Infrared radiative transfer in the 9.6-μm band: Application to TIROS operational vertical sounder ozone retrieval

Richard J. Engelen[1]

Institute for Marine and Atmospheric Research Utrecht, Utrecht University, Utrecht, The Netherlands

Graeme L. Stephens[1]

Cooperative Research Center for Southern Hemisphere Meteorology, Clayton, Victoria, Australia

Abstract. This paper introduces a radiative transfer model for the 9.6-μm ozone band that specifically matches the TIROS operational vertical sounder (TOVS) channel 9. The model is based on a spectral Malkmus band model for transmission. Band parameters were calculated by comparing to MODTRAN3 derived radiances. The effect of pressure on absorption is dealt with using a four-parameter approximation, and the improvements of this approximation over the more common Van de Hulst-Curtis-Godson scaling approximation are assessed. While this new model is exploited in the development of the retrieval described in this paper, the result has wider applicability to ozone climate problems requiring calculation of the radiative forcing associated with changing ozone. A two-layer version of the radiative transfer model is implemented in a retrieval scheme to obtain total ozone amounts from radiances measured by the TOVS instrument. Because the TOVS ozone channel is mainly sensitive to lower stratospheric ozone, ozone columns of the upper layer (above 30 hPa and with mean pressure of 10 hPa) are prescribed as a function of latitude. Ozone columns of the lower layer (mean pressure of 105 hPa) are then retrieved. The retrieval is based on a nonlinear optimal estimation algorithm and provides definition of error characteristics for every retrieval, which makes it possible to obtain a spatial distribution of the errors in the retrieval together with the spatial distribution of the retrieved total ozone column itself. This global distribution of the retrieval error and also of the contribution of a priori knowledge to the retrieval is presented to provide a validity of the ozone retrievals. Total ozone mapping spectrometer (TOMS) statistics are used as a priori information in the retrieval, and the 40-layer model is used to estimate the forward model error of the two-layer model. Comparisons of ozone retrievals for 1989 with TOMS total ozone measurements show good agreement both in time and in space with a rms difference between 1% and 3% for zonal means and 10% for global gridded measurements.

1. Introduction

One of the most significant environmental issues of this century is the observed loss of polar stratospheric ozone referred to as the "ozone hole" and first reported by *Farman et al.* [1985]. This loss is seasonal and occurs largely over the southern pole [*Stolarski et al.*, 1986], although significant losses of ozone have also been reported in the higher latitudes of the northern hemisphere [*Gleason et al.*, 1993; *Planet et al.*, 1994]. Whereas the mechanisms responsible for the loss of ozone are now largely understood, a number of critical is-

[1]Now at Department of Atmospheric Science, Colorado State University, Fort Collins.

sues remain to be addressed. For instance, the evolution of the ozone hole and the role of transport into and from the polar vortex, the life cycle of the ozone hole and the interannual variability of the ozone hole are topics of current research.

Along with the improvements in modeling the ozone hole and with progress toward prediction of its evolution on timescales of a few days to a week or so, comes the need for reliable global measurements of the three-dimensional distribution of ozone. In the polar regions, highly resolved stratospheric ozone profiles are provided by measurements of the UARS satellite [*Waters et al.*, 1993; *Froidevaux et al.*, 1994]. To date, the main satellite instrumentation used for continuous monitoring of the two-dimensional distribution of the ozone layer is the total ozone mapping spectrometer (TOMS) instrument [*Bowman and Krueger*, 1985]. While this instrument has provided the primary source of observations since 1978, recent failure of TOMS on board the Meteor 3 satellite has heightened interest in other ozone sensors. The companion to TOMS is the solar backscattered ultraviolet (SBUV) instrument, and significant effort has been spent recently on the development of operational SBUV retrievals [*Ahmad et al.*, 1994; *Hilsenrath et al.*, 1995]. Both the TOMS and SBUV measure backscattered ultraviolet sunlight and cannot provide retrievals in the polar night region during winter and early spring.

Infrared radiance data in the 9.6-μm channel of the TIROS operational vertical sounder/ high-resolution infrared radiation sounder (TOVS/ HIRS) flown on NOAA operational satellites (for an extensive description of the instruments, see *Smith et al.* [1979]) can also be used to retrieve total ozone amounts. While the retrieval of ozone based on infrared radiance data offers an advantage over UV backscatter measurements in regions of polar night, IR techniques suffer for reasons explored in this paper. The purpose of this paper is to introduce a physically based retrieval of column ozone applied to TOVS radiance data in order to retrieve a useful ozone climatology based on the long time series of TOVS observations. While other retrievals exist [e.g., *Planet et al.*, 1984; *Ma et al.*, 1984; *Lefèvre et al.*, 1991; *Neuendorffer*, 1996], this paper revisits the issue of infrared radiative transfer through ozone and introduces a new retrieval based on this theory. Also, special attention is paid to the errors in the retrieval, which are especially important when measurements have to be compared with models. The extensive treatment of the radiative transfer and the used error analysis improve the characterization of the retrieval product compared to the existing methods.

The theory of radiative transfer at frequencies of the TOVS ozone channel is introduced in the next section, followed by an outline of a simple forward model used as the basis for the retrieval. Section 4 outlines the retrieval approach based on the nonlinear optimal estimation approach of *Rodgers* [1976]. A particular advantage of this approach over others is that it offers a clear characterization of the retrieval uncertainties and the information content of the retrievals. In section 5 the new retrieval is applied to global TOVS data for 1989 and compared with favorable results to the TOMS data for the same period.

2. Radiative Transfer

The basis underlying any satellite retrieval method is a radiative transfer model that calculates the radiation at the top of the atmosphere for a given distribution of trace gases (CO_2, H_2O, and O_3) and temperature (this is referred to as the forward model). For the problem of relevance in this paper, the equation for the monochromatic radiance at the top of the atmosphere for a plane parallel non-refracted path at a certain viewing angle θ is

$$I_\nu(0,\mu) = B_\nu(T(\tau_s))e^{-\tau_s/\mu} + \int_0^{\tau_s} B_\nu(T(\tau))e^{-\tau/\mu}\mu^{-1}d\tau \ , \quad (1)$$

where $I_\nu(\tau,\mu)$ is radiance, μ is $\cos\theta$, τ is optical depth, and $B_\nu(T(\tau))$ is Planck radiance for temperature T as a function of τ. TOVS satellite radiance data are broadband, and simulation of these radiances based on equation (1) requires some kind of spectral integration which must include in these integrals the instrument filter response functions. A practical form of this integration is

$$I(0,1) = \sum_{j=1}^{N} f_j \Delta\nu_j \Big[B_j(T(\tau_{s,j})\mathcal{T}_j(\tau_{s,j}) + \int_0^{\tau_{s,j}} B_j(T(\tau_j))\mathcal{T}_j(\tau_j)d\tau_j\Big] \ , \quad (2)$$

where the spectral integration is carried out as a summation over a finite number of N subintervals chosen to resolve the spectral structure of the sensor filter function f_j and μ is set to 1 (nadir sounding). $\mathcal{T}_j$ is the transmittance from the top of the atmosphere to a specified level

$$\mathcal{T}_j(\tau) = \frac{1}{\Delta\nu_j}\int_{\Delta\nu_j} e^{-\tau_\nu}d\nu \ , \quad (3)$$

where

$$\tau_\nu = k_\nu\, u \ . \quad (4)$$

Here, k_ν is the absorption coefficient and u is the amount of absorbing matter.

Two issues that must be addressed in evaluating the forward model of TOVS channel 9 radiances are a suitable way of evaluating the broadband transmission (equation (3)) and an appropriate way to integrate over optical path, which is especially complex for ozone absorption because of the combined effects of the dependence of absorption on pressure and the variation of ozone concentration with pressure.

Two-Parameter Band Model

We demonstrate that a two-parameter band model adequately represents the broadband transmission along paths of complex pressure variation. We begin with the introduction of the Malkmus band model [*Malkmus*, 1967; *Goody and Yung*, 1989], which expresses the transmittance as a function of absorber amount at fixed pressure and temperature as

$$\mathcal{T}(u) = \exp\left[-\frac{\pi\alpha_{\mathrm{L}}}{2\,\delta}\left(\sqrt{1+\frac{4Su}{\pi\alpha_{\mathrm{L}}}}-1\right)\right] , \quad (5)$$

with S the average line intensity, α_{L} the average Lorentz line width, and δ the average line spacing. Broadband transmission is evaluated given suitable values of the band parameters α_{L} and S. These are obtained from line absorption data by requiring exact agreement in the weak-line and strong-line limits. This gives the following expression:

$$\mathcal{T}(u) = \exp\left[-\frac{2X^2}{Y\Delta\nu}\left(\sqrt{1+\frac{Y^2u}{X^2}}-1\right)\right] , \quad (6)$$

where X and Y are related to the statistical line parameters by

$$X = \sum_i^N (S_i\,\alpha_i)^{\frac{1}{2}} , \quad (7)$$

$$Y = \sum_i^N S_i , \quad (8)$$

and where $\Delta\nu$ is the bandwidth. According to *Goody and Yung* [1989], the error in the band transmittance due to the use of the Lorentz line shape instead of the Voigt line shape is less than 2.6% and for the ozone absorption band is even less than 0.16%. The Malkmus band model parameters X and Y were calculated by fitting to MODTRAN3 [*Berk et al.*, 1989] derived transmittances at a resolution of 1 cm^{-1} as a function of the optical path of the absorbers rather than by summing over spectral line data. For the water vapor absorption only, the line absorption was used. For each TOVS channel the channel transmittance was then calculated as

$$\bar{\mathcal{T}}(u) = \frac{\sum_{j=1}^N f_j \mathcal{T}_j(u)}{\sum_{j=1}^N f_j} , \quad (9)$$

where the summation is over the band defined by the channel filter function f_j and where $\mathcal{T}_j(u)$ are the MODTRAN derived transmittances. The band parameters so derived are given in Table 1 for channels 1, 2, 8, 9, 10 using NOAA10 filter functions.

In Figure 1 the transmittance of TOVS channel 9 as function of constant pressure absorber path length is shown for both MODTRAN and the band model using the parameters of Table 1. The pressure and temperature used in the calculation are 1013 hPa and 235 K, respectively.

As done by *Clough et al.* [1989], the absorption due to the water vapor continuum is parameterized as

$$\mathcal{T}(u) = \exp(-\tau_{\mathrm{cont}}) , \quad (10)$$

where the continuum optical depth is

$$\tau_{\mathrm{cont}} = \nu_0\left[C_s\frac{p_w}{p_0} + C_f\frac{p}{p_0}\right]\left(\frac{T_0}{T}\right)u , \quad (11)$$

where u is the vertical path of water vapor, p_w and p denote the water vapor partial pressure and the ambient pressure, respectively, T is the temperature, C_s and C_f are the self- and foreign-broadening coefficients for water vapor, respectively, ν_0 is the central wavenumber of the band, and T_0 and p_0 are 296 K and 1013 mbar, respectively. The values of ν_0, C_s, and C_f are also given in Table 1 for each channel.

The radiative transfer model using the band transmission functions and band-corrected Planck functions specific to each channel [e.g., *Weinreb et al.*, 1981] was used to simulate channel brightness temperatures for each of the 1761 TOVS initial guess retrieval (TIGR2) atmospheric profiles [*Scott et al.*, 1991]. Each set of TIGR2 profiles consists of an ozone, a water vapor, and a temperature profile.

Pressure Dependence of Transmission

It was mentioned above how the transmission through ozone is complicated by the different dependences of the line absorption on the ozone profile and the pressure. The common approach for dealing with pressure scaling is the Van de Hulst-Curtis-Godson (HCG) method [*Goody and Yung*, 1989]. This method can be applied to the band model in the following way. In the HCG approximation, the scaled absorber amount $\tilde{u}$ is

$$\tilde{u} = \int_{\mathrm{path}} \frac{Y(T)}{Y(\tilde{T})}du , \quad (12)$$

and the scaled pressure $\tilde{p}$ is

$$\tilde{p} = \int_{\mathrm{path}} \frac{X^2(T)}{X^2(\tilde{T})}\frac{du}{\tilde{u}} , \quad (13)$$

where X and Y are as defined before and $\tilde{T}$ is a scaled temperature. If we neglect temperature dependence (MODTRAN

Table 1. Malkmus Band Parameters for NOAA10 HIRS

Channel	Gas	X, $cm^{-1}kg^{-1/2}m$	Y, $cm^{-1}kg^{-1}m^2$	C_s, $kg^{-1}m^2\,cm$	C_f, $kg^{-1}m^2\,cm$	ν_0, cm^{-1}
1	H_2O	0.35	0.82	5.18×10^{-3}	8.49×10^{-6}	667.70
	CO_2	42.19	9087.5			
	O_3	12.96	27.89			
2	H_2O	0.41	0.7	4.54×10^{-3}	6.38×10^{-6}	680.23
	CO_2	64.32	1325.2			
	O_3	32.83	77.44			
8	H_2O	0.05	0.02	1.12×10^{-3}	4.81×10^{-8}	899.50
	CO_2	0.05	0.01			
	O_3	0.01	1.6			
9	H_2O	0.05	0.02	5.18×10^{-4}	6.35×10^{-9}	1029.01
	CO_2	0.08	0.01			
	O_3	201.23	3045.07			
10	H_2O	0.42	0.43	3.51×10^{-4}	3.21×10^{-7}	1224.07
	CO_2	0.03	0.03			
	O_3	0.68	4.17			

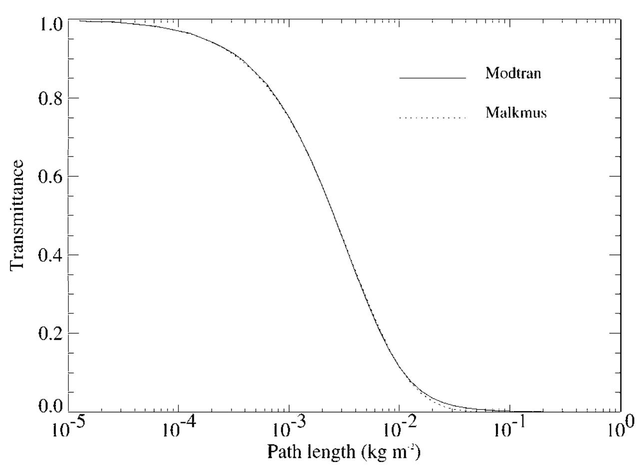

Figure 1. Comparison between MODTRAN and Malkmus band model fit to the transmission derived using the NOAA10 filter function for TOVS channel 9. The transmissions are shown as a function of the constant pressure absorber path length.

$$\int_{\text{path}}$$

The scaled absorber amount is applied directly in (6) and the pressure $\tilde{p}$ is used to scale the X^2 factors in (6). The results of simulated channel 9 radiances using the band model (6) with the parameters of Table 1 and the HCG method are shown in Figure 2 and contrasted against the corresponding brightness temperatures derived using MODTRAN. Each point represents a pair of band model and MODTRAN simulations using a single TIGR2 atmosphere. A very good agreement is observed between the two models, with the MODTRAN brightness temperatures slightly higher than the band model brightness temperatures.

Walshaw and Rodgers [1963] and *Goody* [1964] demonstrate the satisfactory nature of the HCG approximation for the absorption by water vapor and carbondioxide. The method, however, breaks down for ozone where the absorption falls between the strong and weak limits due to high concentrations that exist at low pressure and low concentrations at high pressure. To assess how these pressure effects might affect our ability to simulate radiances in the 9.6-μm band, we adopted the approach of *Walshaw and Rodgers* [1963]. We begin with the Malkmus band model in the spectral integral form,

$$\bar{\mathcal{T}}(\phi, \phi') = \exp\left[-\frac{\beta_s}{\pi}\int_0^\infty \ln(1+\tau_\nu)\, dy\right], \tag{16}$$

where the optical depth of a Lorentz line is

$$\tau_\nu = 2\int_\phi^{\phi'} \frac{\eta\phi}{y^2+\phi^2}\, d\phi\,, \tag{17}$$

where $\phi = p/p_0$, $y = \nu/\alpha_{\mathrm{L}}$. The dimensionless variable η is defined as

$$\eta = \frac{k p_s \zeta}{2\pi\alpha_s g}\,, \tag{18}$$

where k is the mean line intensity, p_s the surface pressure, α_s is the mean line width at surface pressure, g is the gravity constant, and ζ is the ozone mass mixing ratio. With an ozone mixing ratio profile of the form

$$\zeta(\phi) = \zeta_{\max}\frac{4a\phi^2}{(1+a\phi^2)^2}\,, \tag{19}$$

effects of pressure on transmission. This integral was evaluated using a Romberg quadrature scheme on a open interval [*Press et al.*, 1989].

We can use the same model under the HCG approximation in the form

$$\bar{\mathcal{T}}(\phi, \phi') = \exp\left[-\beta_s\left(-\frac{G_1}{G_0} + \sqrt{2G_1 + (G_1/G_0)^2}\right)\right], \tag{21}$$

where

$$G_0 = \int_\phi^{\phi'} \eta\, d\phi, \qquad G_1 = \int_\phi^{\phi'} \eta\phi\, d\phi\,.$$

With (19), these integral functions are

$$G_0 = 2\eta_{\max}\left[\frac{\phi}{1+a\phi^2} - \frac{\phi'}{1+a\phi'^2} + \frac{\arctan(\sqrt{a}\phi') - \arctan(\sqrt{a}\phi)}{\sqrt{a}}\right] \tag{22}$$

$$G_1 = 2\eta_{\max}\left[\frac{1}{a+a^2\phi'^2} - \frac{1}{a+a^2\phi^2} + \frac{\ln(1+a\phi'^2) - \ln(1+a\phi^2)}{a}\right]. \tag{23}$$

The transmittance calculated using the Walshaw and Rodgers model (equations (16) and (17)) is contrasted in Figure 3 with the transmittance derived using equation (21). The transmittances, shown as a function of height, were obtained using the same values for a and $\zeta_{\max}$ as *Walshaw and Rodgers* [1963], and a value of $\eta_{\max}$ and β_s chosen to represent the TOVS channel 9. The values of these parameters relevant to Figure 3 are 1600, 10 ppmm, 11.84, and 2.66 for a, $\zeta_{\max}$, $\eta_{\max}$, and β_s, respectively. The comparisons reveal that the transmittances below 20 km differ significantly, with the transmittance of the HCG model less than the transmittance of the exact model. These transmittances were applied in the radiative transfer model together with the temperature profiles of the TIGR2 data set to determine the effect of these transmission differences on brightness temperatures. The model using the HCG approximation yields brightness temperatures that are 1.2 K (0.5 %) lower on average than the exact model.