Vol. 18 No. 5 Advances in Atmospheric Sciences September 2001

Ozone Profile Retrieval from Satellite Observation Using High Spectral Resolution Infrared Sounding Instrument

Yanni Qu[1], Mitchell D. Goldberg[2] and Murty Divakarla[1]

[1]*Research and Data System Corporation, 7833 Walker Dr. Greenbelt, MD 20770*

[2]*National Environment Satellite Data and Information Service, Office of Research and Application, World Weather Building, 5200 Auth Road, Camp Springs, MD 20746*

(Received September 1, 2000)

ABSTRACT

This paper presents a preliminary result on the retrieval of atmospheric ozone profiles using an improved regression technique and utilizing the data from the Atmospheric InfraRed Sounder (AIRS), a hyper–spectral instrument expected to be flown on the EOS–AQUA platform in 2002. Simulated AIRS spectra were used to study the sensitivity of AIRS radiance on the tropospheric and stratospheric ozone changes, and to study the impact of various channel combinations on the ozone profile retrieval. Sensitivity study results indicate that the AIRS high resolution spectral channels between the wavenumber 650–800 cm^{-1} provide very useful information to accurately retrieve tropospheric and stratospheric ozone profiles. Eigenvector decomposition of AIRS spectra indicate that no more than 100 eigenvectors are needed to retrieve very accurate ozone profiles. The accuracy of the retrieved atmospheric ozone profile from the present technique and utilizing the AIRS data was compared with the accuracy obtained from current Advanced TIROS Operational Vertical Sounder (ATOVS) data aboard National Oceanic and Atmospheric Administration (NOAA) satellites. As expected, a comparison of retrieval results confirms that the ozone profile retrieved with the AIRS data is superior to that of ATOVS.

Key words: AIRS, ATOVS, Regression, Eigenvector, Principal component

1. Introduction

Ozone plays a very important role in global climate change. This is particularly true in the stratosphere, where ultra–violet solar radiation is strongly absorbed by ozone, leading to substantial change in the earths atmospheric thermal, physical and chemical structure. Although the troposphere contains only about 10% of the total atmospheric ozone, the variation of tropospheric ozone may have more significant climatic effect than stratospheric ozone on the earth's surface temperature, because the solar and the infrared effects of tropospheric ozone changes the surface temperature in the same direction (Ramanathan, et al., 1987). Also, being closer to the surface of the earth, the tropospheric ozone has a significant impact on the biosphere, including human life and plants. Strong attention is now being placed on the measurement of the tropospheric ozone, which can be a hazardous pollutant.

To study the climatic effects of the atmospheric ozone and to better understand its role in the radiative, photochemical and meteorological processes of the earth–atmosphere system, it is necessary to know ozone's 3–D distributions, as well as its temporal change in the present atmosphere. Satellite vertical soundings provide a very powerful tool to achieve this goal. Satellite observations provide both temporal and spatial sampling over the whole globe, especially in otherwise inaccessible areas, whereas balloon and aircraft techniques have very limited operational range and are costly when implemented around the world.

The principal technology used for ozone profile measurement in the past and current operational and research satellites is listed in Table 1. An examination of Table 1 reveals that most of the ozone profile measurements from satellites are limited to the stratosphere due to the characteristic limitations of the observing instruments. These measurements are important in the study of the influence on the solar radiation reaching the earth. To determine the long–term implications of ozone change on public health and agriculture, tropospheric ozone retrievals from satellite will become important. A hyper–spectral infrared sounding instrument will provide an opportunity to observe stratospheric and tropospheric ozone simultaneously.

Over the past 30 years, many studies have been done to improve the accuracy of retrieving atmospheric parameters from satellite observations. Since the temperature and water vapor profiling capabilities are needed to support global numerical weather prediction, the emphasis to this point has been placed on improving the vertical resolution of thermodynamic soundings. To achieve the required vertical resolution for temperature and moisture profile, the sounding instrument must have near continuous spectral coverage through the 650–2700 cm^{-1} region with a spectral resolution ($\Delta\lambda / \lambda$, λ is wavelength) of the order 1.0 / 1000 (Smith et al., 1979, 1983; Fleming, 1987). High spectral resolution is needed to avoid smearing the upwelling radiance contributions from the relatively strong but narrow lines with the contributions from the more transparent and broader regions between the absorption lines. Meanwhile, the quasi–continuous spectral radiation observations support a capability to measure atmospheric trace gas profiles, which are important for studying global climate change. As a major trace gas, ozone profiles can be retrieved from such an instrument. The Atmospheric Infrared Sounder (AIRS) is one such instrument. It will fly on the second Earth Observing System (EOS–AQUA), scheduled to be launched in 2002.

Table 1. Satellite ozone observations

BUV	Backscattered Ultraviolet (25–55 km)	BUV
SBUV	Solar Backscattered Ultraviolet (25–55 km)	BUV
SBUV / 2	Solar Backscattered Ultraviolet / 2 (25–55 km)	BUV
LRIR	Limb Radiance Inversion Radiometer (15–60 km)	9.6 μm
LIMS	Limb Infrared Monitor of the Stratosphere (16–60 km)	9.6 μm
SAGE	Stratospheric Aerosol and Gas Experiment (16–60 km)	Solar Occult
SAGE / 2	Stratospheric Aerosol and Gas Experiment (16–60 km)	Solar Occult
CLAES	Cryogenic Limb Array Etalon	9.6 μm
HALOE	Halogen Occultation Experiment	Solar Occult
ISAMS	Improved Stratospheric and Mesospheric Sounder	9.6 μm
MLS	Microwave Limb Sounder	

The satellite retrieval of ozone using infrared absorption bands has been studied by a number of researchers (Heath et al., 1973; Ma et al., 1984; Marshall et al., 1991). Furthermore, the vertical resolution and error components of ozone retrieval from measurements of infrared limb emission has been studied by Gille et al. (1987), although the study was limited to the stratosphere. Using high spectral resolution instrument data, Lee (1992) analyzed ozone profile retrieval only for several individual cases.

This research investigates the capability of inferring 3–D ozone distributions from AIRS observations. While the main focus is on the capability of retrieving tropospheric ozone, the methodology adopted retrieves the entire atmospheric ozone profile at the same time. Principal component (or eigenvector) analysis was performed in this study to reduce the overwhelming data from the AIRS observation global. A statistical eigenvector regression algorithm was used for ozone profile retrieval to utilize as much information from AIRS spectra as possible. The next section describes the details on the AIRS instrument and the transmittance model used in the simulation of AIRS radiances. Section 3 gives the ozone retrieval methodology. Results obtained using the present method are presented in Section 4. The section includes the sensitivity study of AIRS radiance on stratospheric and tropospheric ozone changes, selection of optimum number of AIRS channels and eigenvectors for best ozone profile retrievals, and preliminary results of ozone profile retrieved from AIRS. Finally, conclusions from our study is given in section 5.

2. Data Resources

All studies presented in this paper are based on simulated AIRS radiance by Pressure Layer Fast Algorithm for Atmospheric Transmittance (PFAAST) model developed by University Maryland Baltimore Campus (UMBC) (Hannon et al., 1996). The atmospheric profiles used to simulate AIRS radiance were originally taken from National Center for Environmental Prediction (NCEP) forecast model. The NOAA–NCEP profiles were integrated with other data, like trace gas profiles, surface emissivity etc., by Jet Propulsion Laboratory (JPL). Six level ozone profile from 100 hPa to 10 hPa by NCEP model were appended with Upper Atmosphere Research Satellite (UARS) (10~ 0.1 hPa) and HARVARD (1000~ 100 hPa) climatological data to obtain entire ozone profile from surface to 0.1 hPa (Evan Fishbein, 2000). Two data sets were used in this study. An ensemble of 6030 profiles selected from the whole globe were used as training data to study our retrieval method and to generate regression coefficients. An independent data consisting of 300 profiles was used to verify the accuracy achieved by present algorithm.

AIRS is a nearly continuous spectral coverage spectrometer from 3.7 to 15.4 μm. AIRS has about 2378 detector elements or channels, at its focal plane with a noise level between 0.1–0.2 K at 250 K. The AIRS spectral ranges include the 4.2 and 15 μm CO_2 bands, that are used in the temperature profile retrievals. 6.3 μm is used to retrieve of water vapor, and 9.6 μm to retrieve ozone. There are about 180 channels within the 9.6 μm band alone. 9.6 μm is traditionally used for ozone profile retrieval. The wings of the ozone band and other weaker ozone absorption lines over the entire AIRS spectrum can probe into the lower atmospheric layer ozone, whereas the center channels of the band can measure the upper layer ozone theoretically.

AIRS PFAAST is a monochromatic layer to space transmittance model. It produces equivalent channel averaged optical depths instead of layer transmittance. The current PFAAST model allows water vapor, ozone, methane, carbon monoxide, the temperature, and local scan angle to vary. All other gases are treated as ' fixed' . Pressure layering grid for the AIRS PFAAST model was selected to keep radiative transfer errors well below the instrument noise. Details about the AIRS PFAAST model and its use are documented by Hannon, et al., in 1996. The following relation defines the pressure layer boundaries selected for AIRS

$$P(i) = (ai^2 + bi + c)^{7/2}, \tag{1}$$

where P is a pressure in hPa, i is layer boundary index and ranges from 1 to 101, and the parameters a, b and c were determined by solving this equation with the following fixed value, $P(1)=1100$, $P(38)=300$ and $P(101)=0.005$ hPa.

A typical AIRS upwelling radiance spectrum in brightness temperature units simulated by AIRS PFAAST is shown in Fig.1.

3. Ozone retrieval methodology

A linear statistical technique is used for retrieving atmospheric ozone profiles from satellite measured spectral radiance. This technique combines a statistical eigenvector analysis and a linear statistical regression method. Once a regression relationship is developed, an atmospheric ozone profile can be retrieved from the AIRS spectrum.

3.1 *Regression between principal component score and ozone profile*

Statistical linear regression between principal component score of brightness temperature covariance eigenvector (principal component) and atmospheric parameters had been previously studied (Smith, et. al. 1976). The basic idea of this research stems from that paper. However, some details are different, like using a noise weighted radiance (radiance / noise) covariance matrix instead of brightness temperature to generate the eigenvectors, especially since this study utilizes high spectral resolution radiance observations.

The principal component score D (nsample × npc) can be calculated by

$$D = R\ E, \tag{2}$$

where E (nchan × npc) is a orthogonal eigenvector from the covariance matrix of R (nsample × nchan). R is radiance matrix weighted by expected instrument noise. The nsample is the number of samples in our training data set. The nchan is AIRS channels used in our

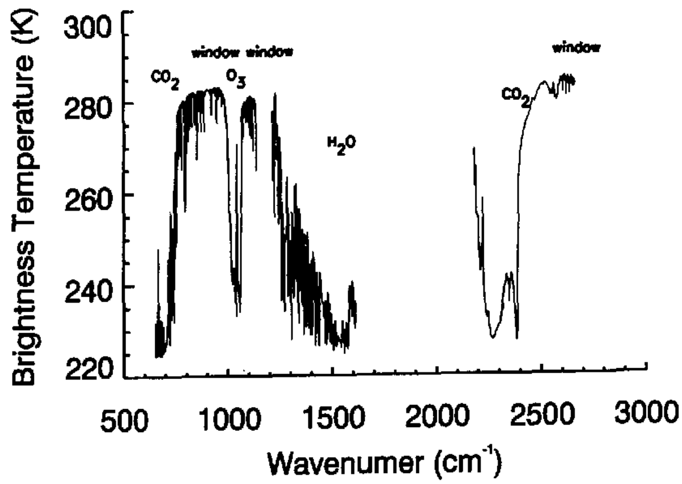


Fig. 1. Simulated AIRS brightness temperature spectrum for clear condition.

regression. It can be an entire set of AIRS channels or a subset. The npc is the number of eigenvector used to reconstruct AIRS radiance spectra.

A regression relationship between the ozone profile O and D can be obtained as follows.

$$O = DG \tag{3}$$

Using the normal equation to solve the least squares problem for G, gives

$$G = (D^T D)^{-1} D^T O, \tag{4}$$

where G represents the ozone profile regression coefficients with dimension npc × nlevel, and nlevel is the atmospheric pressure levels of ozone profiles. Although 100 levels was used to generate ozone regression coefficient, only nine integrated the ozone layers will be displayed. Those nine layers are 1–2, 2–4, 4–8, 8–14, 14–29, 29–61, 61–134, 134–235 hPa and 235 hPa to surface.

3.2 *Retrieval of the ozone profile*

Any observed radiance can be expanded as

$$r = c\ E, \tag{5}$$

where r is a vector. E is the eigenvector matrix from the previous EOF analysis, and c is a vector containing the principal component score for r, respectively. When a spectral radiance r is observed from satellite, its principal component score can be calculated by

$$c = r\ E^T. \tag{6}$$

After determining c, the ozone profile can be found.

$$O = cG. \tag{7}$$

Given a set of AIRS spectral radiance observations, ozone profiles can be retrieved using Eq. (7) with the coefficients obtained from (4) and (6). The retrieved ozone profile can be used as a first guess in another retrieval algorithm that requires a first guess (e.g. physical retrieval) to produce a final retrieval. The final retrieval product depends on the radiance residual. If the residual in 9.6 μm is less than the instrument noise, the final retrieval product would be same as that of generated by the statistical regression (Eq. 7). Otherwise, the final retrieval method will further refine the ozone profile retrieved by statistical regression. Results presented in this paper are based on the statistical regression using Eq. (7).

4. Results

To ascertain the strength of the signal received by AIRS instrument from satellite, the sensitivity study of the AIRS channel radiance to variations of tropospheric and stratospheric ozone was performed. In addition, the number of channels and the number of eigenvectors used to obtain the best ozone regression retrieval were studied. Applications of eigenvector regression algorithm to AIRS observation were also performed. RMS errors of ozone profiles retrieved from 300 different independent samples around the world indicate the possibility of reproducing ozone profiles by AIRS. Three individual retrieved ozone profiles were given to show the regression algorithms accuracy. To further assess the performance of the AIRS instrument on ozone profile retrieval, RMS errors of ozone profiles retrieved using AIRS data were compared with those using ATOVS data aboard the current NOAA operational satellite.

4.1 *Sensitivity of AIRS channels to tropospheric and stratospheric ozone*

The purpose of sensitivity studies is to verify if the signal can be received by the AIRS instrument when only part of atmospheric ozone profile changed. Two separate experiments were conducted to assess the sensitivity of AIRS radiance to variation in tropospheric and stratospheric ozone profile. To begin with, the U.S. Summer Standard atmosphere was used, and stratospheric ozone (100–0.1 hPa) amount was increased to 10% and 50%. The resultant change in the AIRS brightness temperature is shown in Fig. 2a. In the second experiment, the tropospheric ozone was increased to 10% and 50%, and Fig. 2b shows the resultant change in brightness temperature. It is obvious from these figures that the AIRS channels show a higher sensitivity to stratospheric ozone variation. A 10% change in stratospheric ozone has resulted a 1 K change in the center of the ozone absorption band. A 50% change in the stratospheric ozone has resulted a decrease of 4.3 K in several channel radiance. This strong signal from stratospheric ozone indicates that the stratospheric ozone variation can be well monitored by AIRS. With respect to tropospheric ozone change in Fig. 2b, the corresponding changes in AIRS channel brightness temperature are about 0.5 K and 1.8 K respectively. Although these change are not as large as that of stratospheric ozone change, the AIRS channel brightness temperature changes are well above the instrument noise level to retrieve tropospheric ozone profiles. Another interesting spectral region to note is 650–800 cm^{-1} (Fig. 2a), which is affected by weaker ozone lines.

4.2 *Studies of optimum number of channels and eigenvectors*

Selection of the optimum number of channels and eigenvectors to obtain the best ozone profile retrieval was performed on training data set described in Section 2. Five sets of channel combinations were used in channel selection study. All unstable and noisy channels (about 478 channels) for AIRS were excluded from our channel lists. The first set is for the 9.6 μm ozone band only. It includes 176 channels covering wavenumber from 980–1080 cm^{-1}. This is a traditional infrared spectral region for ozone profile retrieval used by most past and current satellite ozone measurements. The second set is whole AIRS spectrum except 9.6 μm ozone band, which has 1784 channels. The possibility of ozone profile retrieval without using ozone absorption band can be studied by this set because ozone absorption has very good correlation with atmospheric temperature distribution from pioneer study (Ma, et. al., 1984). The third set is from 650 to 1300 cm^{-1} spectral region that includes 1142 channels. The 9.6 μm ozone band , the 15 μm CO_2 temperature probing band, and many weaker ozone absorption lines are located in this region. The temperature correlation with ozone and contribution from weaker ozone lines could give additional information on ozone profile retrieval as revealed from the sensitivity study. The fourth set is from 800 to 2700 cm^{-1} containing 1584 channels. This set covers 4.3 μm CO_2 temperature probing band and 9.6 μm ozone absorption without any other weaker ozone lines. The fifth (and final) channel set covers the whole AIRS spectrum with 1960 channels. The effect of using all AIRS channels can be studied by this set. Figure 3 shows the regression results by different channel sets. It is obvious that channel set 5 gives the best result. Although set 2 has 1784 channels, low tropospheric ozone was not retrieved well because of lacking ozone 9.6 μm information. The 9.6 μm ozone band alone could not retrieve ozone profiles well either. The RMS errors are larger than 10% in every layer from 40 to 1000 hPa. The accuracy of retrieved ozone profiles can be improved dramatically with the combination of temperature probing channels and the 9.6 μm ozone

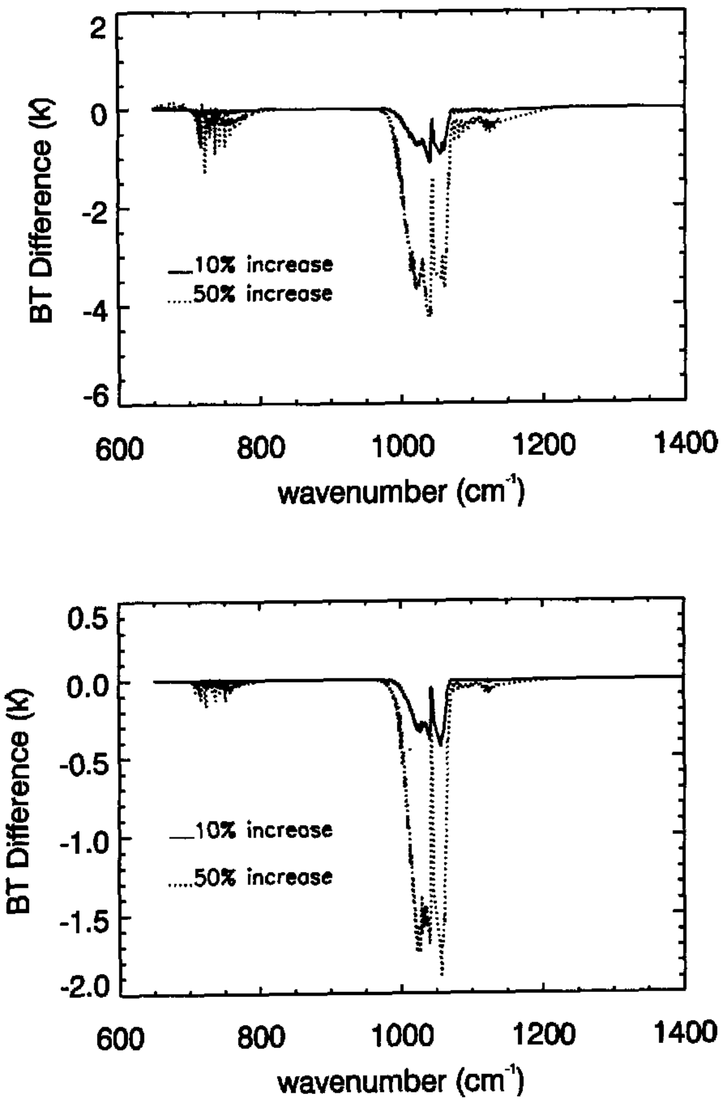


Fig. 2. Sensitivity of brightness temperature on stratospheric (a) and tropospheric (b) ozone changes. The solid lines show a 10% increase in ozone amount and the dotted lines indicate a 50% increase.

channels as revealed by the results from 3, 4 and 5. Low tropospheric ozone from 200 to 1000 hPa is reproduced with very good accuracy by 800–2700 cm^{-1} or 650–1300 cm^{-1} channels. However, ozone profiles for 40–200 hPa are retrieved with better accuracy using 650–

1300 cm^{-1} than by 800–2700 cm^{-1} region. Using all AIRS channels has resulted in improved accuracy for the entire retrieved ozone profiles from the stratosphere to the troposphere.

The retrieval of ozone profiles was performed using an eigenvector regression algorithm. Partial (980–1080 cm^{-1}) and whole AIRS (650–2700 cm^{-1}) spectral radiances were used to study the effect of different number of eigenvectors on the ozone retrieval accuracy. In Fig. 4, there is a little impact in ozone error using 20 or 100 eigenvectors for 980–1080 cm^{-1} region. However, Figure 5 shows that there is significant improvement on ozone error using 100 eigenvectors compared to using 20 eigenvectors for the entire AIRS spectrum. The results are consistent with our confirmation that AIRS spectra cannot be reconstructed well from 20 eigenvectors. Instead, 100 eigenvectors are needed to reconstruct most channels to within the noise level.

Consequently, the number of channels used and the number of eigenvectors used, both affect the ozone profile retrieval accuracy. An examination of the figures reveals that the most accurate ozone profile retrievals are obtained using all AIRS channels and using 100 eigenvectors.

4.3 *Ozone profiles retrieval*

A statistic result of 300 independent retrieved ozone profiles by using all AIRS channel and 100 eigenvectors is shown in Fig. 6. The bias, the RMS error, the percent RMS error and the mean ozone profile are given by dotted, dot–dash, dash and solid black lines respectively. The results confirm that the whole ozone profile can be reproduced well by eigenvector regression algorithm using AIRS data. Retrieval error from the ozone profiles is below 10% over all atmospheric layers and error in stratosphere is smaller than that of troposphere. The maximum RMS error is located in 100 hPa. The retrieved and the truth ozone profiles for three different samples randomly extracted from independent data are displayed in Fig. 7a, 7b and 7c. These three cases show the ability of the regression algorithm in retrieving various

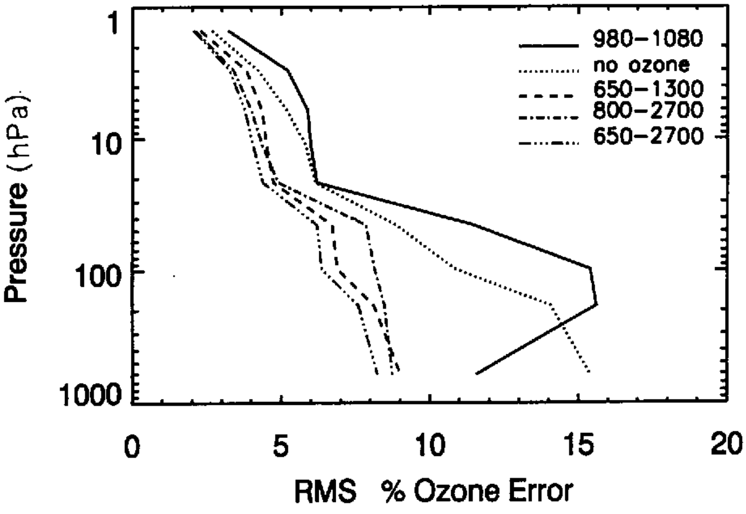


Fig. 3. RMS percentage errors of ozone profile retrievals from different spectral regions (or channels).

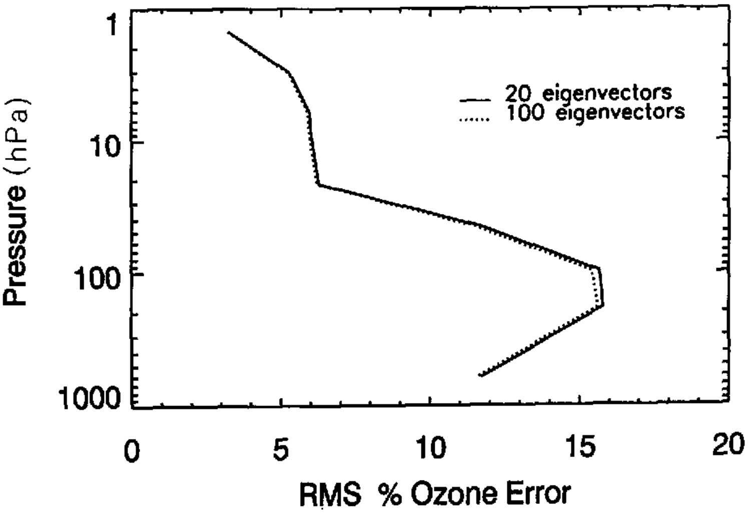


Fig. 4. RMS percentage errors of ozone profile retrievals using different number of eigenvectors for the 980–1080 cm^{-1}.

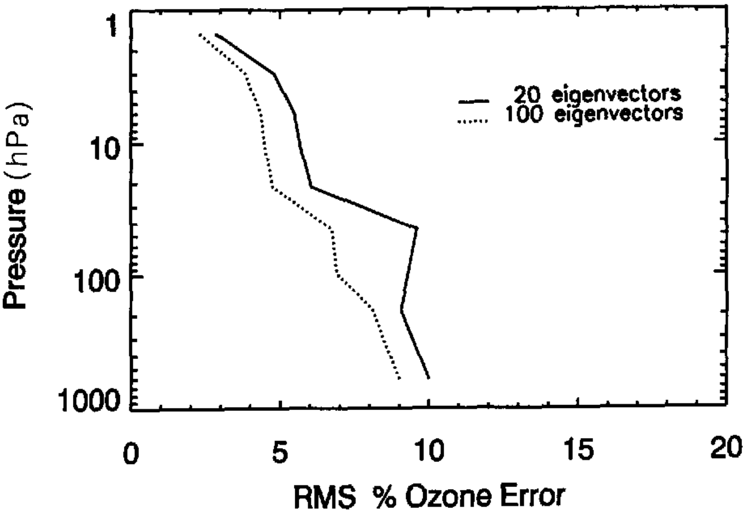


Fig. 5. RMS percentage erors of ozone profile retrievals using different number of eigenvectors for 650–2700 cm^{-1}.

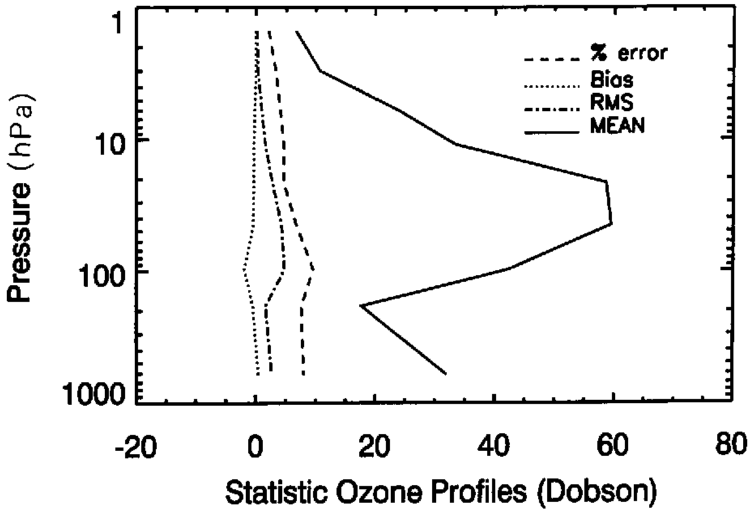


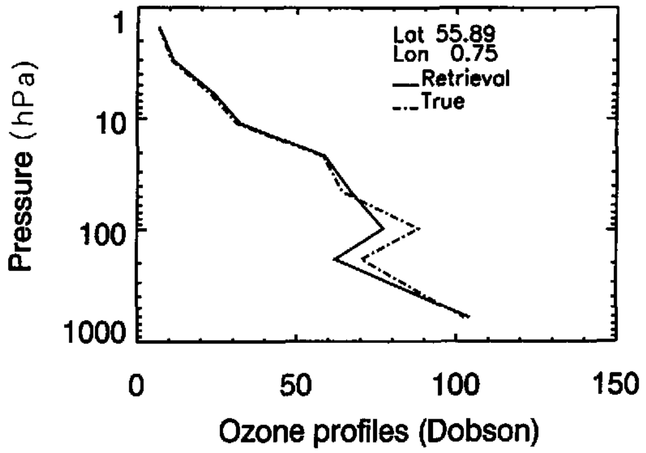
Fig. 6. Statistic error analysis for 300 independent ozone profile retrievals.

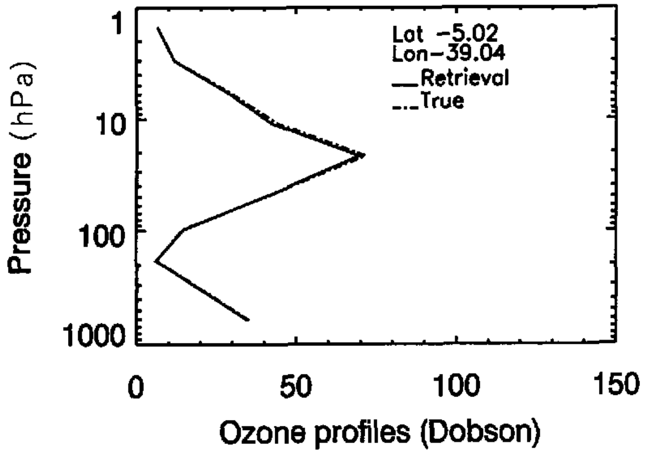
ozone profiles. The sub–tropical ozone profile shown in Fig. 7b has a maximum ozone amount of 70 Dobson units at about 25 hPa, and a minimum of 5 Dobson units at 200 hPa. The mid–latitude result is given in Fig. 7c. Maximum ozone of 70 Dobson units occurs over a broad pressure range around 100 hPa. Fig. 7a gives ozone profile at latitude 55.89 and longitude 0.75 degree. It is obvious that this profile shape is very different from Figs. 7b and 7c. The maximum ozone amount of 100 Dobson units is located in the lower troposphere, which makes tropospheric ozone significantly higher than the other two cases.

To further assess the performance of AIRS instrument, the ozone profile retrievals obtained by the AIRS data were compared with the retrievals from ATOVS data aboard the current NOAA operational satellite. Figure 8 shows the result of comparison. Although the dataset used for this comparison is different from the earlier dataset, the inter–comparison of ozone profile retrievals from AIRS and ATOVS would help to investigate the improvement achievable with AIRS. A radiosonde–rocket match–up data set consisting of 4000 profiles from the year 1988 was used for this comparison. The temperature and water vapor values were extrapolated up to 0.1 hPa using "shape similar" match up rocketsonde. Ozone profile information was obtained from World Ozone Data Center (WODC) global ozone sonde observations based on the latitude, longitude, day and time information. Ozone retrieval from simulated ATOVS uses all AMSU and HIRS channels, and only one ozone channel (9.6 μm) is available from the HIRS instrument. The dashed line in the Fig. 8 gives the global mean and solid line gives background error distributions of ozone profiles. The middle–wide line represents the retrieved profile RMS percentage error from the AIRS instrument and the narrow–wide line represents the retrieved error from ATOVS. An examination of the errors indicates that AIRS provides better ozone retrieval accuracy compared to ATOVS. The error in ATOVS retrieval at 700 hPa is about 20% and the retrieval error from AIRS is 13%.In general, the AIRS retrieval is superior compared to ATOVS over all atmospheric layers. The maximum error in AIRS retrieval occurs at 250 hPa. The total ozone (integrated over all ozone layers) errors indicated by the value at 1000 hPa, are 3.8% and 5.7% for AIRS and ATOVS, respectively.

5. Conclusions

AIRS is a high spectral resolution infrared instrument, which can sense atmospheric trace gas absorption lines and absorption between the lines. Sensitivity studies indicate the possibility of retrieval atmospheric ozone profiles using AIRS. Accurate retrieval ozone profiles can be obtained from eigenvector regression using 100 principal component scores. The ozone retrieval errors are within 10% in every layer when the regression algorithm was





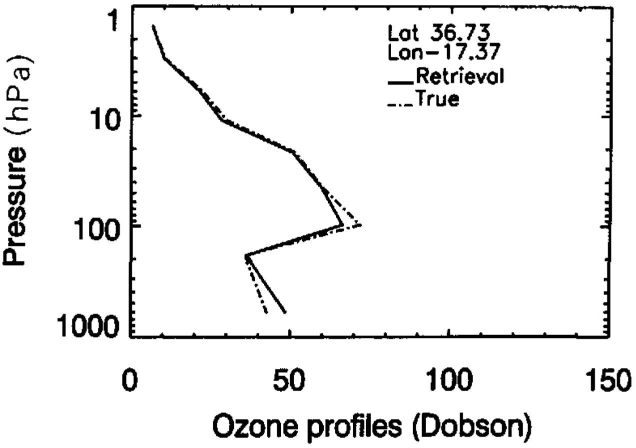


Fig. 7. Three individual ozone profiles retrieved by eigenvector regression algorithm.

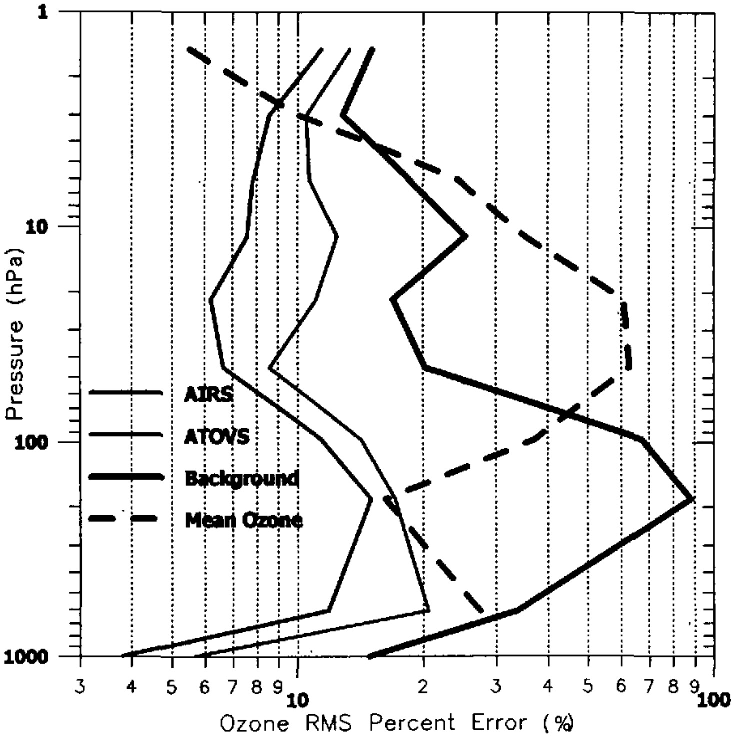


Fig. 8. A comparison of ozone profile retrieved from ATOVS and AIRS.

applied on a diverse dataset. Three hundreds independent ozone profiles showed very encouraging RMS and percentage errors. Three randomly selected individual ozone profiles give a general impression that eigenvector regression retrieval can be very accurate for very different ozone profile shapes. The conclusion from the presented study is that AIRS can provide better stratospheric and tropospheric ozone profile retrievals with respect to the current ATOVS.

REFERENCES

Fishbien, E., 2000: (Personal Communications).

Fleming, H. E., and L. Barnes, 1987: Satellite topographic remote sensing retrieval methods. RSRM 87: *Advances in Remote Sensing Retrieval Methods.* A Deepak Publishing, Hampton, VA.

Gille, J. C., and P. L. Bailey, 1987: Vertical resolution and error components of ozone retrievals from measurements of infrared limb emission. RSRM 87: *Advances in Remote Sensing Retrieval Methods.* A Deepak Publishing, Hampton, VA.

Hannon, S. E., L.L. Strow, and W.W. McMillan, 1996: *Atmospheric infrared fast transmittance models: a comparison of two approaches.* SPIE 2830, 94–105.

Heath, D.F., C.L. Mateer, and A. J. Krueger, 1973: The NIMBUS–4 backscatter ultraviolet (BUV) atmospheric ozone experiment – two years operation. *Pure Appl. Geophys.*, 106–108, 1238–1253.

Lee, S. C., 1992: Retrieval of atmospheric ozone from aircraft interferometer observations. M.S. Thesis, University of Wisconsin–Madison, Department of Meteorology, 64 pp.

Ma, X.L.,W.L. Smith, and H.M. Woolf, 1984: Total ozone from NOAA satellites – A physical model for obtaining measurements with high spatial resolution. *J. Clim. Appl. Meteor.*, **23**, 1309–1314.

Marshall, J.L., Z.J. Wu and G. Mills, 1991: Determining total ozone using TOVS data from NOAA satellites. *Technical Proceedings of Sixth International TOVS Study Conference*, 293–299.

Ramanathan, V., L. Callis, R. Cess, J. Hansen, I. Isaksen, W. Kuhn, A. Lacis, F. Luther, J. Mahlman, R. Reck, and M. Schlesinger, 1987: *Climate–chemical interactions and effects of changing atmospheric trace gases.*

Smith, W.L., and H.M. Woolf, 1976: The use of eigenvectors of statistical convariance matrices for interpreting satellite sounding radiometer observations, *J. Atmos. Sci.*, **33**, 1127–1140.

Smith, W. L., H. B. Howell, and H. M. Woolf, 1979: The use of interferometric radiance measurements for sounding the atmosphere. *J. Atmos. Sci.*, **36**, 566–575.

Smith, W. L., H. E. Revercomb, H. B. Howell, and H. M. Woolf, 1983: HIS – A satellite instrument to observe temperature and moisture profiles with high vertical resolution, *Proceedings of the Six Conference on Atmospheric Radiation*, AMS, Boston, MA. 10.