

Non-Grey Radiative Transfer

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May 25, 2011

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1 Non Grey Absorption

In many cases, the absorption of light can be modelled adequately using Beer’s law. Here the transmittance of light, with a wavelength range of λ to $\lambda + \Delta\lambda$, and through a mass of gas m with an absorption coefficient κ is given by

$$T = \exp(-\kappa m). \quad (1)$$

The assumes that all photons in the wavelength range “see” the same κ . When this is true the material is said to be “grey”. If κ varies very rapidly as a function of wavelength then Beer’s law cannot apply, and the material is said to be “non-grey”. In atmospheric applications m is usually given in terms of molecules per square centimetre, and so κ has units of area.

An example is given below in Fig.1 where the value of κ for O₂ is plotted over a very

small wavelength range close to 760nm. (This is an oxygen absorption feature.)

Oxygen Absorption

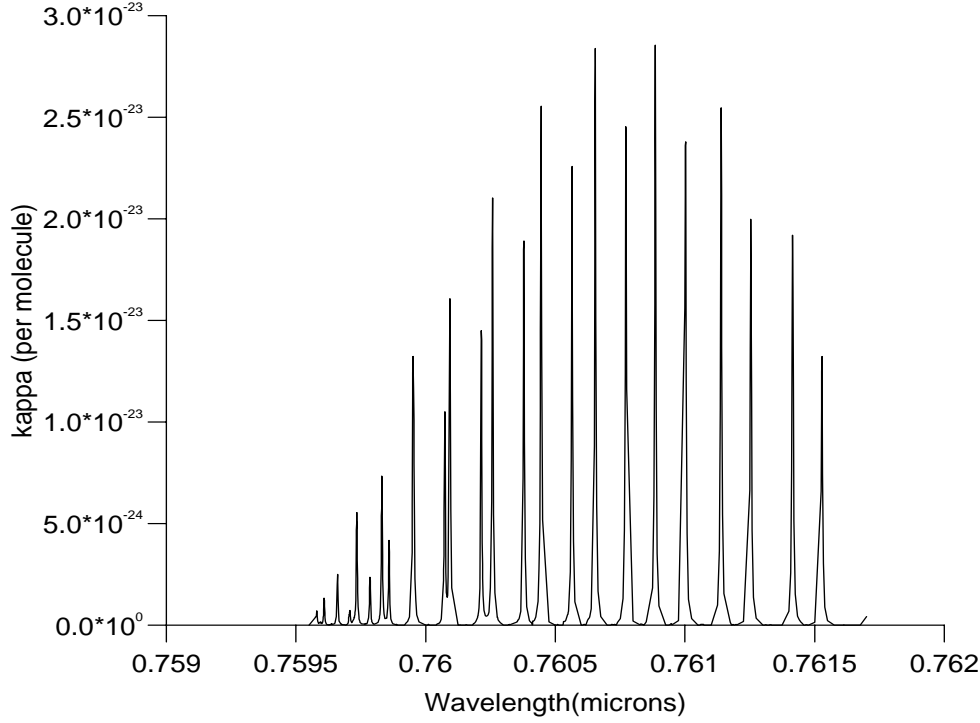


Figure 1: Oxygen absorption aoefficient in the lower atmosphere

The function $\kappa(\tilde{\nu})$ is obtained from

$$\kappa(\tilde{\nu}, p, T) = \sum^I S_I(\tilde{\nu}, T) f_I(\tilde{\nu}, p, T), \quad (2)$$

where κ is the absorption coefficient (cm^2), S_I is the line intensity (cm) of the I th line, and f_I is the normalised line shape for the I th line. The units given here are appropriate for use with the HITRAN database [1]. (This can be obtained via the website <http://cfa-www.harvard.edu/hitran>.) Other variables are the wavenumber $\tilde{\nu}$ (cm^{-1}), the temperature T (Kelvin), and pressure p (Pa). For an individual line, centred at $\tilde{\nu}_0$,

$$\kappa(\tilde{\nu}, p, T) = \kappa_0 V(x, y) = \kappa_0 \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{y^2 + (x - t)^2} dt. \quad (3)$$

Here $V(x, y)$ is the *Voigt function*. The details of the calculation of this function and the *HUMLIK* program are given by Wells [2].

In this notation, if $S(T)$ is the temperature dependent line strength,

$$\kappa_0 = \frac{S(T)}{\alpha_D(T)} \sqrt{\frac{\ln 2}{\pi}}, \quad (4)$$

$$x = \frac{\tilde{\nu} - \tilde{\nu}_0}{\alpha_D(T)} \sqrt{\ln 2}, \quad (5)$$

$$y = \frac{\alpha_L(p, T)}{\alpha_D(T)} \sqrt{\ln 2}. \quad (6)$$

The Doppler width (half width at half maximum) α_D and the Lorentz width α_L are given by

$$\alpha_D(T) = \frac{\tilde{\nu}_0}{c} \sqrt{\frac{2kT}{m} \ln 2}, \quad (7)$$

and

$$\alpha_L(p, T) = \alpha_L(p_0, T_0) \frac{p}{p_0} \left(\frac{T_0}{T} \right)^n. \quad (8)$$

There are slightly differing formula depending on whether the width is half or full, or whether the value of Doppler width is quoted at half maximum of $1/e$ of the maximum. Also, some authors incorporate the y/π into κ_0 . Also c is the speed of light *in vacuo* ($cm s^{-1}$), k is Boltzmann's constant (JK^{-1}), and m is the molecular weight (kg). Lastly p_0 and T_0 are reference pressures and temperatures, and n is a dimensionless coefficient of temperature dependence. In the lower atmosphere, where pressure broadening dominates over Doppler broadening, k can be approximated by the Lorentz profile

$$\kappa(\tilde{\nu}, p, T) = \frac{S(T)}{\pi} \frac{\alpha_L}{(\tilde{\nu} - \tilde{\nu}_0)^2 + \alpha_L^2} \quad (9)$$

The line intensity's temperature dependence, for a transition from state η to η' is given by

$$S_{\eta\eta'} = \frac{h\tilde{\nu}_{\eta\eta'}}{c} \frac{n_{\eta}}{N} \left(1 - \frac{g_{\eta}n_{\eta'}}{g_{\eta'}n_{\eta}} \right) B_{\eta\eta'}. \quad (10)$$

The prime demotes the upper state, the g s are state statistical weights, the n 's are the state populations and N is the molecular number density. The transition frequency converted to wavenumber is $\tilde{\nu}_{\eta\eta'}$, and B is the Einstein B coefficient. In thermodynamic equilibrium this simplifies to

$$S(T)_{\eta\eta'} = S(T_0) \frac{Q(T_0)}{Q(T)} \frac{\exp(-c_2 E_{\eta}/T) (1 - \exp(-c_2 \tilde{\nu}_{\eta\eta'}/T))}{\exp(-c_2 E_{\eta}/T_0) (1 - \exp(-c_2 \tilde{\nu}_{\eta\eta'}/T_0))}. \quad (11)$$

Here E_{η} is the lower state energy, c_2 is the second radiation constant $= hc/k$, and $Q(T)$ is the partition function. The latter is supplied as a table in HITRAN, and the lower state energy is also provided. The Lorentz width is obtained from

$$\alpha(T, p) = \left(\frac{T_0}{T} \right)^n \left(\alpha_{air}(p_0, t_0) \left(\frac{p - p_s}{p_0} \right) + \alpha_{self}(p_0, t_0) \frac{p_s}{p_0} \right), \quad (12)$$

where $\alpha_{air}(p_0, t_0)$, $\alpha_{self}(p_0, t_0)$, and n are taken from HITRAN tables, and p_s is the partial pressure. This is a more complicated version of eqn.8 which takes into account the collisions between molecules of the same species which have a larger effect than collisions with different species due to resonances; this is most important for oxygen.

Suppose more is required than just the direct transmittance T , and wanted to find the radiance field at the TOA (Top Of Atmosphere) say. It is possible, given the solar spectral irradiance curve, to find the radiance in a given direction, for a particular solar position.

An example is shown below in Fig.2

TOA Radiance

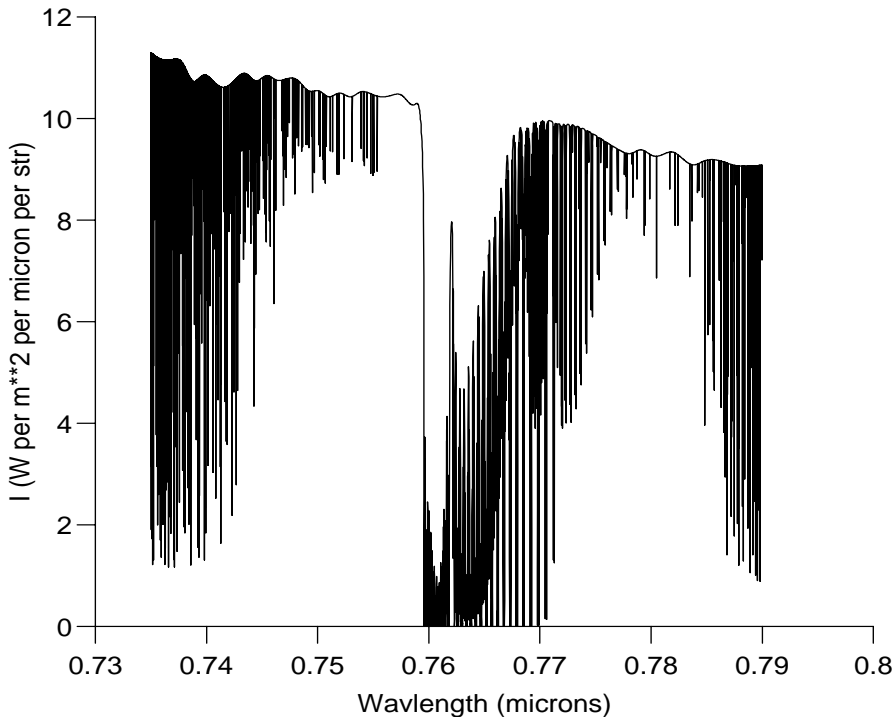


Figure 2: The upwelling radiance in a given direction at the TOA.

Here the wavelength interval is larger than that in Fig.1, the radiance in this wavelength interval is just the average of the radiances in the many (over 4000) expensive multiple scattering calculations.

An earlier method of coping with the non-grey nature of the atmosphere was to use band models. These are dealt with in well known books by Goody, and by Liou [3] [4]. In some applications these have the merit of capturing the non-grey nature of the atmospheric

radiation in tables which are small in size. However, where multiple scattering calculations are required the band models in themselves are of no use.

If greater accuracy is required and/or multiple scattering takes place, other methods must be used. Exponential sum fitting is one approach [5]. An early approach was to calculate the photon path length distribution [6] [7] [8]. It was realised that this was related to the inverse Laplace transform of the atmospheric transmittance. That is, the κ distribution function is the inverse Laplace transform of the atmospheric transmittance with the mass of gas as the transform variable.

$$T(m) = \int_0^\infty f(\kappa) e^{-\kappa m} d\kappa \quad (13)$$

Then the inverse transform $f(\kappa)$ is known as the κ distribution.

The κ distributions of the Malkmus band model are given by Goody[9]. The κ distribution for the exponential band model is given by Domoto [10], and by Godslove [11] in a form that is far more efficient for computation.

If more accuracy is required we must then return to the actual details of the spectra. We must directly calculate the κ distribution, and in a multiple layer atmosphere with varying temperature and pressure, we must use the cumulative distribution as discussed below.

1.1 The κ - and Correlated- κ approach

The correlated κ approach is given in some detail in [12] [13] [14] [15] [16]. We shall just look at the basic principles here.

On looking at Fig.3, it can be seen that the same values of κ are repeated many times over. Therefore, if only an average of many calculations is required rather than the full detail of Fig.2, it is clear that there is an opportunity for reducing the number of calculations needed drastically.

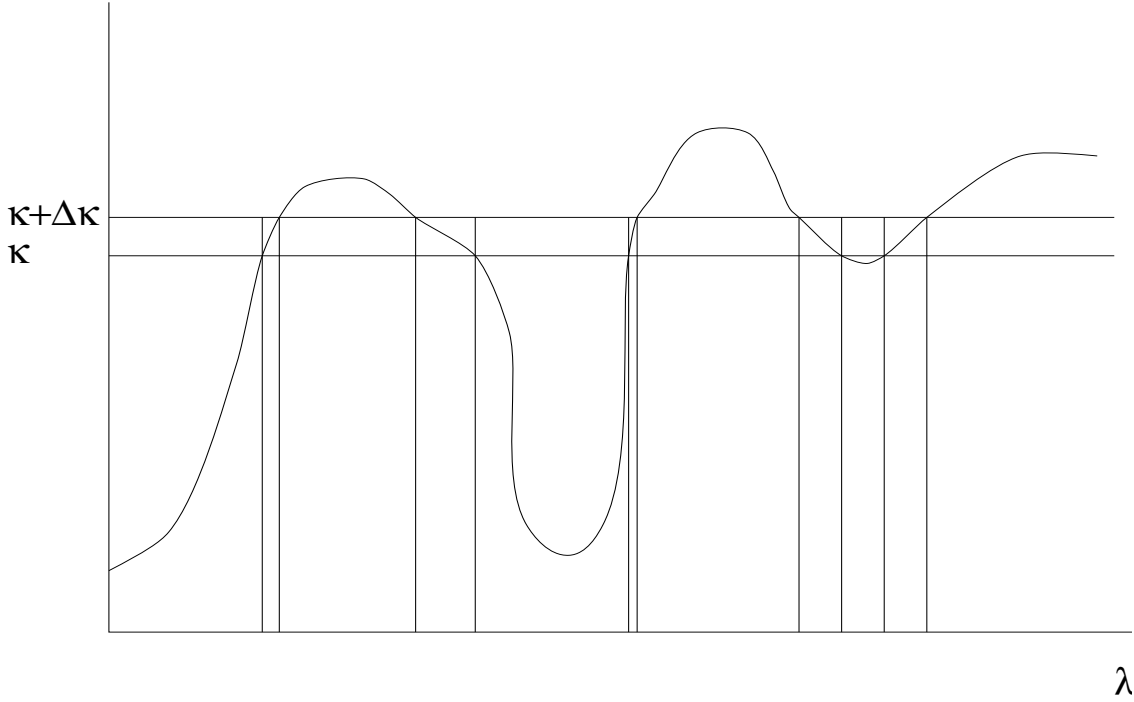


Figure 3: The fraction of photons that “see” an absorption coefficient between κ and $\kappa + \Delta\kappa$.

So, if radiance values were calculated for one wavelength with an absorption coefficient of κ , then several other wavelengths have values of κ very close to this value, and as an approximation, they can be lumped together in order to save CPU time (which can be considerable). If this is done for the whole range of κ values in the interval, then each radiance must be added in a weighted sum. The weight is simply the fraction of the λ interval that represents the subinterval of κ in the weighted sum. In other words the weight is the probability that a photon picked at random wavelength between λ and $\lambda + \Delta\lambda$ ‘sees’ an absorption coefficient between κ and $\kappa + \Delta\kappa$. If Q is any radiative quantity, then in the continuum limit, the average \overline{Q} is given by

$$\overline{Q} = \int_0^\infty f(\kappa') Q(\kappa) d\kappa \quad (14)$$

where $f(\kappa')$ is the probability density of finding a κ in the range κ and $\kappa + \Delta\kappa$. For instance, the transmittance is

$$\overline{T} = \int_0^\infty f(\kappa') \exp(-\kappa m) d\kappa. \quad (15)$$

In practice, the integrals are replaced by discrete sums, and the function f is also discrete. Suppose the function $\kappa_i(\lambda_i)$ is found for a large number of $i = 1, N$ at evenly spaced intervals $\delta\lambda = \Delta\lambda/N$ in the required wavelength range. Even if N is large enough to resolve the spectrum, there may be gaps where the difference between successive κ is

larger than the chosen bin size for κ . These gaps are unpredictable, and the same computer code must find the discrete probability density function for different gases, pressures and temperatures. Because of this, it is preferable to choose that M regular bins for the κ (subscript i), and values of λ (subscript j) so that the grid on λ to $\lambda + \Delta\lambda$ is not regular. Once this is done, we have M values for κ_i and an unpredictable N' values of λ_j . The

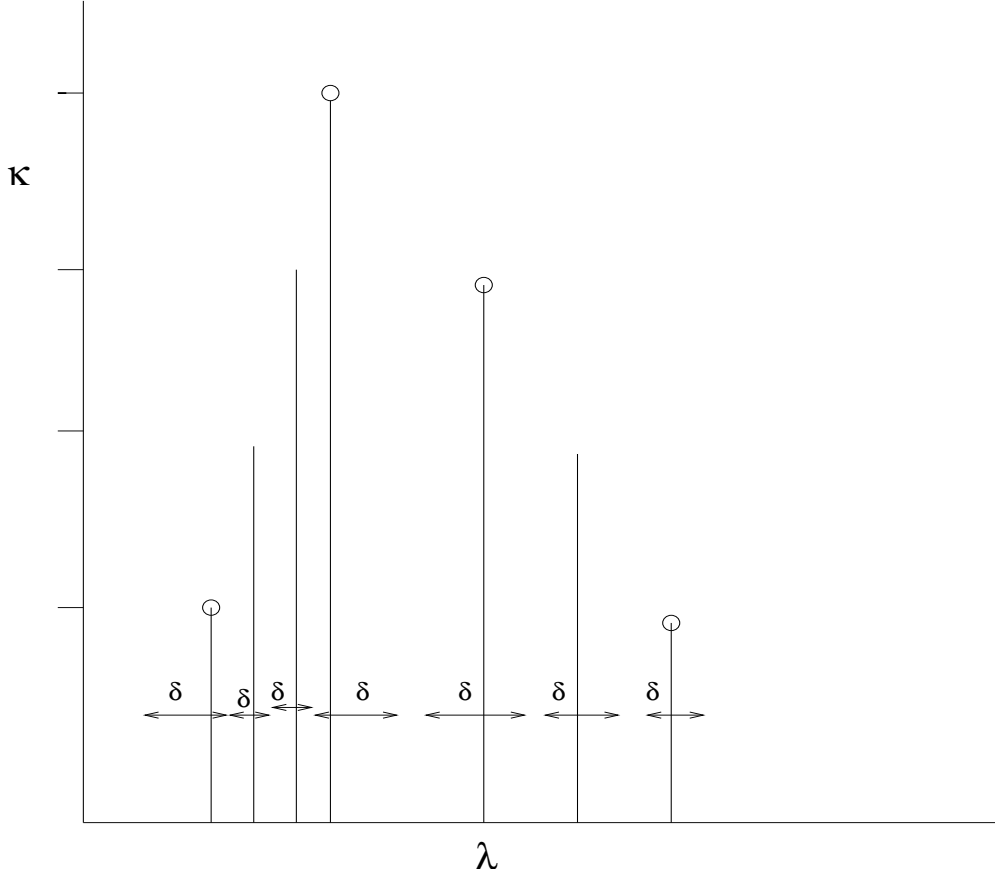


Figure 4: It is better to choose irregular bins over λ and regular bins over κ .

The function H_n is defined as follows.

$$H_n = \begin{cases} 1 & \text{if } n\delta\kappa < \kappa < (n+1)\delta\kappa \\ 0 & \text{otherwise.} \end{cases} \quad (16)$$

Here n ranges from 0 to M . Thus, for any given n , the κ distribution function is given by

$$f(\kappa)|_{(n+1/2)\delta\kappa} = \frac{1}{\lambda_2 - \lambda_1} \sum_{j=1}^{j=N'} H_j(n) \delta\lambda_j, \quad (17)$$

which is the fraction of the wavelength interval that is represented by the n th bin. The $\delta\lambda$ are the fractions of the total wavelength range associated with each of the λ_i . Clearly

$$\sum_{n=0}^{n=M} f_n = 1. \quad (18)$$

Given that a discrete approximation of $f(n)$ is calculated, the κ distribution function can be used to calculate any radiative quantity via eqn.13. However there is a real snag. In a real atmosphere, there are variations in temperature and pressure as a function of height. In a single layer, it can be said that a certain fraction of photons see such and such a κ value, but when these photons enter another layer at a different temperature and pressure, there is no way of saying what κ values should be assigned in the second layer. It has been shown that, for the Lorentz profile and a few others, that this problem can be overcome by using the cumulative distribution instead, i.e.

$$g(k) = \int_0^k f(\kappa') d\kappa'. \quad (19)$$

Then eqn.14 transforms into

$$\overline{T} = \int_0^1 \exp(-\kappa(g)m) dg, \quad (20)$$

or in general

$$\overline{Q} = \int_0^1 Q(\kappa(g)) dg. \quad (21)$$

So, for certain absorption line profiles, the κ values used in a quadrature approximation to

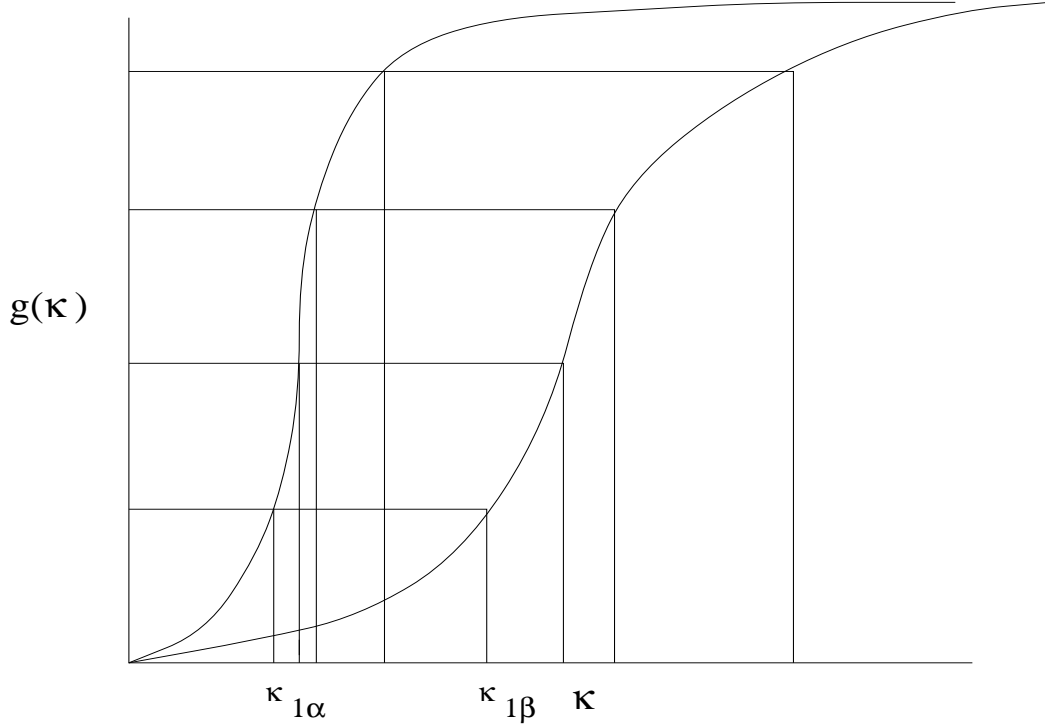


Figure 5: The two cumulative distributions correspond to different pressures and temperatures.

eqns.18 and 19 are 100% correlated. All the photons that see the value of $\kappa_{1\alpha}$ in one layer

see the value $\kappa_{1\beta}$ in the other. Because of this, when the cumulative distribution is used rather than using the κ distribution directly, the method may be described as the *correlated* κ method. In general this is not exactly true, but the correlations are high enough for this correlated κ method to be a good approximation.

1.2 Snags

All seems well so far, but this is not the case if actual radiance values are needed in some wavelength interval. This is because the solar spectral irradiance $S(\lambda)$ will vary across the wavelength interval. what is more, if a prediction of a given instrument reading is required, the instrument response function $R_{esp}(\lambda)$. If exact calculations are required, each κ value ‘sees’ a whole range of response function values, so in a numerical approximation of eqn.18

$$\bar{T} = \sum_{p=1}^{p=P} w_p \exp(-\kappa_p(g)m) \quad (22)$$

would turn into a double summation

$$\bar{T} = \sum_{p=1}^{p=P} \sum_{q=1}^{q=Q} w_q w_p R_{esp\,q} \exp(-\kappa_p(g)m) \quad (23)$$

in order to take into account the range of response function variation across each κ_p . This would then turn into a triple sum when the solar variation was included. This could easily turn out to be just as expensive as doing the fine detail calculations of Fig.2. Instead, we might use the approximation that

$$\bar{T} = \sum_{p=1}^{p=P} \overline{R_{esp} S_p} w_p \exp(-\kappa_p(g)m). \quad (24)$$

Here $\overline{R_{esp} S_p}$ is the mean value of the solar response times the response function calculated for each κ_p . This goes some way to taking into account how the absorption coefficient varies across the response function.

The final problem is how to deal with the radiance at the top of the atmosphere.

$$\bar{I} = \sum_{p=1}^{p=P} \overline{R_{esp} S_p} w_p I(\kappa_p, R), \quad (25)$$

where R is the reflectance at the ground level. The problem here as things stand is that if R varies with wavelength in the wavelength interval covered by the response function, then it is longer a matter calculating predefined weights for a given problem. The solution of the radiative transfer problem itself depends on the reflectance spectrum as well as the κ values inserted into each layer of atmosphere. What is needed is a list of what reflectance value, on average, is needed for each κ_p , then

$$\bar{I} = \sum_{p=1}^{p=P} \overline{R_{esp} S_p} w_p I(\kappa_p, R_p). \quad (26)$$

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