Ozone Corrections for Rayleigh-Scatter Temperature Determinations in the Middle Atmosphere

R. J. SICA, Z. A. ZYLAWY, AND P. S. ARGALL

Department of Physics and Astronomy, The University of Western Ontario, London, Ontario, Canada

(Manuscript received 7 August 2000, in final form 11 October 2000)

ABSTRACT

A well-established technique for the determination of temperature in the middle atmosphere is the retrieval of temperature profiles from density profiles of air. The measurement of air density profiles from the ground and from space are typically determined from measurements of Rayleigh-scattered light. Most researchers using the Rayleigh-scatter temperature technique do not state whether they correct their measurements for the absorption of light due to ozone in the upper stratosphere. Such corrections may have been less significant for initial studies of temperature, but with the current need for temperature measurements of sufficient quality to access atmospheric change, these corrections take on an added importance. Significant improvement to the temperature measurements in the stratosphere are shown to result by including this effect for any reasonable choice of ozone profile. Simple correction functions are presented for temperature measurements, appropriate for low, middle, and high latitudes evaluated at two of the three most common Rayleigh-scatter wavelengths, 532 and 589 nm. Though the 350nm wavelength is also commonly used for Rayleigh-scatter measurements, the effects of ozone at this wavelength are found to be negligible. The correction functions increase the temperature in the middle stratosphere by about as much as 4 K, with the largest corrections at the low latitudes and the longer wavelength, 589 nm. Deviations from these baseline values due to seasonal variability in the ozone profile change the temperature correction by less than 10%. Despite increases of two to three times of ozone in the mesosphere during the spring season, mesospheric temperatures are found to not require any correction for ozone. Hence, even without explicit knowledge of the ozone profile, experimenters can still significantly improve their Rayleigh-scatter stratospheric temperature measurements compared to not correcting for ozone absorption.

1. Introduction

The determination of temperatures from Rayleighscattering measurements is an important remote sensing technique for temperature determination, particularly in the middle atmosphere, which is optically thin to visible light. This technique is used by Rayleigh-scatter lidar systems to retrieve temperature from photocount height profiles above the region of aerosol scattering (approximately 25 to 30 km). The retrieval of temperature from the photocount measurement is possible by assuming hydrostatic equilibrium and using the Ideal Gas law. This method has been described in detail by Hauchcorne and Chanin (1980) for an ozone-free atmosphere and expanded on by Keckhut et al (1993). Leblanc et al. (1998) have simulated this method in detail and present estimates of the accuracy of the retrieval. Their analysis includes (among other effects) ozone absorption and mentions both the necessity of a correction and that the correction is not strongly dependent on the choice of ozone profile. However, they do not explicitly show the effect of ozone absorption on temperature retrievals and do not offer a correction for existing profiles in the literature. Keckhut et al. (1990) discuss ozone corrections for the determination of temperature in the troposphere and lower stratosphere using vibration Raman scattering from N_2 . Here, the correction is even more important than for the middle and upper stratospheric Rayleigh-scatter measurements.

In addition to the work of Chanin and colleagues, numerous other groups have reported Rayleigh-scatter temperatures, but with the exception of Chanin and colleagues, most groups do not claim to correct their measurements for ozone absorption. Perhaps one reason such corrections are neglected is that most systems do not have access to simultaneous measurements of ozone profiles, so the experimenter may feel that a reasonable correction is not possible. Also, many current and all older Rayleigh-scatter lidar have low to moderate power-aperture products, meaning that photon noise is the predominant error source at most heights. For larger power-aperture lidars, such as the Purple Crow Lidar, the photon noise in the stratosphere becomes negligible for integration times greater than about 15 min and height resolutions greater than about 1000 m (Sica et

Corresponding author address: Dr. R. J. Sica, Department of Physics and Astronomy, The University of Western Ontario, London, ON N6A 3K7, Canada. E-mail: sica@uwo.ca

^{© 2001} American Meteorological Society



FIG. 1. Mean ozone number density profiles used for the temperature correction calculation.

al. 1995). Thus, the Purple Crow Lidar, as well as other high power-aperture systems in operation or in the planning stages, allows temperature determinations relevant to weather, as well as climate, to be measured. A standard correction for ozone is thus important both for temperature studies as well as for evaluating stratospheric change.

2. Methodology

Absolute temperature profiles are obtained from Rayleigh-scatter lidar measurements of relative density by assuming hydrostatic equilibrium and integrating the Ideal Gas law from the greatest altitude downward. At heights within about 15 km of the greatest altitude, the accuracy of the temperature determination can be affected by the choice of initial temperature (or pressure) required to seed the integration. For most Rayleigh lidars currently in operation, the uncertainties in temperature due to the choice of top temperature are negligible below the stratopause. To quantitatively evaluate the effects of ozone absorption, stratospheric temperature profiles were calculated from density profiles with and without a correction for ozone absorption as a function of latitude and wavelength. An atmospheric transmission function for ozone is computed using the relevant cross section and the appropriate ozone density profile, as described below (e.g., Leblanc et al. 1998). First, the



FIG. 2. Percent departures from the mean of the seasonal ozone profiles used for the temperature correction calculation for high latitudes (top), middle latitudes (middle), and low latitudes (bottom).

absorption coefficient at a given wavelength is calculated from knowledge of the cross section, σ , using

$$k_a(\lambda) = \sigma(\lambda)[n(O_3)], \qquad (1)$$

where $n(O_3)$ is the number density of ozone.

TABLE 1. Polynomial coefficients for the ozone temperature correction at 589 nm.

| Location | a_0 | a_1 | <i>a</i> ₂ | <i>a</i> ₃ |
|-------------------------------|-------|---------|-----------------------|------------------------|
| Low latitudes | 11.3 | -0.0736 | $-1.36 	imes 10^{-2}$ | 2.14×10^{-4} |
| Middle latitudes | 14.2 | -0.561 | 4.79×10^{-3} | 1.53×10^{-5} |
| High latitudes equinox/summer | 10.4 | -0.442 | 5.27×10^{-3} | -1.19×10^{-5} |
| High latitudes winter | 19.3 | -1.36 | 3.29×10^{-2} | -2.70×10^{-4} |

TABLE 2. Polynomial coefficients for the ozone temperature correction at 532 nm.

| Location | a_0 | a_1 | a_2 | <i>a</i> ₃ |
|-------------------------------|-------|---------|------------------------|------------------------|
| Low latitudes | 5.38 | -0.0485 | -5.87×10^{-3} | 9.54×10^{-5} |
| Middle latitudes | 6.65 | -0.0267 | 2.43×10^{-3} | 5.15×10^{-6} |
| High latitudes equinox/summer | 4.83 | -0.208 | 2.53×10^{-3} | -6.36×10^{-6} |
| High latitudes winter | 8.88 | -0.627 | 1.52×10^{-2} | -1.24×10^{-4} |

The calculations at 589 nm are performed with a Chappius band absorption cross section of 4.8×10^{-25} m², while at 532 nm, the cross section is 2.2×10^{-25} m² (Brasseur and Solomon 1984). Ozone DIAL lidars commonly make Rayleigh-scatter measurements in the region of 355 nm (the "offline" wavelength), but the



FIG. 3. Temperature profiles used for the correction calculation for high latitudes (top), middle latitudes (middle), and low latitudes (bottom).

ozone absorption at this wavelength is so small, on the order of one-thousandth of the ozone absorption cross section at 308 nm $(1.05 \times 10^{-26} \text{ m}^2 \text{ at } 355 \text{ nm})$, that the corresponding Rayleigh-scatter temperature correction is negligible (Cacciani et al. 1989).

Average ozone density profiles appropriate for low and middle latitudes for winter, spring, summer, and fall are taken from Klenk et al. (1983) and are shown in Fig. 1. The equinox and summer high latitude ozone profiles are also from Klenk et al. (1983). These climatologies, above 20 km, are from the Nimbus-7 solar backscattered ultraviolet (SBUV) instrument. Low latitude is defined as below 25° latitude, middle latitude is from 25° to 65° , and high latitude is from 65° to 80° . Since this experiment requires sunlight to retrieve ozone, profiles were not available for the polar night. For the high latitude winter case a zonally average profile from the model of de Grandpré et al. (1997) was used. These model calculations use only homogeneous chemistry. The effect of polar ozone holes on the ozone densities above 25 km is small. However, at these heights, additional scattering from polar stratospheric clouds is possible. Temperature corrections for cloudscattering effects are beyond the scope of this paper.

The seasonal deviations from the mean for these profiles is shown in Fig. 2. The deviations are calculated as a percent difference of the individual profiles and the mean of the four profiles at each latitude range. The largest deviations are at high latitudes while the smallest are at low latitudes, where the ozone number density is largest. Figure 2 serves two purposes. First, it highlights the magnitude of the ozone seasonal variability. Second, it allows the reader to develop a feel for the amount of correction necessary for a given change in ozone. For example, if one is concerned about what uncertainty a change in ozone of 5% would have on the standard correction given in (4), they can look at regions of 5% changes in variability in ozone profiles and see the corresponding changes in temperature correction in Figs. 4 and 5. As will be discussed in section 4, for changes of this level, the change in temperature correction is small (a few percent) relative to the average value of the temperature correction.

The calculation also requires the appropriate seasonal averages for the total density and temperature. These profiles are taken from the compilation given by Kantor and Cole (1985), appropriate for the same latitudes and seasons. The temperature profiles used are shown in Fig. 3.



FIG. 4. Corrected minus the uncorrected temperature as a function of height for high latitudes (top), middle latitudes (middle), and low latitudes (bottom) at 589 nm. The thin solid line on the left-hand side of each panel is the standard deviation of the profiles from their mean.

The optical depth, τ , is then found in the usual manner from

$$\tau(z, \lambda) = \int_{z_0}^z \sigma(\lambda) n(z') \, dz', \qquad (2)$$

where z_0 is the altitude of the lidar, taken here to be sea level. If considering satellite measurements of Rayleigh scattering, the integral would be from the top of the atmosphere to the height of interest.

Once the optical depth is known, the transmission is given by Beer's law:

$$T(z, \lambda) = e^{-\tau(z, \lambda)}.$$
 (3)

For the calculations presented here, the true atmospheric density is known. For a Rayleigh-scatter lidar sounding, the experimenter obtains the product of the true relative density and the transmission function. If ozone absorption is present, the transmission from the surface to altitudes above the absorption is constant but diminished relative to the lower heights. Hence, above the absorption, the temperatures retrieved from the relative densities are not affected by absorption. However, the relative densities in the absorption region are larger than the actual relative densities, since measurements from these height are affected by the absorption to a lesser extent than densities above the absorption region. Hence, these measured higher



FIG. 5. Corrected minus the uncorrected temperature as a function of height for high latitudes (top), middle latitudes (middle), and low latitudes (bottom) at 532 nm. The thin solid line on the left-hand side of each panel is the standard deviation of the profiles from their mean.

densities cause the retrieved temperatures to be lower than the actual temperatures.

For the calculations here, we do the inverse problem. Corrected temperatures are found directly from the known densities. Uncorrected temperatures are found by the dividing the model densities by a normalized transmission function. The transmission function in (3) is normalized to unity at the "top" of the calculation (e.g., 60 km), decreasing below unity where ozone absorption is present.

3. Results

Figures 4 and 5 show the difference between the corrected and uncorrected temperature profiles for the four seasons for backscatter returns at 589 and 532 nm. The temperature changes are larger at 589 nm due to the greater ozone absorption. The average correction for all seasons is largest at low latitudes and smallest at the pole due to the greater upper stratospheric ozone densities at the lower latitudes.

Also shown in Figs. 4 and 5 is the standard deviation of the temperature corrections due to seasonal variability. The seasonal variability in the correction is largest at the highest latitudes, particularly in the winter. Note that for the high latitude case, the variability shown is only for the equinox and summer seasons, as the winter temperature correction is significantly smaller than the other cases. Except for the high latitude winter case, the standard deviation of the correction is much less than the magnitude of the correction itself. Hence, significant improvements to Rayleigh-scatter temperature estimates in the stratosphere can be made without detailed knowledge of the ozone profile compared to neglecting the correction.

Temperature measurements (K) reported without an ozone correction can be increased by an amount given by

$$\Delta T = a_3 z^3 + a_2 z^2 + a_1 z + a_0, \tag{4}$$

where z is altitude and 25 < z < 50 km. The polynomial coefficients, which give the mean temperature correction for the appropriate latitude, are given in Table 1 for 589 nm and Table 2 for 532 nm. Of course, individual experimenters can correct the shape of their density profiles using whatever ozone profiles are most appropriate. What is important is to provide a correction for existing measurements in the literature, which have not been corrected.

It is well known that the midlatitude mesospheric ozone densities can show increases of factors of 3 to 5 during the spring equinox in the 70-km altitude region. Ozone profiles with a secondary peak in the upper mesosphere were used to determine if mesospheric ozone could have a significant effect on retrieved temperatures. Mesospheric ozone was found to have an insignificant effect on temperature retrievals (changes on the order of a few hundredths of a degree). Thus, corrections for Rayleigh-scatter temperature retrievals for ozone absorption are only necessary in the stratosphere.

4. Summary

The result of these calculations show the need to correct Rayleigh-scatter measurements for ozone absorption. Fortunately, for most circumstances, the improvements of the temperatures using the ozone climatological mean is an order of magnitude or more better than not applying a correction. Though the corrections are small, they are not negligible. In the past, before large power-aperture product lidars became available, such corrections may have been less important, as the statistical noise of the measurement was dominant, even in the stratosphere. The photon noise in the middle stratosphere for the Purple Crow Lidar is negligible for integrations greater than tens of minutes. For studies of possible anthropogenic temperature change, such as the Stratospheric Processes and their Role in Climate (SPARC) initiative to study stratospheric temperature trends, corrections on the order of 1 K become critical, particularly if measurement sets with and without the correction are compared. It is important for the community to be aware of this effect and to correct for it.

In conclusion, correcting Rayleigh-scatter density profiles for ozone absorption causes temperature increases of 3 to 4 K at 589 nm and 1 to 2 K at 532 nm around 30 km altitude. Seasonal variability in ozone causes changes on the order of 10% of the above values, except in the winter at high latitudes, where the decreased upper stratospheric ozone densities cause temperature differences between corrected and uncorrected temperature profiles 30% less than the other seasons. Thus, improvements in Rayleigh-scatter temperature estimates are obtained in most situations using any reasonable estimates or measurements of the ozone height profile. Though the ozone changes used for these calculations are based on seasonal changes, nightly or hourly changes in ozone of the same magnitude produce almost identical changes in the temperature derived by Rayleigh-scatter lidars. Hence, these corrections can be equally well applied to shorter timescales.

Acknowledgments. We would like to thank Dr. T. Leblanc for alerting us to the need for this correction in our measurements, J. de Grandpré and J. C. Mc-Connell for providing us with ozone profiles, and the National Research and Engineering Research Council of Canada, the Meteorological Service of Canada, and CRESTech for their support of this project. We would also like to thank the reviewers for improving this paper with their helpful comments.

REFERENCES

- Brasseur, G., and S. Solomon, 1985: Aeronomy of the Middle Atmosphere. D. Reidel, 156 pp.
- Cacciani, M., A. D. Sarra, G. Fiocco, and A. Amoruso, 1989: Absolute determination of the cross-section of ozone in the wavelength region 339 to 355 nm at temperatures of 220 to 293 K. *J. Geophys. Res.*, **94**, 8485–8490.
- de Grandpré, J., J. W. Sandilands, J. C. McConnell, S. R. Beagley, P. C. Croteau, and M. Y. Danilin, 1997: Canadian middle atmosphere model: Preliminary results from the chemical transport module. *Atmos.-Ocean*, 35, 385–431.
- Hauchecorne, A., and M. L. Chanin, 1980: Density and temperature profiles obtained by lidar between 35 and 70 km. *Geophys. Res. Lett.*, 7, 565–568.
- Kantor, A. J., and A. E. Cole, 1985: Handbook of geophysics and the space environment. Section 15.2, A. S. Jursa, Ed., Air Force Geophysics Laboratory Tech. Rep. 85-0315. [NTIS ADA-167000.]
- Keckhut, P., M. L. Chanin, and A. Hauchecorne, 1990: Stratosphere temperature measurement using Raman lidar. Appl. Opt., 29, 5182–5186.
- —, A. Hauchecorne, and M. L. Chanin, 1993: A critical review of the database acquired for the long-term surveillance of the middle atmosphere by the French Rayleigh lidar. J. Atmos. Oceanic Technol., 10, 850–867.
- Klenk, K. F., P. K. Bhartia, E. Hilsenrath, and A. J. Fleig, 1983: Standard ozone profiles from balloon and satellite data sets. *J. Climate Appl. Meteor.*, **22**, 2012–2022.
- Leblanc, T., I. S. McDermid, A. Hauchecorne, and P. Keckhut, 1998: Evaluation of optimization of lidar temperature analysis algorithms using simulated data. J. Geophys. Res., 103, 6177–6187.
- Sica, R. J., S. Sargoytchev, P. S. Argall, E. F. Borra, L. Girard, C. T. Sparrow, and S. Flatt, 1995: Lidar measurements taken with a large-aperture liquid mirror. 1. Rayleigh-scatter system. *Appl. Opt.*, 34, 6925–6936.