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

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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-

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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 (CO₂, H₂O, and O₃) 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

\[ I_\nu(0, \mu) = B_\nu(T) e^{-\tau_\nu / \mu} + \int_0^{\tau_\nu} B_\nu(T(\tau)) e^{-\tau_\nu / \mu} \mu^{-1} d\tau, \]

where \( I_\nu(\tau, \mu) \) is radiance, \( \mu = \cos \theta \), \( \tau \) is optical depth, and \( B_\nu(T(\tau)) \) is Planck radiance for temperature \( T \) as a function of \( \tau \). 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

\[ I(0, 1) = \sum_{j=1}^{N} f_j \Delta \nu_j \left[ B_j(T(\tau_{s,j})T_j(\tau_{s,j}) \right. \]

\[ + \int_0^{\tau_{s,j}} B_j(T(\tau)) T_j(\tau) d\tau_j \right], \]

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 \( \mu \) is set to 1 (nadir sounding). \( T_j \) is the transmittance from the top of the atmosphere to a specified level

\[ T_j(\tau) = \frac{1}{\sum f_j \Delta \nu_j} \int \frac{e^{-\tau_\nu}}{\Delta \nu_j} d\nu, \]

where

\[ \tau_\nu = k_\nu u. \]

Here, \( k_\nu \) 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 es-
specially complex for ozone absorption because of the com-
bined 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 ade-
quately represents the broadband transmission along paths of
complex pressure variation. We begin with the introduction
of the Malkmus band model \cite{Malkmus1967, Goody1989}, which expresses the transmittance as a function
of absorber amount at fixed pressure and temperature as
\[ T(u) = \exp\left[-\frac{\pi \alpha_1}{2 \delta} \left(1 + \frac{4Su}{\pi \alpha_1} - 1 \right)\right], \tag{5} \]
with \( S \) the average line intensity, \( \alpha_1 \) the average Lorentz line
width, and \( \delta \) the average line spacing. Broadband transmis-
sion is evaluated given suitable values of the band parameters
\( \alpha_1 \) 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:
\[ T(u) = \exp\left[-\frac{2X^2}{Y \Delta \nu} \left(1 + \frac{Y^2u}{X^2} - 1 \right)\right], \tag{6} \]
where \( X \) and \( Y \) are related to the statistical line parameters by
\[ X = \sum_{i=1}^{N} (S_i \alpha_i)^+, \tag{7} \]
\[ Y = \sum_{i=1}^{N} S_i, \tag{8} \]
and where \( \Delta \nu \) is the bandwidth. According to Goody and
Yung \cite{Goody1989}, the error in the band transmittance due to the
use of the Lorentz line shape instead of the Voigt line shape is
less than 0.16\%.

The Malkmus band model parameters \( X \) and \( Y \) were calculated by fitting to MODTRAN3 \cite{Berk1989} 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 ab-
sorption only, the line absorption was used. For each TOVS
channel the channel transmittance was then calculated as
\[ \tilde{T}(u) = \frac{\sum_{j=1}^{N} f_j T_j(u)}{\sum_{j=1}^{N} f_j}, \tag{9} \]
where the summation is over the band defined by the chan-
nel filter function \( f_j \) and where \( T_j(u) \) 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 func-
tion 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 calcu-
lation are 1013 hPa and 235 K, respectively.

As done by Clough et al. \cite{Clough1989}, the absorption due to the
water vapor continuum is parameterized as
\[ T(u) = \exp(-\tau_{cont}) \tag{10} \]
where the continuum optical depth is
\[ \tau_{cont} = \nu_0 \left[C_s \frac{p_w}{p_0} + C_f \frac{p}{p_0} \right] \left(\frac{T_0}{T}\right) u, \tag{11} \]
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, respec-
tively, \( \nu_0 \) is the central wavenumber of the band, and \( T_0 \) and
\( p_0 \) are 296 K and 1013 mbar, respectively. The values of \( \nu_0, \)
\( C_s, \) 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 \cite[e.g.,][]{Weinreb1981} was used to simulate
channel brightness temperatures for each of the 1761 TOVS
initial guess retrieval (TIGR2) atmospheric profiles \cite{Scott1991}.
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 com-
mon approach for dealing with pressure scaling is the Van
de Hulst-Curtis-Godson (HCG) method \cite{Goody1989}. This method can be applied to the band model in the
following way. In the HCG approximation, the scaled ab-
sorber amount \( \tilde{u} \) is
\[ \tilde{u} = \int \frac{Y(T)}{Y(T)} du, \tag{12} \]
and the scaled pressure \( \tilde{p} \) is
\[ \tilde{p} = \int \frac{X^2(T)}{X^2(T)} \frac{du}{\tilde{u}}, \tag{13} \]
where \( X \) and \( Y \) are as defined before and \( \tilde{T} \) is a scaled tem-
perature. If we neglect temperature dependence (MODTRAN
Table 1. Malkmus Band Parameters for NOAA10 HIRS

<table>
<thead>
<tr>
<th>Channel</th>
<th>Gas</th>
<th>( X_n ) ( cm^{-1} kg^{-1/2} m \cm^{-1} )</th>
<th>( Y_k ) ( kg^{-1} m^2 )</th>
<th>( C_{\nu_0} ) ( kg^{-1} m^2 cm )</th>
<th>( C_{\nu_0}^{+} ) ( kg^{-1} m^2 cm )</th>
<th>( \nu_0 ) ( cm^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H(_2)O</td>
<td>0.35</td>
<td>0.82</td>
<td>5.18 \times 10^{-3}</td>
<td>8.49 \times 10^{-6}</td>
<td>667.70</td>
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<td></td>
<td>CO(_2)</td>
<td>42.19</td>
<td>9087.5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>O(_3)</td>
<td>12.96</td>
<td>27.89</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>H(_2)O</td>
<td>0.41</td>
<td>0.7</td>
<td>4.54 \times 10^{-3}</td>
<td>6.38 \times 10^{-6}</td>
<td>680.23</td>
</tr>
<tr>
<td></td>
<td>CO(_2)</td>
<td>64.32</td>
<td>1325.2</td>
<td></td>
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</tr>
<tr>
<td></td>
<td>O(_3)</td>
<td>32.83</td>
<td>77.44</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>H(_2)O</td>
<td>0.05</td>
<td>0.02</td>
<td>1.12 \times 10^{-3}</td>
<td>4.81 \times 10^{-8}</td>
<td>899.50</td>
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<td>O(_3)</td>
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<td>1.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>H(_2)O</td>
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<td>0.02</td>
<td>5.18 \times 10^{-4}</td>
<td>6.35 \times 10^{-9}</td>
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<td>CO(_2)</td>
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<td>0.01</td>
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<tr>
<td></td>
<td>O(_3)</td>
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<td>3045.07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>H(_2)O</td>
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<td>0.43</td>
<td>3.51 \times 10^{-4}</td>
<td>3.21 \times 10^{-7}</td>
<td>1224.07</td>
</tr>
<tr>
<td></td>
<td>CO(_2)</td>
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<td>0.03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>O(_3)</td>
<td>0.68</td>
<td>4.17</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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.
calculations showed that the temperature dependence of the TOVS ozone absorption band is small), the HCG approximation becomes
\[
\tilde{u} = \int_{\text{path}} du = u ,
\]
and
\[
\tilde{p} = \int_{\text{path}} p \, du / \tilde{u} .
\]
The scaled absorber amount is applied directly in (6) and the pressure \( \tilde{p} \) is used to scale the \( \chi^2 \) 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 carbon dioxide. 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-\( \mu \)m band, we adopted the approach of Walshaw and Rodgers [1963]. We begin with the Malkmus band model in the spectral integral form,
\[
\tilde{T}(\phi, \phi') = \exp \left[ -\frac{\beta_\phi}{\pi} \int_0^\infty \ln(1 + \tau_\nu) \, dy \right] ,
\]
where the optical depth of a Lorentz line is
\[
\tau_\nu = 2 \int_\phi^{\phi'} \frac{\eta \phi}{y^2 + \phi^2} \, dy ,
\]
where \( \phi = p / p_0 , \) \( y = \nu / \alpha_1 . \) The dimensionless variable \( \eta \) is defined as
\[
\eta = \frac{k p_s \zeta}{2 \pi \alpha_s g} ,
\]
where \( k \) is the mean line intensity, \( p_s \) the surface pressure, \( \alpha_1 \) is the mean line width at surface pressure, \( g \) is the gravity constant, and \( \zeta \) is the ozone mass mixing ratio. With an ozone mixing ratio profile of the form
\[
\zeta(\phi) = \zeta_{\text{max}} \frac{4 a \phi^2}{(1 + a \phi^2)^2} ,
\]
the optical depth can be written as [see Walshaw and Rodgers, 1963]
\[
\tau_\nu = \frac{4 \eta_{\text{max}}}{b^2} \left\{ (1 + b) \ln \frac{1 + b \chi}{1 + b \chi'} + b(\chi' - \chi) \right\} ,
\]
where \( b = a \phi^2 - 1 \) and \( \chi = (1 + a \phi^2)^{-1} . \)

The transmission along a path from pressure \( \phi \) to pressure \( \phi' \) is evaluated explicitly by integrating (16) providing exact effects of pressure on transmission. This integral was evaluated using a Romberg quadrature scheme on an open interval [Press et al., 1989].

We can use the same model under the HCG approximation in the form
\[
\tilde{T}(\phi, \phi') = \exp \left[ -\beta_\phi \frac{(G_1 \mp \sqrt{2G_1 + (G_1 / G_0)^2})}{G_0} \right] ,
\]
where
\[
G_0 = \int_\phi^{\phi'} \eta \, d\phi , \quad G_1 = \int_\phi^{\phi'} \eta \phi \, d\phi .
\]
With (19), these integral functions are
\[
G_0 = 2 \eta_{\text{max}} \int_\phi^{\phi'} \frac{\phi}{1 + a \phi^2} - \frac{\phi'}{1 + a \phi'^2} \, dy + \arctan(\sqrt{a \phi'}) - \arctan(\sqrt{a \phi}) ,
\]
\[
G_1 = 2 \eta_{\text{max}} \int_\phi^{\phi'} \frac{1}{\alpha + a \phi^2 \phi'} - \frac{1}{\alpha + a \phi'^2} \, dy + \ln(1 + a \phi^2) - \ln(1 + a \phi'^2) \, \frac{dy}{a} .
\]

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 \( \zeta_{\text{max}} \) as Walshaw and Rodgers [1963], and a value of \( \eta_{\text{max}} \) and \( \beta_\phi \) chosen to represent the TOVS channel 9. The values of these parameters relevant to Figure 3 are 1600, 10 ppm, 11.84, and 2.66 for \( a , \zeta_{\text{max}} , \eta_{\text{max}} , \) and \( \beta_\phi , \) 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.
Figure 2. Comparison of calculated channel 9 brightness temperatures using MODTRAN and the band model with water vapor continuum absorption included.

Figure 3. Comparison of the transmission as a function of height using the exact Walshaw model and the same model with the HCG approximation and the four-parameter approximation. The dash-dotted line represents the ozone profile used for the calculations.
Four-Parameter Band Model

It is straightforward to improve on the HCG, as Goody [1964] and Rodgers [1968] have demonstrated. Here this extension of the HCG, referred to as a four-parameter approximation, is applied to the Malkmus band model. The conceptual view of this four-parameter method is to consider a path composed of two contiguous elements, one at pressure \( p_1 \) and the other at pressure \( p_2 \). The optical depth of two superimposed Lorentz lines at standard temperature then follows as

\[
\tau_\nu = \frac{S\alpha_1 u_1}{\pi(\nu^2 + \alpha_1^2)} + \frac{S\alpha_2 u_2}{\pi(\nu^2 + \alpha_2^2)},
\]

(24)

with

\[
\alpha_i = \alpha_0 \frac{p_i}{p_0}.
\]

This equation gives us the following three equations:

\[
\tilde{u}_1 + \tilde{u}_2 = \int du
\]

\[
\tilde{u}_1 \tilde{p}_1 + \tilde{u}_2 \tilde{p}_2 = \int p du
\]

\[
\tilde{u}_1 \tilde{p}_1^2 + \tilde{u}_2 \tilde{p}_2^2 = \int p^2 du.
\]

(25)

With the following parameters

\[
\mu_i = \frac{\tilde{u}_i}{\tilde{u}}
\]

\[
\lambda_i = \frac{\tilde{p}_i}{\tilde{p}}
\]

(26)

\[
\rho = \frac{\int p^2 du}{\tilde{p}^2 \tilde{u}},
\]

where \( \tilde{u} = \int du \) and \( \tilde{p} = \int p du/\tilde{u} \), these equations have the dimensionless form

\[
\mu_1 + \mu_2 = 1
\]

\[
\mu_1 \lambda_1 + \mu_2 \lambda_2 = 1
\]

\[
\mu_1 \lambda_1^2 + \mu_2 \lambda_2^2 = \rho.
\]

(27)

With the ad hoc constraint [Goody, 1964]

\[
\lambda_1 = \frac{1}{\rho},
\]

(28)

we have a solvable set of four equations, which can be used to calculate \( \tilde{p}_1, \tilde{p}_2, \tilde{u}_1, \) and \( \tilde{u}_2 \). The dimensionless parameter \( \rho \) is a measure of the bimodal character of the distribution. For a single layer, \( \rho = 1 \); for two layers, \( \rho > 1 \), and it increases as the pressure difference between the two layers increases.

This four-parameter approximation was used in the Malkmus band model with the same band parameters \( X \) and \( Y \) as described before. The transmission is now

\[
\tau = \exp[-(\gamma - \tilde{\alpha}_1 - \tilde{\alpha}_2)],
\]

(29)

where

\[
\tilde{\alpha}_i = \frac{2X^2 \tilde{p}_i}{Y \Delta \nu p_0},
\]

(30)

and

\[
\gamma = \left[ \tilde{\alpha}_1^2 (1 + m_1) + \tilde{\alpha}_2^2 (1 + m_2) \right]
\]

\[
+ 2\tilde{\alpha}_1 \tilde{\alpha}_2 \sqrt{1 + m_1 + m_2}\right]^{1/2},
\]

(31)

where

\[
m_i = \frac{Y^2 p_0}{X^2 \tilde{p}_i} \tilde{u}_i.
\]

(32)

The transmission is also presented as a function of height in Figure 3. The transmissions were derived for the analytical ozone profile introduced above. The superior performance of the model over that of the HCG is evident.

3. A Simple Forward Model

The retrieval approach introduced here is built around a simple two-layer version of the radiative transfer model described above. The rationale for the two-layer model derives from the work of Neuendorffer [1996], who notes the limited vertical information implied in the 9.6-μm TOVS radiances. The model consists of two layers from 1000 – 30 hPa and 30 – 0 hPa. The radiance at the top of the atmosphere can be described with

\[
I_\theta = B(T_s) T_l + B(T_l) (T_u - T_l) + B(T_u) (1 - T_u),
\]

(33)

where the subscripts \( s, l, u, \) and \( t \) correspond to surface, lower layer, upper layer, and total atmosphere, respectively. For the upper layer, \( \rho = 1 \), and \( T_u \), the transmittance from the top of the atmosphere to 30 hPa, is described by

\[
T_u = \exp \left[ \alpha_u - \alpha_u \sqrt{1 + m_u} \right],
\]

(34)

with

\[
\alpha_u = \frac{2X^2 \nu}{Y \Delta \nu p_0},
\]

\[
m_u = \frac{Y^2 p_0}{X^2 \nu} \tilde{u}_u.
\]
and $u_\ell$ is the ozone amount of the layer. For both layers together, $\rho$ is not equal to 1 and the transmittance $T_\ell$ is calculated with equation (29), where $\tilde{\alpha}_i$ and $\gamma_i$ are as defined in (30) and (31).

The actual model adopted in the retrieval is similar to that of Neuendorffer [1996]. The surface temperature required in equation (33) is approximated by a weighted sum of the brightness temperatures of TOVS channel 8 and 10:

$$T_s = 0.6 T_8 + 0.4 T_{10}. \tag{35}$$

The mean temperature of the lower layer is defined as the average of the brightness temperatures of HIRS channel 2 and microwave sounding unit (MSU) channel 4:

$$T_\ell = (T_2 + 2 T_{MSU4})/3. \tag{36}$$

The temperature of the upper layer is taken to be the brightness temperature of HIRS channel 1. Following Neuendorffer [1996], the amount of ozone in the upper layer is prescribed as a function of latitude by

$$u_\ell = 102 [0.9 + 1.1 \cos(\text{latitude } \pi/180)], \tag{37}$$

and the only unknown variable is the total ozone amount of the lower layer $u_\ell$.

Figure 4 shows the radiances calculated with this two-layer model versus radiances calculated with the 40-layer model for a subset of the TIGR2 atmospheres. The subset was chosen to give a good representation of the TIGR2 atmospheres. In the two-layer model the mean pressures of the two layers ($p_\ell$ and $p_\ell$) are taken to be 10 hPa and 105 hPa, respectively. These mean pressures were chosen to give the best results compared to the 40-layer model. It can be seen that the two-layer model performs well for most of the atmospheres. In the tropical regions (denoted by the diamonds in Figure 4) a bias exists. This can possibly be explained by noticing that for the tropical profiles the ozone amount in the upper layer is the main contributor to the total ozone amount. Because this amount is prescribed in the model, there is little flexibility to deal with variations in the real profile.

The difference between the two-layer model with the 40-layer model is used for the error estimate of the two-layer model. This estimate is needed in the retrieval procedure described in the next section. Assuming that the 40-layer model represents the “truth,” the forward model variance $S_f$ can be calculated [Marks and Rodgers, 1993]. Because there is a difference in model performance between low latitudes and high latitudes, $S_f$ is calculated separately for latitudes either side of 30° latitude. The bias of the model for the two latitude regions is also used in the retrieval in the same way as proposed by Marks and Rodgers [1993].

### 4. Retrieval of Total Ozone

To retrieve total ozone from the TOVS measurements, we used the approach described by Rodgers [1990] and Marks and Rodgers [1993], which expresses a measurement $y$ as

$$y = \mathcal{F}(x, b) + \epsilon_y, \tag{38}$$

where $\epsilon_y$ is the error in the measured radiance, $x$ is the total ozone value, $\mathcal{F}$ is the atmospheric “forward function,” representing the detailed physics of the measurements (and given by the simple two-layer forward model introduced above), and $b$ denotes all unretrieved quantities that affect the radiance and which must be specified a priori. The measurement $y$ represents the channel 9 brightness temperature.

Using estimates $\hat{x}$ and $\hat{b}$, our forward model provides a synthetic radiance $\hat{y}$. Following Marks and Rodgers [1993], we can find the optimal solution $\hat{x}$ by minimizing the function $\Phi$

$$\Phi = \frac{(\hat{x} - x_a)^2}{S_a} + \frac{(y - \mathcal{F}(\hat{x})^2}{S_y}, \tag{39}$$

with respect to $\hat{x}$. An a priori value $x_a$ for $x$ is used to improve the noise characteristics and stability of the solution relative to an “exact” solution ($\hat{x} = \mathcal{F}^{-1}(y)$). $S_a$ and $S_y$ are the error covariances of the a priori value and the measurement. $S_y$ also contains the error estimate of the forward model $S_f$. This error was estimated by comparing the two-layer model with the more sophisticated 40-layer band model as shown in the last section, and is much larger than the actual TOVS measurement errors because it contains all the uncertainties in the simple forward model.

After linearizing about the current estimate $x^i$, the minimization calculation yields

$$x^{i+1} = \frac{S_a^{-1} x_a + K S_y^{-1} (y - \mathcal{F}(x^i) + K x^i)}{S_a^{-1} + K^2 S_y^{-1}}, \tag{40}$$

where $K = \partial \mathcal{F} / \partial x$ and is calculated with a simple perturbation method:

$$K = \frac{\mathcal{F}(1.01 \hat{x}) - \mathcal{F}(0.99 \hat{x})}{0.02 \hat{x}}. \tag{41}$$

Because $K$ has to be calculated in every step of the retrieval, the forward model, which is used three times in each step, has to be computationally efficient.

The error covariance of the retrieved $x$ is

$$S_x^{-1} = S_a^{-1} + K^2 S_y^{-1}. \tag{42}$$
As a convergence test, the following equation is used:

\[
\frac{(x^{i+1} - x^i)^2}{S_x} \ll 1
\]  \hspace{2cm} (43)

Only a few iteration steps are needed to converge to the solution. Following the error analysis described by Marks and Rodgers [1993], we used $\chi^2$ as an extra quality test for the retrieval. The approximate $\chi^2$ to use is

\[
\chi^2 = \frac{(y - \mathcal{F}(x^i))^2}{S_y} + \frac{(x_\alpha - \hat{x})^2}{S_\alpha}
\]  \hspace{2cm} (44)

This should follow a $\chi^2$ distribution with one degree of freedom, as we have one measurement ($y$) and one virtual measurement ($x_\alpha$) with one parameter ($\hat{x}$) being retrieved. A typical value of $\chi^2$ for a moderately good retrieval is then 1. We regarded a convergent retrieval as acceptable only if $\chi^2$ is not significant at the 1% level.

The retrieval scheme was applied to a subset of the TIGR2 profiles. The 40-layer model was used to calculate the radiances of the channels, needed in the retrieval, for each set of profiles. Monthly averaged zonal mean ozone statistics for the years 1987 – 1991 obtained from measurements of the total ozone mapping spectrometer (TOMS) [Bowman and Krueger, 1985] were used for the a priori ozone values ($x_\alpha$) and error covariances ($S_\alpha$). If no ozone statistics were available (e.g., in the polar night), an a priori value of 180 DU with an error of 150 DU was used for the lower layer.

Figure 5 shows the retrieved total ozone amounts contrasted against the integrated ozone profile amounts. It can be seen that relative to the integrated profiles, the retrieval scheme gives values generally within 25 DU. This is better illustrated by Figure 6, which shows the difference between the retrieved total ozone amounts and the integrated ozone profile amounts as a function of latitude. The bottom part of this figure shows the retrieval errors. The triangles denote retrievals, which have to be discarded because $\chi^2$ is too large or because they rely too much on the a priori information. This dependence on a priori information is denoted by the parameter $A$, which is explained in the next paragraph. The figure shows that although the estimated retrieval error can be quite large (especially at higher latitudes), the difference between retrieved and real total ozone amounts is smaller than 10% for most of the cases. The estimated retrieval errors are probably too large compared to the actual differences because it is hard to provide accurate error estimates for the a priori data and the forward model, and because the direct inversion of our forward model is not as ill-conditioned as in some other retrievals. Therefore the ozone retrieval can perform better than the retrieval error estimates indicate.

It is important to determine the dependence of the retrieval on the a priori information. This dependence can be characterized by a parameter that reflects the amount of a priori information retained in the retrieval. According to Rodgers [1990], we can write our retrieved total ozone value as a linear combination of the true value and the a priori value with weights $A$ and $(1 - A)$ plus contributions from experimental error in the forward model parameters and the measurement,

\[
\hat{x} = Ax + (1 - A)x_\alpha + D_y e_y
\]  \hspace{2cm} (45)

where $D_y$ is the derivative of the inverse model with respect
**Figure 5.** Scatterplot of the retrieved total ozone columns versus the real total ozone columns for a subset of the TIGR2 profiles.

**Figure 6.** Difference between retrieved total ozone and integrated TIGR2 profile total ozone as a function of latitude (upper part), and estimated retrieval error as a function of latitude (lower part). Crosses denote accepted retrievals; triangles denote discarded retrievals (for details, see text).
to $y$. $A$ can be calculated with
\[ A = 1 - D_a = 1 - \frac{\partial \tilde{x}}{\partial x_a} = 1 - \frac{1}{1 + R^2 \frac{\bar{S}}{S_0}}. \]  

Figure 7 shows the parameter $A$ as a function of latitude for each retrieval. The contribution of the a priori information varies widely between 0 and 100%. The reason for this is that the forward model is very insensitive to changes in the ozone concentration when the contrast between the surface temperature and the mean temperature of the lower layer is very low. The retrieval is then unstable [e.g., Lefèvre et al., 1991] and relies mainly on the a priori information. How much the retrieval is relying on the a priori information is determined by the ratio between the forward model error and the a priori error. This is illustrated by the triangles in Figure 7, which represent the parameter $A$ when an a priori value of 180 DU with an standard deviation of 150 DU is used in the retrieval. Because this standard deviation is much larger than the standard deviation of the TOMS statistics, the retrieval depends less on the a priori information. This effect is also illustrated in Figure 8, which shows the contribution of the a priori error and the forward model error to the total error. For most retrievals the total error is dominated by the forward model error. Only in the low-contrast cases, the contribution of the a priori error becomes large, which means that the retrieval heavily relies on the a priori information.

5. Application to Global TOVS Measurements

The new ozone retrieval scheme was applied to NOAA10 TOVS radiances for 1989 [Smith et al., 1979]. The radiances are cloud-cleared and corrected for the limb-darkening effect [McMillin and Dean, 1982]. The retrieved total ozone amounts are compared to similar data available from TOMS [Bowman and Krueger, 1985]. These data are available on a 1.25° by 1° grid for the years 1979 to 1992 (GRIDTOMS version 6 available on CD-ROM from NASA). Figure 9 and Figure 10 show the annual cycles for 1989 of zonal averaged total ozone for both TOMS and TOVS between 0°N and 5°N, and between 45°N and 50°N, respectively. The two forms of ozone data agree reasonably well with each other. A rms difference of 2.9% and 1.4% was found for 50°N and 5°N, respectively. Differences at 5°N can probably be explained by the effect of the quasi-biennial oscillation (QBO), which impacts the higher stratosphere where the ozone amount is prescribed for the TOVS retrieval.

Figure 11 shows the global total ozone distribution derived by TOVS for August 7, 1989. The agreement with the TOMS total ozone field (Figure 12) is reasonable with an rms difference of 10%. Patterns are similar with regions of maxima and minima in total ozone matching in location and magnitude. For example, small-scale structures such as the minimum over Nova Zembla and the extension of ozone-poor air from the tropics over Japan are detected in both data sets. The advantage of the TOVS data in the polar night region is evident.

A particular advantage of the retrieval introduced in this paper is illustrated in Figure 13, which shows the percent error of the retrieved total ozone amounts. A global picture of the reliability of our retrieval is thus obtained. The figure shows that in the tropics the error is small but that above ice or snow surfaces, like the Antarctic and the northern hemispheric snow fields, the error of the retrieval becomes much larger and is due to the large sensitivity of the forward model in cases of low thermal contrast between the surface and the lower stratosphere. Although the test retrievals in the last section showed that the difference between the retrieved total ozone and the real total ozone is often smaller than the retrieved error estimate, one has to be cautious interpreting the retrieved ozone values when the error estimate is large.

6. Conclusions

A radiative transfer model is introduced that uses a spectral band model for transmission based on the Malkmus line distribution. The effect of pressure on absorption is dealt with using an extended version of the widespread Van de Hulst-Curtis-Godson approximation, the four-parameter approximation. The methods were tested using a solution introduced by Walshaw and Rodgers to test the two pressure scaling approximations. We showed that for the absorption in the 9.6-µm ozone band the four-parameter approximation provides a significant improvement over the more common HCG approximation. While this result is then exploited in the development of the retrieval described in this paper, the result has wider applicability to ozone climate problems involving calculation of the radiative forcing associated with changing ozone.

A two-layer version of the radiative transfer model was implemented in a retrieval scheme to obtain total ozone amount from radiances measured by the TOVS instrument on board the NOAA satellites. The approach described by Marks and Rodgers [1993] was followed. This method provides good 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 is different from other existing infrared retrieval schemes for ozone, which provide only general error estimates. The main differences between our approach and the approach of Neuendorffer [1996] are the radiative transfer modeling and the retrieval error char-
Figure 7. Parameter $A$ (for details, see text) as a function of latitude in case of the TOMS a priori data (upper part) and in case of the simple a priori data (bottom part).

Figure 8. Total error of the retrieved total ozone values for a subset of the TIGR2 profiles (light grey) and the contributions to this error of the forward model error (grey) and the a priori error (dark grey).
**Figure 9.** Annual cycle of zonal averaged total ozone columns between 0°N and 5°N retrieved by TOMS (grey line) and TOVS (black line).

**Figure 10.** Annual cycle of zonal averaged total ozone columns between 45°N and 50°N retrieved by TOMS (grey line) and TOVS (black line).
Figure 11. Total ozone (DU) measured by TOVS on August 7, 1989.

Figure 12. Total ozone (DU) measured by TOMS on August 7, 1989.
acterization. This global distribution of the retrieval error and also of the contribution of a priori knowledge to the retrieval gives much more insight in the validity of the ozone retrievals.

Ozone retrievals for 1989 were compared with TOMS total ozone measurements. This comparison showed good agreement between the two ozone retrievals both in time and in space (a rms difference between 1% and 3% for zonal means and 10% for global gridded measurements). In contrast with the TOMS measurements, the infrared TOVS measurements allow ozone retrieval twice a day (daytime and nighttime retrievals) and in the polar night. A disadvantage is the unstable retrieval when the difference between surface temperature and lower stratospheric temperature is small.

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**Figure 13.** Percent error in the total ozone columns measured by TOVS on August 7, 1989.


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