde{q}\tilde{P}}{\tilde{T}} = \frac{1}{L}\int_0^L \frac{q(z)P(z)}{T(z)}\,dz \qquad (2)$$

This can be more simply written in terms of the density, $\rho(z) = P(z)/RT(z)$, where $R \approx 286.9\ \mathrm{J\ kg^{-1}\ K^{-1}}$ is the gas constant for dry air:

$$\tilde{q}\tilde{\rho} = \frac{1}{L}\int_0^L q(z)\rho(z)\,dz \quad . \qquad (3)$$

If we define the effective density as

$$\tilde{\rho} = \frac{1}{L}\int_0^L \rho(z)\,dz \quad , \qquad (4)$$

the effective mixing ratio must satisfy

$$\tilde{q} = \frac{1}{L\tilde{\rho}}\int_0^L q(z)\rho(z)\,dz\,. \qquad (5)$$

To determine $\tilde{T}$ and $\tilde{P}$ from $\tilde{\rho}$, we first find the effective density height, $\tilde{z}_\rho$, namely the height where the local density equals the effective density. (This assumes we know the density explicitly throughout the layer. In the next section we consider the case where the conditions are known only at the boundaries of the layer.)

Finally, evaluating

$$\tilde{T} = T(\tilde{z}_\rho) \quad \text{and} \quad \tilde{P} = \tilde{\rho}R\tilde{T} \qquad (6)$$

completes our search for effective mixing ratio, temperature and pressure values.

Modeling a layer from only boundary values

Often we do not know $q(z)$, $P(z)$ and $T(z)$ explicitly, so calculating the effective conditions from Eq.s (4-6) is not possible. However, if their boundary values, q_0, P_0 and T_0 at the bottom and q_L, P_L and T_L at the top, are known, we can proceed with some reasonable assumptions.

First, to evaluate Eq. (4), we assume the density decreases exponentially with altitude as $\rho(z) = \rho_0 e^{-z/h}$, where h is the scale height (typically ~6-11 km) and $\rho_0 = P_0 / RT_0$. The local scale height, h, can be determined from the layer boundary values by

$$\frac{L}{h} = \lambda = \log\left(\frac{P_0 T_L}{P_L T_0}\right). \tag{7}$$

where $\lambda = L/h$ is the dimensionless layer thickness. With this exponential model for ρ, Eq. (4) can be integrated:

$$\tilde{\rho} = \frac{\rho_0}{L}\int_0^L e^{-z/h}\, dz = \rho_0 \frac{1-e^{-\lambda}}{\lambda}. \tag{8}$$

Next, to evaluate Eq. (5) we assume linear model for the mixing ratio: $q(z) = q_0 + \alpha z$, where $\alpha = (q_L - q_0)/L$ is the mixing ratio gradient. Then,

$$\begin{aligned} \tilde{q} &= \frac{1}{L\tilde{\rho}}\int_0^L \left(q_0 + \alpha z\right)\rho_0 e^{-z'/h}\, dz \\ &= q_0\left[1 + \frac{\left(q_L - q_0\right)}{q_0}\left(\frac{1}{\lambda} - \frac{e^{-\lambda}}{1-e^{-\lambda}}\right)\right] \end{aligned} \tag{9}$$

Fig. 1 compares the effective density to the midpoint density, $\rho_{1/2}$, as a function of layer thickness, $\lambda = L/h$. For thin layers, the effective density approaches the midpoint density, but as the thickness is increased it approaches the density of the layer bottom.

By setting $\rho_0 e^{-z/h} = \tilde{\rho}$ we find the effective density height $\tilde{z}_\rho$:

$$\frac{\tilde{z}_\rho}{L} = \frac{1}{\lambda}\ln\left(\frac{\lambda}{1-e^{-\lambda}}\right). \tag{10}$$

Note that the effective density height is not in general equal to the corresponding effective mixing ratio height, which is found by inspection from Eq. (9).

$$\frac{\tilde{z}_q}{L} = \frac{1}{\lambda} - \frac{1}{e^{\lambda} - 1} \quad . \tag{11}$$

These two effective heights are compared in Fig. 2.

We determine $\tilde{T}$ by again assuming a linear model: $T(z) = T_0 + \beta z$, where $\beta = (T_L - T_0)/L$. Eq. (6), $\tilde{T} = T(\tilde{z}_\rho)$, produces

$$\tilde{T} = T_0\left[1 + \frac{T_L - T_0}{T_0}\frac{1}{\lambda}\ln\left(\frac{\lambda}{1-e^{-\lambda}}\right)\right]. \tag{12}$$

The effective pressure is also obtained from Eq. (6): $\tilde{P} = \tilde{\rho}R\tilde{T}$.

This completes our calculation of the effective conditions. A uniform layer with mixing ratio $\tilde{q}$, temperature $\tilde{T}$ and pressure $\tilde{P}$, calculated as prescribed above, will produce the same transmittance as layer with exponentially decreasing density and linear mixing ratio and temperature variations. The effective conditions, $\tilde{q}$ $\tilde{T}$ and $\tilde{P}$, are determined from boundary values alone.

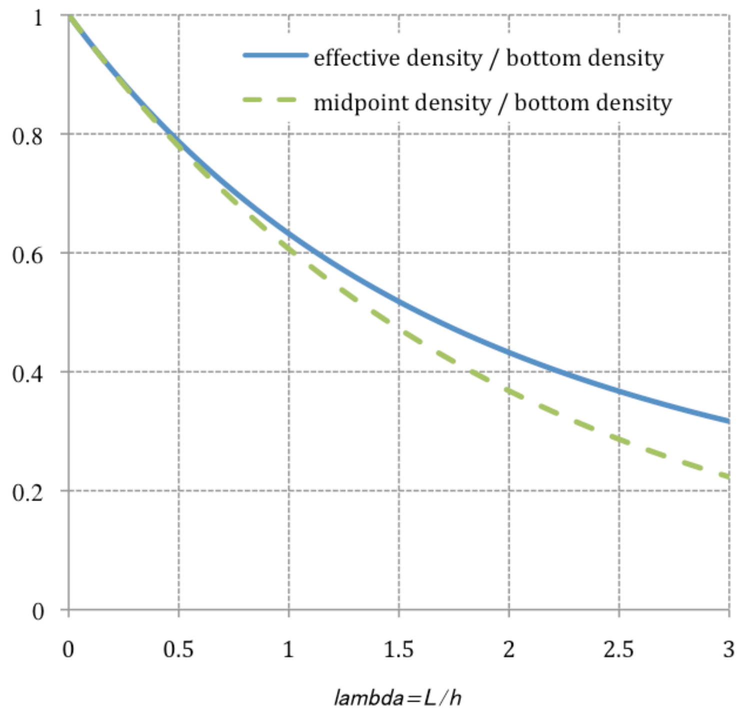

Fig. 1—Effective density. The effective density (blue curve) is plotted as a function of layer thickness. For comparison, the layer-midpoint density is shown (green dashed curve). For thin layers ($L < h$), the effective density is only slightly greater than the midpoint density, but for thicker layers it becomes substantially greater. For $L = h$, the effective density is only 4% greater than the midpoint density. For $L = 3h$, the effective density is 50% greater than the midpoint.

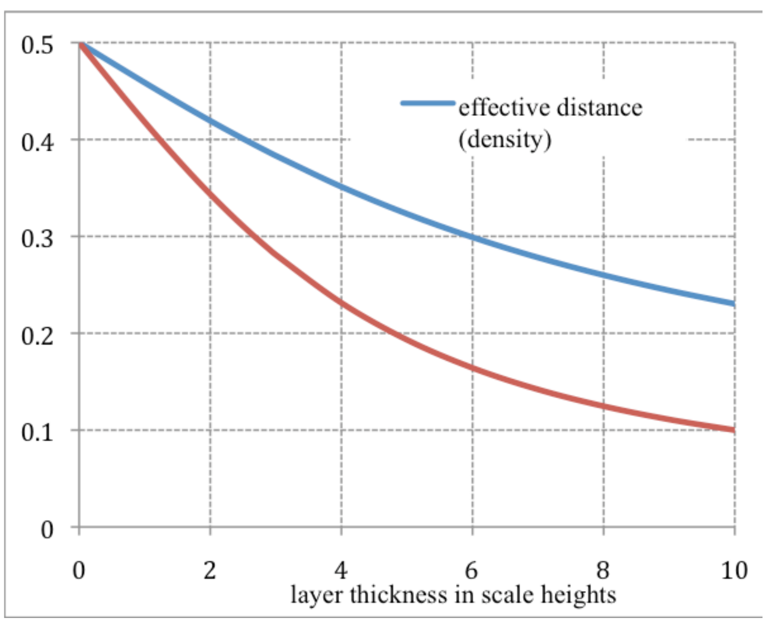

Fig. 2—Effective distance. The effective distance is the fractional distance from the layer bottom at which the effective density or mixing ratio occurs. For very thin layers, both the effective density and mixing ratio occur very near the midpoint of the layer. As the layer thickness grows, they occur closer to the bottom of the layer. For a 1-scale-height layer, the effective density occurs 46% of the way up from the bottom, whereas the effective mixing ratio occurs below this, only 42% from the bottom.