

Total ozone from NOAA satellites in the Australian region

Zhen-jia Wu and John Le Marshall

Bureau of Meteorology Research Centre, Australia

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High Resolution Infrared Radiation Sounder (HIRS) radiance measurements from the TIROS-N/NOAA series satellites have been used to calculate total ozone amounts in real time for the Australian region. The method used to calculate ozone amount has been developed from that of Ma, Smith and Woolf, which is the basis of the algorithms used in the International TOVS Processing Package (ITPP). The method described here employs the radiative transfer equation and uses the statistical relationships between HIRS channel 1 to 4 radiances and ozone amount to establish a first-guess profile. Several changes have been made to the Ma et al. algorithm to improve the estimation of total ozone. Results from the new algorithm are compared with those from the original and with surface-based observations of total ozone taken using Dobson spectrophotometers.

Introduction

Satellites play an important role in monitoring the trends in ozone distribution on a global basis. From the late 1960s instruments to determine the global ozone distribution have been flown in space and have employed several techniques to remotely sense ozone distribution (Le Marshall 1989). These include nadir or limb viewing to measure the backscattered ultraviolet radiation from different layers in the stratosphere and mesosphere with processing principles similar to the Umkehr method (Heath et al. 1973; Thomas et al. 1980), observing infrared emission usually around the 9.7 μm ozone absorption band as the instrument limb scans (Gille et al. 1975) or scans subsatellite (Muller and Cayla 1983; Planet et al. 1984; Ma et al. 1984; Planet et al. 1988; Lienesch and Pandey 1985; Lienesch 1988), and measuring the absorption in the ultraviolet or visible ozone bands as the sun or a star is occulted by the earth (McCormick et al. 1979). Although there have been significant problems in measurement associated with operating instruments in space, satellite-based observations provide important information on the global distribution of ozone. Satellite data may also prove to be critical to analyse the long-term trend of ozone amount.

Corresponding author address: Dr J. Le Marshall, Bureau of Meteorology Research Centre, GPO Box 1289K, Melbourne, VIC 3001, Australia.

The Australian Bureau of Meteorology (BoM) has been receiving data, at its Melbourne and Perth tracking stations, from all the operational TIROS/NOAA series satellites (including NOAA-9, NOAA-10 and NOAA-11) traversing the Australian region. In particular, data from the TIROS Operational Vertical Sounder (TOVS), which includes the High Resolution Infrared Sounder (HIRS) and Microwave Sounding Unit (MSU), are processed in real time to obtain temperature and water vapour profiles, and cloud parameters. The HIRS 9.7 μm ozone absorption band is also used in conjunction with other HIRS thermal infrared bands, and temperature and water vapour profiles to obtain total ozone column density (Le Marshall et al. 1989). To retrieve the temperature and water vapour parameters from the instrument observations, a physical solution of the radiative transfer equation, expressed in perturbation form, is used. The solution uses ancillary data, including numerical weather prediction model-based or statistically-based first-guess temperature and moisture fields and real-time surface temperature and moisture analyses. Instrument bias and transmittance corrections are determined locally.

The purpose of this paper is to present recent improvements in the retrieval scheme for total ozone used at the Australian Bureau of Meteor-

ology. Several changes have been made to the original ozone retrieval scheme which was based on the algorithm of Ma et al. (1984) and derived from the software in the ITPP (Smith et al. 1984) to achieve more accurate results.

The total ozone retrieval algorithm of Ma et al.

The Ma et al. and ITPP total ozone retrieval algorithm can be summarised as follows. HIRS channels 1 to 4 (stratospheric temperature channels) are used to specify the first-guess vertical profile of ozone concentration, according to regression relations between the radiances of these channels and the ozone concentration. The first-guess ozone profile is further adjusted vertically using regression relations between the ozone peak position and the latitude of the retrieval site, and the difference between the observed radiance and the radiance calculated from the first-guess profile. The total ozone concentration is then given by the inverse solution of the radiative transfer equation (RTE).

In detail, the RTE, which is used for the retrieval of total ozone and other meteorological parameters, may be expressed as

$$I(\nu, \theta) = B(\nu, T(P_s))\tau(\nu, \theta, p_s) - \int_0^{P_s} B(\nu, T(P))d\tau(\nu, \theta, p) \quad \dots 1$$

Integrating by parts, we have

$$I(\nu, \theta) = B(\nu, T(P=0)) + \int_0^{P_s} \tau(\nu, \theta, P)dB(\nu, T(P)) \quad \dots 2$$

where $I(\nu, \theta)$ is the observed radiance at a particular wavelength ν for a zenith angle of observation θ , $\tau(\nu, \theta, P)$ is the transmittance from the atmospheric pressure level P to the observing satellite along a straight line of zenith angle θ , and $B(\nu, T)$ is the Planck function for temperature T . The subscript s denotes surface value, either ground or cloud top. The path of integration is a straight line of zenith angle θ from the satellite to the surface.

In the process of total ozone estimation, the temperature profile and the Planck function $B(\nu, T)$ are fixed with respect to the pressure level P , hence the 'perturbation' form of Eqn 1 or 2 can be expressed as

$$\delta I = \int_0^{P_s} \delta\tau(P)dB(T(P)) \quad \dots 3$$

where δ denotes the change or 'perturbation' of the quantities I and τ . Variables θ and ν are omitted from the equation for the sake of simplicity. This equation explicitly relates the changes of radiance I to changes in the transmittance profile $\tau(P)$, which in turn result from changes in the ozone profile.

If we assume that the width of the observational wavenumber band is infinitesimally narrow and that the transmittance is only affected by a single absorber, e.g., ozone, then according to the Beer's Law, we have

$$\tau(P) = e^{-k_\nu\mu(P)} \quad \dots 4$$

where k_ν is the absorption coefficient at wavenumber ν , and μ is the path length between the satellite and pressure level P .

The path length $\mu(P)$ is given by

$$\mu(P) = \sec\theta \int_0^P q g^{-1}dP$$

where q is the ozone mixing ratio and g is the acceleration due to gravity.

Thus for the factor $\delta\tau(P)$ in Eqn 3, we have

$$\begin{aligned} \delta\tau(P) &= \delta e^{-k_\nu\mu(P)} \\ &= e^{-k_\nu\mu(P)} (-k_\nu) \delta\mu(P) \\ &= \tau(P) \ln\tau(P) \frac{\delta\mu(P)}{\mu(P)} \quad \dots 5 \end{aligned}$$

Inserting Eqn 5 into Eqn 3 we obtain

$$\delta I = \int_0^{P_s} \tau(P) \ln\tau(P) \frac{\delta\mu(P)}{\mu(P)} dB(T(P))$$

In order to ensure that the radiance calculated using Eqn 1 matches the observed radiance of the 9.7 μm ozone channel, the ozone mixing ratio profile $q(P)$ and hence the ozone path length $\mu(P)$ are varied by the same fractional change at all pressure levels. Thus we have

$$\frac{\delta q(P)}{q(P)} = \frac{\delta\mu(P)}{\mu(P)} = \frac{\delta I}{\int_0^{P_s} \tau(P) \ln\tau(P) dB(T(P))} \quad \dots 6$$

for all P .

This is an inverse solution of the RTE and for the case of ozone retrieval, in which only one channel (9.7 μm band) is utilised. An equivalent expression was achieved by Ma et al. (1984) in Eqn 3 of their paper.

Using Eqn 6, corrections to $q(P)$ or $\mu(P)$ can be made to match the observed and calculated radiances. If necessary an iteration involving Eqns 1 and 6 for the quantities $\delta q/q$ and δI may be undertaken to ensure that δI does not exceed certain limits.

The enhanced algorithm

Several enhancements have been made to the above algorithm. In the new scheme the provision of the first-guess profile is as in Ma et al. (1984) and in the ITPP. Subsequent key changes are described below.

First, the expression for $\delta\tau$ in Eqn 5 has been modified. In the TOVS 9.7 μm channel, transmittance is affected by water vapour absorption and the total transmittance is given by

$$\tau(P) = \tau_{\text{O}_3}(P) \tau_{\text{H}_2\text{O}}(P)$$

where τ_{O_3} and $\tau_{\text{H}_2\text{O}}$ refer to ozone and water vapour transmittances respectively. This equation was used in the forward calculation for the total transmittance, however, the water vapour contribution to the total transmittance appears to have been inadvertently omitted in deriving the inverse solution Eqn 6 from Eqns 4 and 5.

Second, in the case of the 9.7 μm ozone channel, Eqn 4 was not used in the forward calculation for the total ozone transmittance. τ_{O_3} was actually obtained from a numerical data table which related values of τ_{O_3} to values of a 'transmittance scaling factor' q^* (see Ma et al. 1984). q^* was defined by the equation

$$q^* = 2.41 + \log_{10}\gamma$$

where γ is the ozone equivalent path length given by

$$\gamma = \sec\theta \int_0^P q \left(\frac{P}{P_0}\right)^{2/5} \left(\frac{T_0}{T}\right)^{1/5} dP \quad \dots 7$$

and T is the atmospheric temperature, and P_0 and T_0 are standard atmospheric pressure and temperature.

Consequently, Eqn 5 can be replaced by

$$\begin{aligned} \delta\tau &= \delta(\tau_{\text{H}_2\text{O}} \tau_{\text{O}_3}) \\ &= \tau_{\text{H}_2\text{O}} \delta\tau_{\text{O}_3} \\ &= \tau_{\text{H}_2\text{O}} \frac{d\tau_{\text{O}_3}}{dq^*} \frac{1}{\ln 10} \frac{\delta\gamma}{\gamma} \end{aligned}$$

which can be again inserted into Eqn 3 to give

$$\delta I = \frac{1}{\ln 10} \int_0^P \tau_{\text{H}_2\text{O}} \frac{d\tau_{\text{O}_3}}{dq^*} \frac{\delta\gamma}{\gamma} dB$$

From Eqn 7 we know that if $q(P)$ has the same fractional change at all pressure levels, then γ would have the same fractional change. Thus we find

$$\frac{\delta q}{q} = \frac{\delta u}{u} = \frac{\delta\gamma}{\gamma} = \frac{\delta I \ln 10}{\int_0^P \tau_{\text{H}_2\text{O}} \frac{d\tau_{\text{O}_3}}{dq^*} dB} \quad \dots 8$$

in which $d\tau_{\text{O}_3}/dq^*$ can be obtained from the numerical table which links τ_{O_3} to q^* . In the new scheme, Eqn 8 has replaced Eqn 6 and this change has resulted in a quicker convergence to the final ozone profile.

In addition to the changes above, the iteration between quantities of $\delta q/q$ and δI in Eqns 6 and 8, as previously described in the paper of Ma et al. (1984), has been used in this scheme (this iteration is missing in the ITPP). The iteration terminates when the difference between the measured ozone brightness temperature and that calculated is less than 0.02 K, approximately a tenth of the measurement noise level, instead of 0.2 K, as previously suggested by Ma et al. (1984). The 0.02 K difference represents an error of 0.4–0.5 Dobson units (DU), which is about an order of magnitude less than the error of 4–5 DU resulting from the measurement noise. In practice, two to three iterations are required on average to reach the 0.02 K requirement.

Another change to the scheme is to ensure that the vertically adjusted ozone profile is fully modified by the fractional change which is given by Eqn 6 or 8. This was inadvertently omitted in the ITPP.

This change and the change to include the water vapour transmittances in the inverse solution have been subsequently made in the ITPP package which is maintained at the Cooperative Institute for Meteorological Satellite Studies at the University of Wisconsin, Madison.

Accuracy of the algorithm

Figure 1 compares the total ozone amounts computed by the new retrieval algorithm and the earlier one. The computed values are also compared with ground-based Dobson instrument observations for the period 9 January to 12 January 1991 for Melbourne and Brisbane. Each satellite-observed datum in the figure is an average of cloud-free observations over a square of three degrees latitude by three degrees longitude around the related ground station.

From Fig. 1, we can see that the TOVS observations of both the previous and present algorithms are well correlated with the ground instruments and that the data of the improved scheme generally are closer to the ground 'truth', although the corrections are not all in the right direction or of the correct amount.

Figure 2 shows scatter diagrams of the surface observations of total ozone taken via Dobson spectrophotometer versus TOVS measurements using Ma et al.'s algorithm (left column) and versus the present algorithm (middle column), and of Ma et al.'s algorithm versus the present (right column), for Melbourne and Brisbane from 1 January to 30 April 1991. In these scatter dia-

Fig. 1 Total ozone amount observed by Dobson spectrophotometers and from NOAA-10 for (a) Melbourne and (b) Brisbane, for the period of January 9 to January 21, 1991. All observations were made under the 'clear sky' condition.

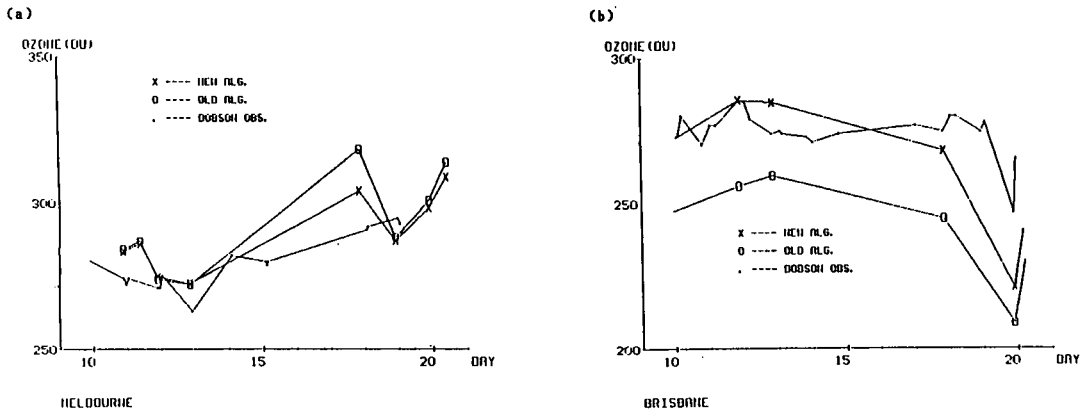
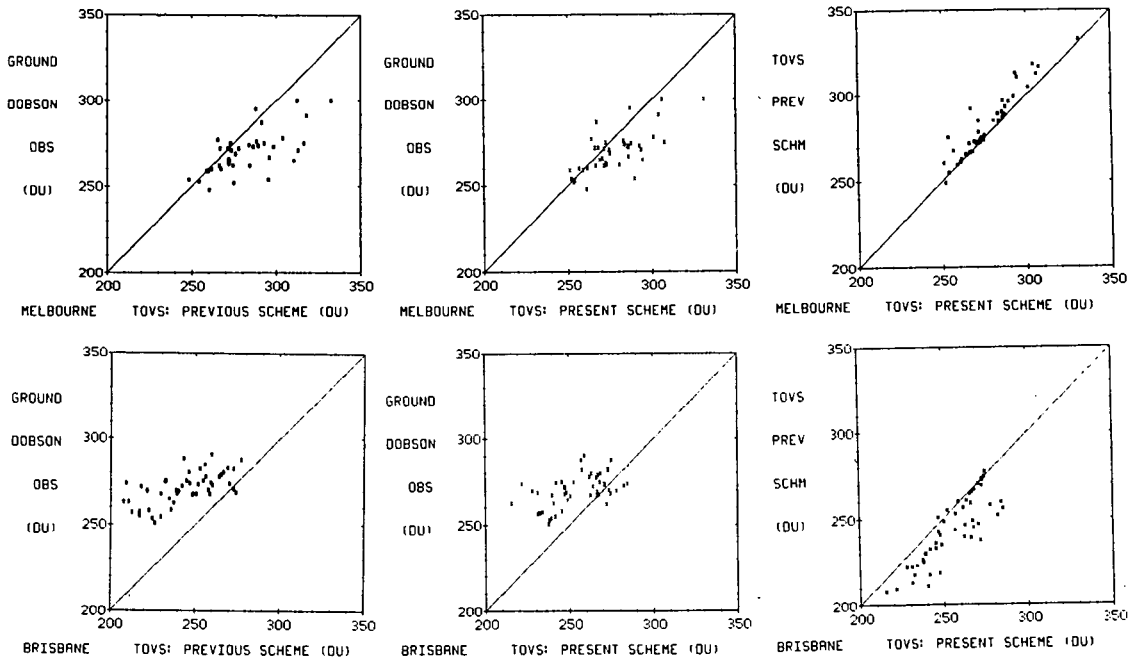


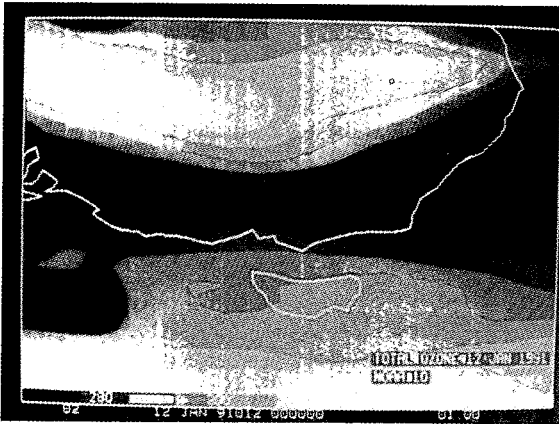
Fig. 2 Scatter diagrams of Dobson spectrophotometer observations versus satellite TOVS retrievals using Ma et al.'s (1984) algorithm (left column) and the present algorithm (middle column), and of Ma et al.'s algorithm versus the present (right column) for Melbourne (top row) and Brisbane (second row) during 1 January to 30 April 1991.



grams, each ground Dobson value is actually a linear time interpolation between the nearest two clear-sky observations, i.e., the observations which use the direct sunlight or the light from the zenith blue sky. The term 'nearest' here means that the Dobson measurements taken are within 16 hours of the compared satellite measurement. In the case where only one 'nearest' Dobson datum is available, the 'interpolation' consists of this one only. Hence, part of the ground and satellite observational discrepancies can be attributed to the temporal and spatial variation of the natural atmospheric ozone content.

As can be seen from these diagrams, the present scheme generally reduces the differences compared to the ground measurements. This is particularly obvious in the case of Brisbane where the data points of the present scheme are clearly closer to the central diagonal line than those of the previous.

Fig. 3 Mean total ozone amount over southeastern Australia on 12 January 1991 estimated from NOAA-10 observations. All observations were made under the 'clear sky' condition.



In general, the variations in the TOVS data are greater than the surface measurements. That is, the satellite retrievals in comparison to the Dobson spectrophotometer data show larger variations of the ozone absorption. However, the present scheme noticeably reduces this variation, in effect increasing the smaller values and decreasing the bigger values.

The root mean square (rms) deviations and the biases from the measurements made with Ma et al.'s algorithm, the present algorithm, and the ground truth, are all shown in Table 1. These results are calculated from the same data set used in Fig. 2. The table shows that the rms deviations and biases between satellite ozone retrievals using the present algorithm and Dobson observations are generally reduced from those using the previous algorithm. For both Melbourne and Brisbane, the average rms deviation is reduced from 26.7 DU previous to 18.5 DU present, and the bias is reduced from -9.2 DU to -4.9 DU. This implies that the improvement of the rms deviations in the present scheme is not solely due to the corrections of the bias. A more important factor contributing to this improvement is the overall accuracy of the retrieval itself. The rms deviations and the bias between the present scheme and the previous one are also listed in the right column of Table 1 for reference. These data (although from a limited verification period), when compared with the results from earlier satellite observations derived by Planet et al. (1984) and Lienesch (1988), also suggest that the data are of good quality.

Of course, the clear advantage of satellite measurements compared to ground-based observations is their spatial coverage and Fig. 3 shows the mean total ozone over southeastern Australia for 12 January 1991, estimated using NOAA-10 clear sky observations. This figure shows lower ozone values over the State of Victoria with higher values over New South Wales, Tasmania and further south. The figure clearly illustrates the utility of those data to show the spatial and temporal variation of the total field in areas which cannot be viewed by conventional means.

Table 1. The root mean square (rms) differences and the biases for Ma et al. and the present scheme versus the Dobson spectrophotometer observations, and those for the present scheme versus Ma et al. for Melbourne and Brisbane. The units are Dobson units (DU) and the period of comparison from 1 January to 30 April 1991.

Site	No. of obs.	Ma et al. alg. vs Dobson data		Present alg. vs Dobson data		Present alg. vs Ma et al. alg.	
		Bias	rms diff.	Bias	rms diff.	Bias	rms diff.
Melbourne	39	13.4	19.7	8.1	14.8	-5.3	8.4
Brisbane	49	-27.3	31.2	-15.3	21.0	12.0	15.8
Both sites	88	-9.2	26.7	-4.9	18.5	4.3	13.0

Summary and conclusion

In summary, an improved algorithm for estimating total ozone amounts from HIRS radiosondes has been presented.

This new scheme, (a) uses Eqn 8 instead of Eqn 6 to provide a more accurate ozone inverse solution of the RTE; (b) re-introduces the iteration suggested by Ma et al. (1984) to reduce the calculated residual error to less than 0.5 DU; and (c) ensures that the vertically adjusted ozone profile is modified as required by Eqn 6 or 8.

Results indicate that the present scheme achieves a higher accuracy in the Australian environment than the previous one.

The rms deviation between the satellite ozone retrievals and the ground-based Dobson observations was reduced from an average of 26.7 DU to 18.5 DU during the period January to April 1991 at 2 sites, namely Melbourne and Brisbane. In other words, the fractional differences were reduced from about 9 per cent to 6 per cent.

The satellite retrievals and the ground truth which are used for these comparisons can have a time difference as large as 16 hours and a spatial difference of up to 1.5 degrees of latitude and longitude. The satellite also observes a weighted volume average. The differences, therefore, can be partially attributed to these collocation differences and natural temporal and spatial variation of the atmospheric ozone.

In conclusion, the important role of stratospheric ozone in shielding life from harmful solar ultraviolet radiation and the clear advantage of measuring the distribution of ozone on a global scale from space, has resulted in a significant satellite-based ozone observation program over the last twenty years. Several instruments are presently being used to monitor ozone from space, these include the Solar Backscatter Ultra-Violet radiometer (SBUV/2), the Total Ozone Mapping Spectrometer (TOMS) and TOVS. In comparison with the SBUV/2 and TOMS, the main shortcoming of the TOVS instrument is that there is only one infrared channel in the TOVS 9.7 μm ozone absorption band. The accuracy of the TOVS ozone retrieval is thus constrained.

This shortcoming will be overcome with the advent of the next generation of satellite-borne infrared sounders. The Advanced Infrared Sounder (AIRS) with approximately four thousand infrared channels is to be launched into space in the late 1990s onboard the Earth Observing System (EOS) satellites.

The Australian Bureau of Meteorology intends to continue to improve its ability to monitor ozone distribution from space using the TOVS instrument. At the same time the Bureau plans to use AIRS data to provide ozone profile information for the Australian region in the late 1990s. Development work to this end is proceeding.

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