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Technique to retrieve solar EUV flux and neutral thermospheric O, O₂, N₂, and temperature from airglow measurements

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ABSTRACT

We describe a method for retrieving neutral thermospheric composition and solar EUV flux from optical measurements of the O⁺(²P) 732 nm and O(¹D) 630 nm airglow emissions. The parameters retrieved are the neutral temperature, the O, O₂, and N₂ density profiles, and a scaling factor for the solar EUV flux spectrum. The temperature, solar EUV flux scaling factor, and atomic oxygen density are first retrieved from the 732 nm emission, which are then used with the 630 nm emission to retrieve the O₂ and N₂ densities. Between the altitudes of 200 and 400 km the retrieval technique is able to statistically retrieve values to within 3.1% for thermospheric temperature, 3.3% for atomic oxygen, 2.3% for molecular oxygen, and 2.4% for molecular nitrogen. The solar EUV flux scaling factor has a retrieval error of 5.1%. We also present the results of retrievals using existing data taken from both groundbased and spacebased instruments. These include airglow data taken by the Visible Airglow Experiment on the Atmosphere Explorer spacecraft and the Imaging Spectrometric Observatory flown on the ATLAS 1 shuttle mission in 1992.

1. INTRODUCTION

It has long been believed that optical measurements of the twilight sky could be used to obtain information about thermospheric composition¹. The first major achievement was the development of a technique to retrieve thermospheric atomic oxygen density and temperature profiles from mid-latitude ground-based twilight measurements of the O⁺(²P) 732 nm emission^{2,3}. The technique required the unattenuated solar extreme ultraviolet (EUV) flux to be known or accurately modeled in order to accurately retrieve atomic oxygen density profiles. This is a problem because measurements of the unattenuated solar EUV flux are not made on a regular basis. However, McDade et al.⁴ demonstrated that it is possible to retrieve both the atomic oxygen density and the solar EUV flux by changing the viewing geometry to include measurements made in the zenith and at a small elevation angles ($\leq 30^\circ$). This new viewing geometry has been incorporated into the technique of Fennelly et al.³ to allow the retrieval of thermospheric atomic oxygen density, neutral temperature, and the unattenuated solar EUV flux from ground-based twilight measurements of the 732 nm emission. With this retrieved information and the measured twilight 630 nm emission it is then possible to retrieve the O₂ and N₂ densities. The retrieval of mid-latitude twilight thermospheric composition and a linear scaling factor for the solar EUV

flux spectrum from ground-based optical measurements represent major developments in the field of aeronomy. This technique is a promising method for monitoring the mid-latitude thermosphere composition and solar EUV flux.

2. THE RETRIEVAL TECHNIQUE

The excursion of the shadow line up (or down) the observing line of sight during a twilight period provides height-dependent measurements of the 732 nm and 630 nm emission intensities from the ground (Figure 1). Measurements taken at low elevation provide information on the height dependence of the thermospheric composition while observations in the zenith direction provide information on the solar EUV flux. The combination of the low elevation and zenith measurements allows the linear dependence of the 732 nm emission on the solar EUV flux to be distinguished from the nonlinear atomic oxygen density dependence.

The local photochemical models employ the Bates-Walker neutral thermospheric density and temperature model⁵ which has been parameterized to include time dependence³. In the Bates-Walker model, once the temperature profile is known, the scale height of O₂ and N₂ is determined, and the model only requires the densities at the lower boundary of the thermosphere to produce the entire O₂ and N₂ profiles. The strong dependence of twilight 630 nm emission on the O₂ density is employed to determine the O₂ density at 120 km. The 630 nm emission also has a dependence on the N₂ density below 250 km at twilight due to quenching.

Modeling the simple twilight chemistry of the emissions coupled with the time-parameterized Bates-Walker thermospheric composition model and an appropriate solar EUV flux model allows the application of the iterative minimization of the Levenberg-Marquardt method⁶ and Brent's method⁷. The Levenberg-Marquardt method iteratively solves a set of nonlinear equations to find the Bates-Walker parameters for the temperature and atomic oxygen density and solar EUV flux scaling parameter which gives the best agreement between the measured and modeled 732 nm emission intensities. Brent's method finds the values for the molecular oxygen and nitrogen Bates-Walker parameters by minimizing the chi-squared merit function of the measured and modeled 630 nm emission.

2.1 732 nm emission model

The retrieval technique is based on the 732 nm emission of O^{+(2P)}, principally because of the simple nature of its production and loss mechanisms. The dominant production source of the O^{+(2P)} ion is photoionization of O by solar EUV radiation at wavelengths of 66.5 nm and less. A second but minor source is photoelectron impact ionization of O. The O^{+(2P)} ion is destroyed by radiation loss and quenching by O and N₂. (The quenching mechanism is altitude dependent, with quenching by N₂ typically becoming significant below 250 km.) During twilight, the production of O^{+(2P)} is completely dominated by photoionization and loss by radiation. During the day the photoelectron impact production increases (but never becomes competitive with photoionization) and the quenching due to N₂ and O become competitive with radiative loss at low altitudes. Hence the 732 nm emission is a function of the O and N₂ densities.

Thus the volume emission rate of the 732 nm doublet is given by

$$\eta_{732} = \frac{0.781 A_{2P} (J + J_e) [O]}{A_{2P} + k_{N_2} [N_2] + k_O [O] + k_e [e]} \quad (1)$$

where 0.781 is the branching ratio for the 2D - 2P transition, J is the photoionization frequency, J_e is the photoelectron excitation frequency, A_{2P} is the inverse lifetime of the 2P state, and k_{N₂}, k_O, and k_e are the quenching rate coefficients for molecular nitrogen, atomic oxygen, and electrons, respectively. Photochemical equilibrium is assumed to apply. The integration of the volume emission rate along the line of sight yields the 732 nm intensity.

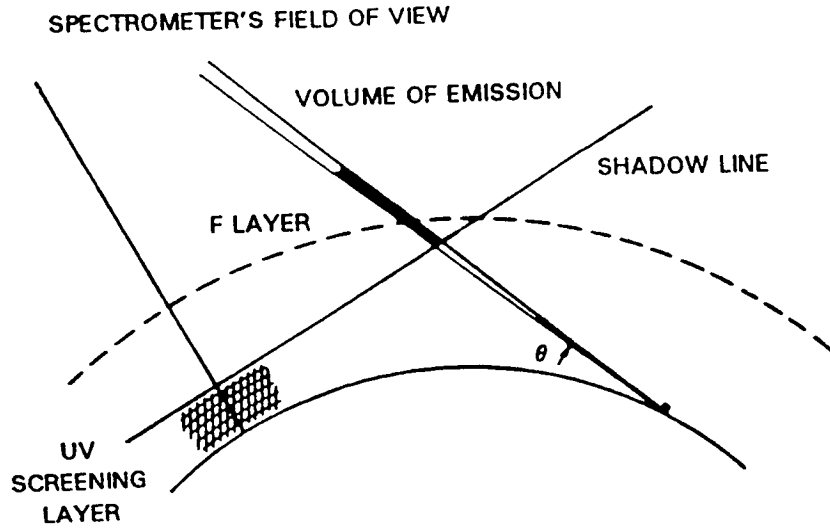


Figure 1. Viewing geometry for groundbased twilight measurements.

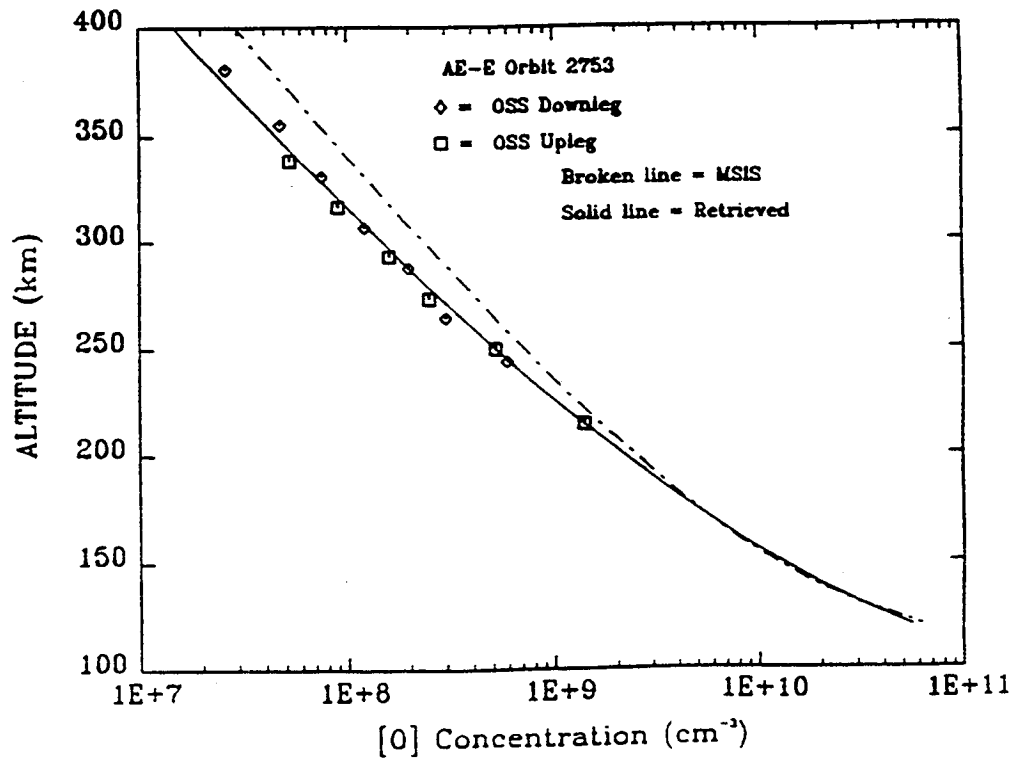


Figure 2. Comparison of the atomic oxygen profile retrieved from twilight 732 nm intensity measurements with *in situ* measurements of O made by AE-E during an overflight.

2.2 630 nm emission model

The 630 nm emission arises from the atomic oxygen transition of $O(^3P - ^1D)$. The three main excitation mechanisms of $O(^1D)$ are photodissociation of molecular oxygen by the Schumann-Runge UV bands, dissociative recombination of O_2^+ , and photoelectron impact excitation of O. The main loss mechanisms for the $O(^1D)$ state are radiation and quenching by N_2 and O. The 630 nm emission is particularly sensitive to the production of $O(^1D)$ by photodissociation of O_2 in the bright twilight. As the twilight advances into the night, the 630 nm emission production is dominated by the dissociative recombination of O_2^+ . During the period of the early twilight, quenching by N_2 becomes the dominant loss mechanism of $O(^1D)$ in the lower thermosphere, whereas radiation dominates the loss mechanisms at larger solar zenith angles and altitudes.

The volume emission rate for 630 nm is given by

$$\eta_{630} = \frac{A_{630}[\beta_{1D}\alpha_{tot}[O_2^+][e] + J_{SR}[O_2] + J_e[O_2]]}{A_{1D} + k_{N_2}[N_2] + k_O[O] + k_{O_2}[O_2]} \quad (2)$$

where A_{630} is the Einstein transition probability for emission at 630 nm; A_{1D} the total Einstein emission probability; β_{1D} , the efficiency for $O(^1D)$ production due to dissociative recombination of O_2^+ ; α_{tot} , the total dissociative recombination rate; J_{SR} , the Schumann-Runge UV attenuated photoionization frequency; J_e , the photoelectron excitation frequency; and k_{N_2} , k_{O_2} , and k_O , the quenching rates of N_2 , O_2 , and O, respectively.

The O_2^+ chemistry during the night simplifies to

$$[O_2^+] = \frac{k_1[O_2][O^+]}{\alpha_{tot}[e]} \quad (3)$$

where k_1 is given by Chen et al.⁸ and is represented by the analytical expression

$$k_1 = 2.1 \times 10^{-11} \left[\frac{T_n + 2.0 T_i}{900} \right]^{-0.763} \quad (4)$$

where T_n and T_i are the neutral and ion temperatures, respectively. Below 400 km the ion temperature is approximately equal to the neutral temperature. This rate coefficient is only good for temperatures less than 900 K. Above that temperature it is known that it may slightly underestimate the rate coefficient for ionospheric conditions.

For the twilight it was found that the approximation adopted for the O_2^+ production Eq. (3) is still valid. Substituting Eq. (3) into Eq. (2), the volume emission rate becomes

$$\eta_{630} = \frac{A_{630}[(\beta_{1D}k_1[O^+] + J_{SR})[O_2] + J_e[O_2]]}{A_{1D} + k_{N_2}[N_2] + k_O[O] + k_{O_2}[O_2]} \quad (5)$$

3. EXPERIMENTAL VERIFICATION OF THE RETRIEVAL PROCESS

Opportunities for validation of the ground-based retrieval algorithm are limited as they require simultaneous airglow observations and *in situ* measurements from the same thermospheric volume. However, one case exists³ of a ground-based airglow measurement of the 732 nm $O^+(^2P)$ emission made by Meriwether et al.⁹ during an overflight of the Atmosphere Explorer C satellite. In this case, the retrieved atomic oxygen concentration could be compared with *in situ* measurements of O. The retrieved atomic oxygen density from the ground-based measurements of 732 nm is compared to the measurements of AE in Figure 2. Excellent agreement was obtained between the measured and retrieved values. The

good agreement obtained, however, is dependent on the corrections for extinction and water vapor absorption which were estimated by Meriwether et al. Since we have only recently developed quantitatively mature techniques for applying these corrections, the good results obtained for AE comparison is somewhat fortuitous, and should be regarded only as supportive evidence that the technique appears to work.

The most recent demonstration of the likely validity of the technique using groundbased data is a retrieval by Fennelly et al.¹⁰ using data taken at McDonald Observatory in which the tropospheric water vapor content was measured *in situ* by a radiosonde. Figure 3 shows the retrieved O profile compared with MSIS-86¹¹ values. Figure 4 shows the percentage difference between retrieved O densities and the MSIS-86 model values. We are in the process of demonstrating that the water vapor content can be reliably deduced by differential absorption techniques by simultaneously monitoring water vapor absorption features in the visible spectrum.

4. COMPUTER VERIFICATION OF THE RETRIEVAL PROCESS

Ideally, to validate the retrieval technique there should be simultaneous ground-based measurements of emissions and electron density, as well as *in situ* neutral thermospheric composition at points along the line of sight and the solar EUV flux. Unfortunately, there are no simultaneous measurements of both the 630 and 732 nm emissions which could be used to validate the full retrieval technique. Until an experiment can be developed and deployed to validate the retrieval process, this technique can only be verified by computer simulations.

In a numerical method of verification, a known neutral thermosphere and solar EUV flux is chosen from which synthetic measurements of the 732 and 630 nm emission are created. We assumed the measurements are made with the CEDAR narrow-band photometer (0.1 nm bandpass) with a sensitivity of 100 counts $R^{-1} s^{-1}$ reported in a companion paper¹². The synthetic measurements include effects from random noise consistent with the expected performance characteristics of the instrument and from the primary noise source in the twilight, namely Poisson noise associated with the sky background produced mainly by Rayleigh scattering of sunlight. In practice, the algorithms that are used to extract the desired airglow signals from the twilight continuum provide detailed diagnostic output on the measured statistical errors¹³. The largest component in the total statistical error is the component due to sky background subtraction. As the solar zenith angle (SZA) decreases, the Rayleigh scattering increases, as does the error due to the background subtraction. Typically, errors due to instrumental effects such as thermal noise can be neglected (because these can be effectively eliminated by adequate cooling) compared with the statistical noise associated with counting the bright twilight sky continuum photons.

We have estimated the upper bounds for the retrieved quantities by creating 50 unique synthetic data sets of the 732 and 630 nm emissions from a known twilight thermosphere and applying the retrieval process to each set. The retrieved quantities were then compared to the known values and absolute errors calculated. For each retrieval, a vertical profile of the absolute percent errors were calculated for atomic O, O₂, N₂, and temperature. In order to estimate the errors of the retrieval, the absolute percent errors of O, O₂, N₂, and temperature, from 120 to 400 km at 10 km intervals, were averaged for the 50 data sets. These averaged absolute percent error profiles are shown in Figure 5. The weighted average error for the retrieved temperature is 3.1%, 3.3% for O, 2.3% for O₂, 2.4% for N₂, and 5.1% for the EUV scaling factor.

5. SPACE-BASED OBSERVATIONS: ISO AND AE

In order to validate the retrieval approach further we have used the Atmosphere Explorer (AE-C) measurements of 732 nm emission made by the Visible Airglow Experiment¹⁴ (VAE) to retrieve atomic oxygen, which is then compared with *in situ* measurements of O made by the Open Source Spectrometer¹⁵ (OSS). The difference between the retrieved and measured O then allows an assessment to be made of the relative errors of measurement.

Figure 6 shows the selected VAE emission data, forward modeled emissions based on our retrieved profiles, and emissions obtained with MSIS-86 model densities. Note that the emissions computed using our retrieved results yield a significantly better fit at all altitudes to the VAE data than the MSIS-86 values. The calculated emissions in Figure 6

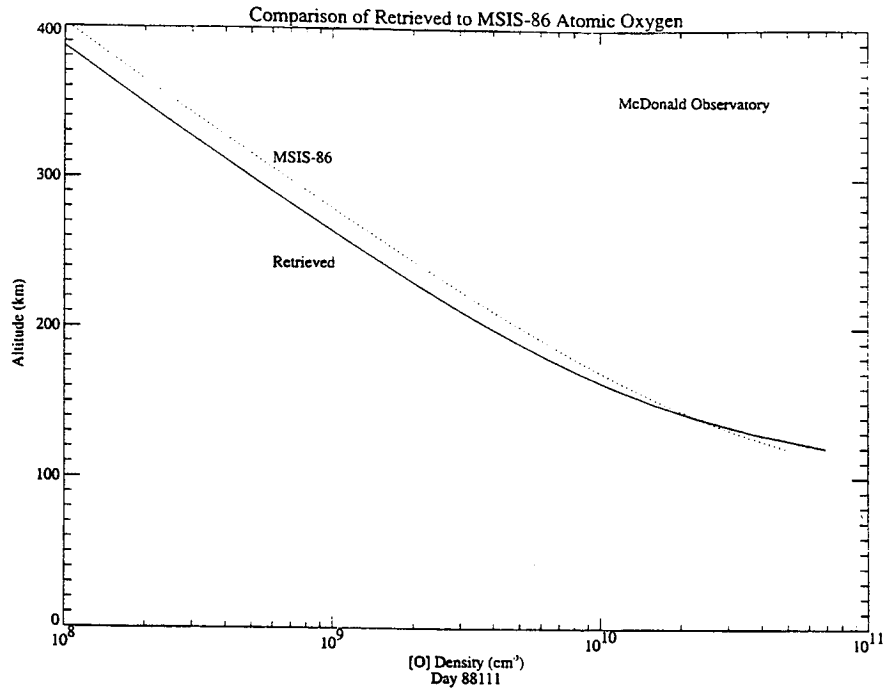


Figure 3. Comparison of the atomic oxygen profile retrieved from twilight 732 nm intensity measurements with MSIS-86 values.

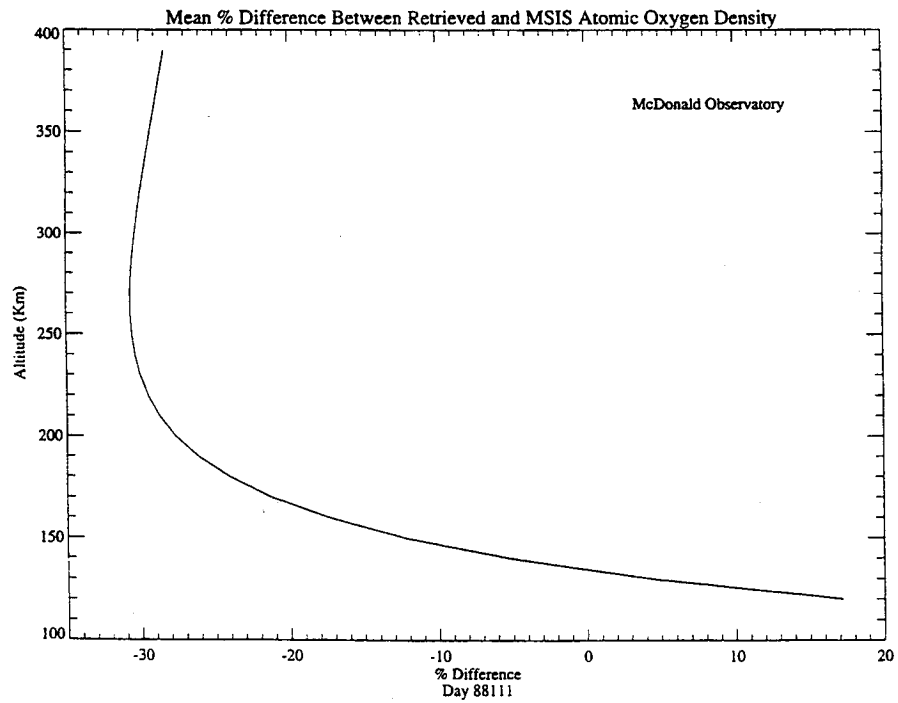


Figure 4. Percent difference between the retrieved and MSIS-86 O profiles shown in the previous figure.

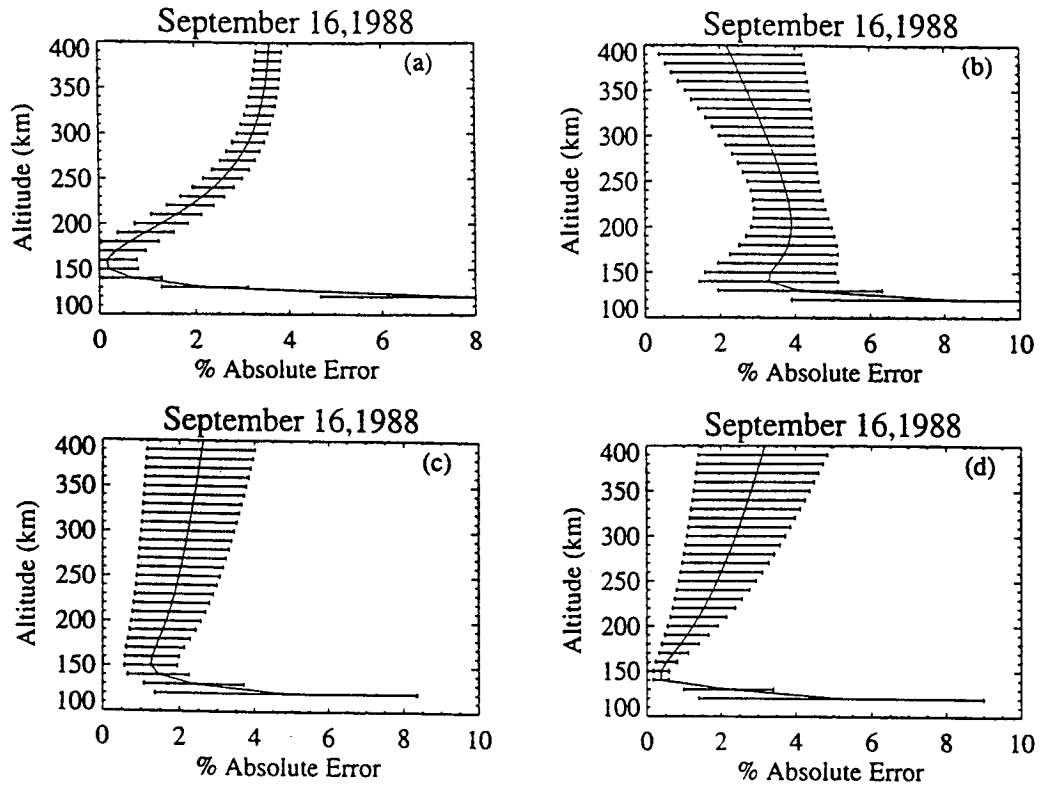


Figure 5. (a) Averaged absolute error and two sigma errors for temperature from 120 to 400 km in 10 km intervals. (b) Same as (a) except for atomic oxygen. (c) Same as (a) except for molecular oxygen. (d) Same as (a) except for molecular nitrogen.

represent line-of-sight integrations through 3-D modeled volume emission rates. The retrieved emission values are based on the atomic oxygen profiles returned from the retrieval algorithm. Figure 7 shows our retrieved atomic oxygen profile compared to the MSIS-86 profile, and *in situ* measurements from the AE OSS. There is excellent agreement between the retrieved and measured atomic oxygen densities.

Figure 8 shows the percent difference between the OSS and the retrieved atomic oxygen. The error increases from -15% at high altitudes to +15% at low altitudes. This is not a systematic error in a real sense, but rather illustrates the errors associated with the retrieval of Bates-Walker boundary values at both the upper and lower boundaries, *i.e.* exospheric temperature, temperature at 120 km and atomic oxygen at 120 km. The retrieval is currently naturally weighted by the large intensities in the vicinity of the layer peak.

We have also applied our technique to airglow observations from the ISO which flew as part of the NASA ATLAS-1 mission¹⁶. Because of the lack of *in situ* observations, these retrievals are compared with MSIS-86 model values. A total of five limb scans, covering a tangent altitude range of approximately 36 km, were utilized. The 732 nm emission measurements are shown in Figure 9 along with MSIS-86 neutral thermospheric values and best fit emissions from the retrieval technique.

6. SUMMARY

The twilight thermospheric composition and solar EUV flux can be retrieved from optical airglow measurements when there is also a simultaneous measurement of the bottomside electron density profile. The results demonstrate clearly that if the measurements are only limited by errors due to Poisson noise, height profiles of twilight thermospheric temperature, O, N₂, and O₂ can be reasonably accurately retrieved given an instrument which can spectrally isolate the spectral feature and which has a sensitivity of 100 counts R⁻¹ s⁻¹. Also, a scaling parameter for a solar EUV flux spectrum model can be retrieved accurately as well. Thus the solar EUV flux for a particular day can be estimated with greater confidence than can be obtained with empirical models of the solar EUV flux based on solar indices. Similar retrievals have been performed with space-based geometries.

While the simulation validation techniques referred to above may be viewed with suspicion, in that some crucial element of the actual observational process may have been overlooked, there are two important mitigating factors: 1) the simulations are based on the retrieval of aeronomic parameters from a synthetically generated database, for which the input parameters are known and which can be configured to include any conceivable scenario that could affect the measurement and retrieval process; and 2) with several years experience, we believe we have encountered or anticipated every significant trap or pitfall in the system. The value of the simulation approach lies in the fact that the errors on retrieved parameters can be precisely determined simply by noting the difference between the known inputs and the retrieved results. The sensitivity of the retrieval algorithms to any conceivable influence can, therefore, be quantitatively determined.

For example, we have evaluated sensitivities of the retrieval of neutral composition to: various kinds of noise (instrumental and geophysical) and to extremes in possible range, degrees of freedom, sampling frequency, temporal sampling window, extinction, absorption, absolute calibration and model uncertainties, and constraints on the number of measured parameters available^{2,3,17}. We have performed comprehensive simulations of the retrievals for widely varying geophysical conditions and found that to insure adequate sensitivity to the parameters retrieved over realistic variations in conditions (which may result in dramatic changes in the dominant processes or excitation mechanisms), it is important to extend the twilight observations into the bright twilight/dayglow regime (solar zenith angle $\leq 95^\circ$), and to continue the observations up to $\sim 110^\circ$ SZA. Some of this work has been published in the Journal of Geophysical Research¹⁷.

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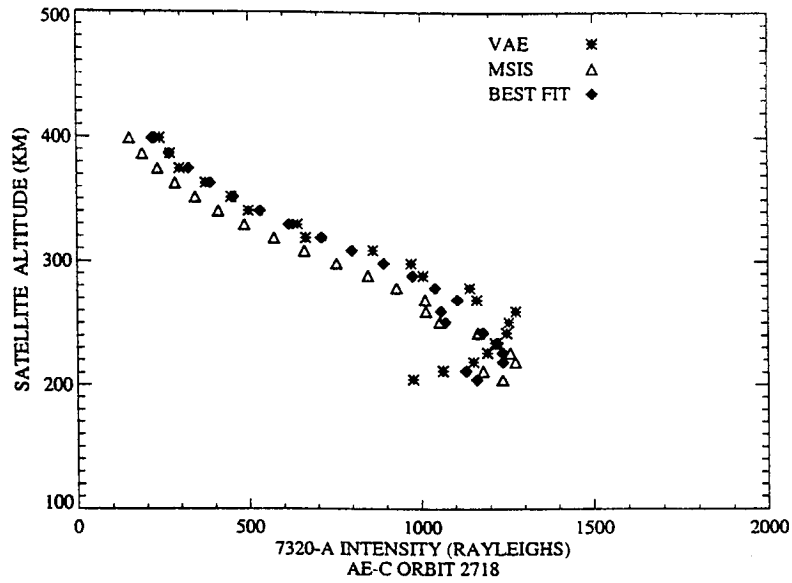


Figure 6. Modeled (triangles) and fitted (diamonds) 732 nm intensity compared with VAE measurements taken on the down-leg of (elliptical) AE-C orbit 2718 on day 74221.

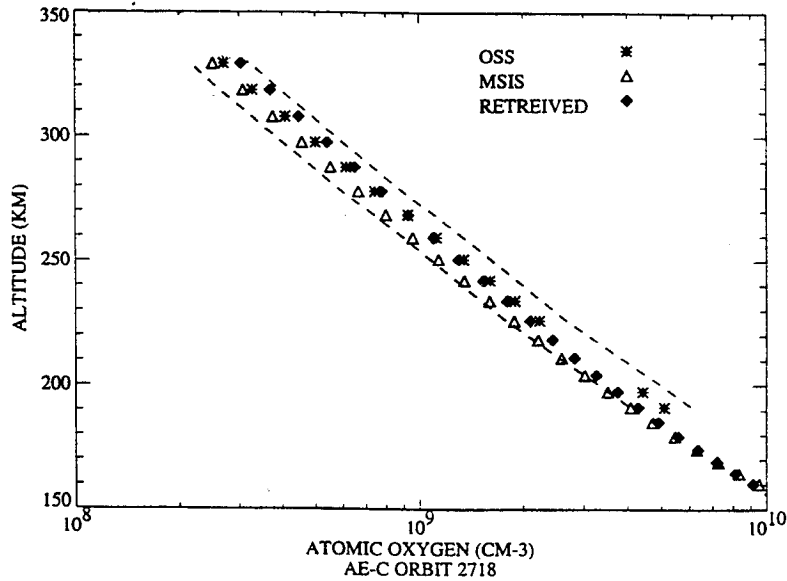


Figure 7. Comparison of the atomic oxygen profile retrieved from VAE 732 nm intensity measurements with in situ OSS measurements of O made on the down-leg of (elliptical) AE-C orbit 2718 on day 74221. The dashed line is an assumed (conservative) error.

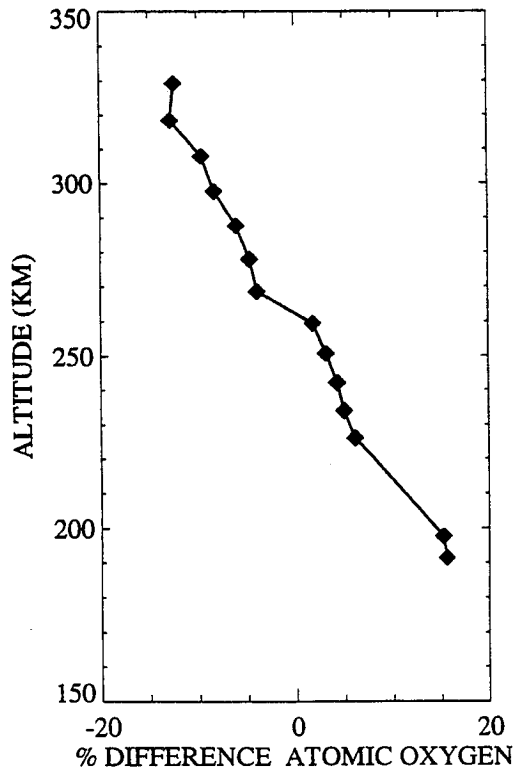


Figure 8. The percent difference between OSS atomic oxygen measurements and retrieved atomic oxygen densities from VAE 732 nm measurements.

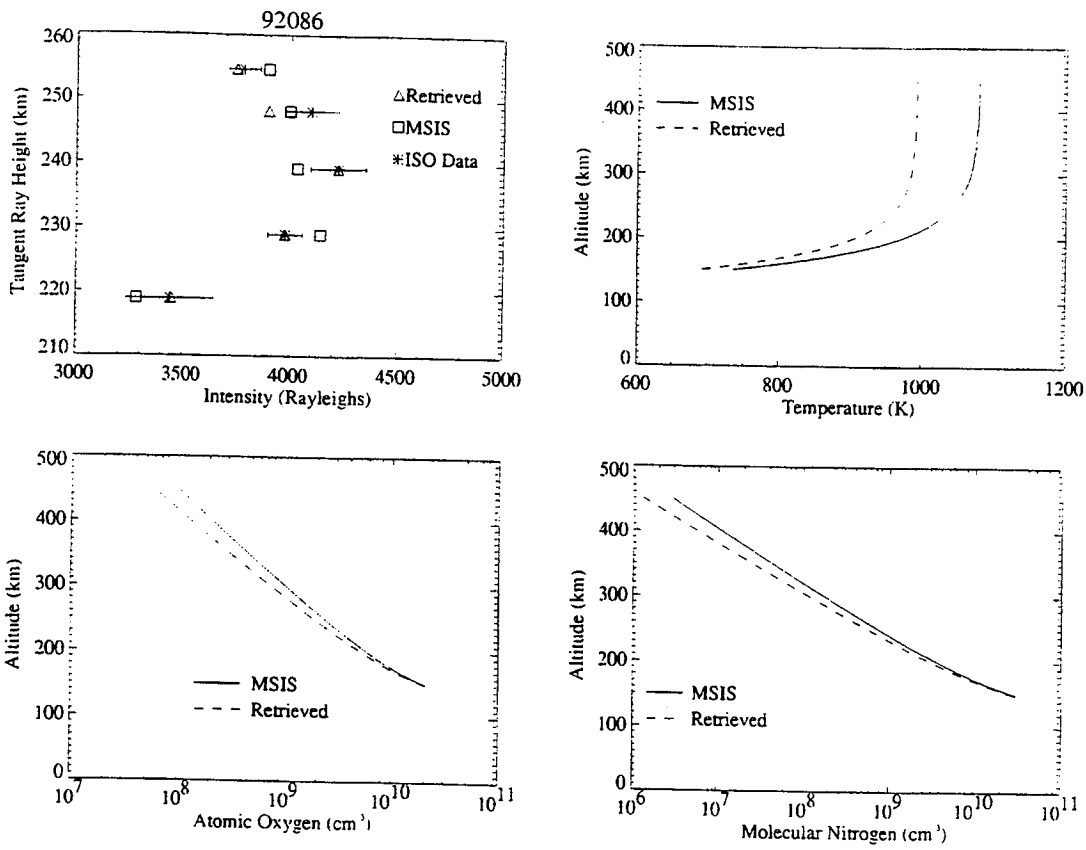


Figure 9. Retrieval from ATLAS-1 ISO data. (a) Measured, modeled (MSIS-86), and retrieved 732 nm emissions. (b) Retrieved altitude temperature profile compared to MSIS-86. (c) Same as (b) except for O. (d) Same as (c) except for N₂.

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