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UNIVERSITY OF WYOMING

FINAL REPORT

FOR

NASA CONTRACT NO. NSG-1518

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ABSTRACT

As a result of NASA Grant No. NSG-1518, we constructed a software system for reducing PAM-II data. The data reduction process concatenates the Air Force's data tapes; determines ephemeris; and inverts full-sun extinction data. Tests of this data reduction process show that PAM-II data can be compared with data from other, similar satellites; these tests also suggest future detailed study of ozone profiles in the polar latitudes.

October 1982

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Approximately one year and a half prior to the launch of the P78-1 satellite carrying the Office of Naval Research (ONR)-601 instrument, we began preparing to analyze the satellite data under a grant from the National Aeronautics and Space Administration (NASA)(Grant Number NSG-1518). The data reduction algorithms have since been constructed, and under other contracts, portions of the resulting data set have been and are being inverted to determine atmospheric constituents. This report summarizes the preparation of the software system being used to analyze PAM-II data and identifies some of the obstacles that had to be overcome in the process of preparing for data reduction.

BACKGROUND

In 1970 an experiment referred to as Stratospheric Aerosol Measurement (SAM) was proposed to NASA for flight on the OSO-J spacecraft. This spacecraft, in fact, was never built; only preliminary design work was ever accomplished. Later, the Office of Naval Research offered to fly an instrument, similar to that proposed for the earlier SAM experiment, on a military satellite. Referred to as PAM (Preliminary Aerosol Measurement), this second experiment was built and was launched on the P72-2 spacecraft in early 1975. Unfortunately, the sustainer motor of the Atlas missle boosting the spacecraft misfired and the spacecraft was destroyed over the Pacific Ocean. A third effort to fly an experiment for remote sensing of the stratospheric aerosols (again referred to as SAM) was successful in 1975 (Pepin, et al., 1977).

A few years later, under contract from NASA, the University of Wyoming built a similar experiment, the SAM-II, which was launched in the fall of 1978 on board Nimbus-7 (McCormick, et al., 1981). Meanwhile, after the loss of the original PAM instrument in 1975, the Office of Naval Research tried to find another ride for the backup instrument of the PAM experiment and did, the P78-1 mission. The backup instrument, PAM-II, was extensively modified prior to its launch in February 1979. Another experiment, the SAGE instrument (Stratospheric Aerosol and Gas Experiment), was also launched in February (McCormick, et al., 1979). In fact, the SAGE and the PAM-II instruments were launched in the same week in February, 1979.

Because of their orbital paths, optical configurations and wavelengths of observation, the SAM-II, SAGE, and PAM-II instruments collect different data. The concurrent nature of these experiments does, however, allow for significant comparisons and the acquisition of complementary atmospheric data. The orbital altitudes of SAGE and PAM-II are approximately 600 km, SAGE in an equitorially-inclined orbit and PAM-II in a sun-synchronous, polar orbit. SAM-II, also in a sun-synchronous, polar orbit, is at an altitude of approximately 900 km. The PAM-II experiment looks at the full sun, unlike the SAM-II and SAGE experiments which are able to resolve a small portion of the solar disk and thus provide higher vertical resolution. All three experiments have channels at 1000 nm allowing for the remote measurement of extinction due to stratospheric aerosol. SAM-II is only a single channel radiometer. PAM-II also has a channel at 600 nm, which is centered in the Chappuis band of ozone, and a third channel located at 430 nm. SAGE has a total of four channels, at 1000, 600, 450, and 385 nm.

PAM-II, the three-channel radiometer (at 1000, 600, and 430 nm), measures the total transmission of electromagnetic radiation traversing the earth's atmosphere. Inversions of the measured data can be used to determine wavelength-dependent, atmospheric extinction coefficients as a function of altitude.

THE DATA REDUCTION PROCESS OF PAM-II DATA

The data reduction process of PAM-II consists of three stages: the transfer of the data tapes to the University of Wyoming; the determination of ephemeris; and the inversion of full-sun data.

I. Transference of PAM-II Data Tapes:

As a result of our NASA grant in 1977, we began developing the software systems required for the analysis of the PAM-II data. The manner of transferring the data tapes to the University of Wyoming ,however, slowed the production of our data-reduction software system.

The Air Force, unlike NASA, uses a very large number of stations for receiving satellite transmissions. Each station collects one small snatch of data and records it on analog-data tape during a pass of the orbitting satellite. The stations then send their tapes to a central Air Force processing station to translate the analog-data tapes into the digital-data tapes necessary for later computer analysis.

For the P78-1 (PAM-II) project, computer facilities at the Western Test Range originally were to translate the anolog-tape data. Unfortunately, quite a few months after the launch of the P78-1, the Air Force determined that those facilities could not be devoted to the P78-1 project, thus requiring another contractor or government facility to translate the data tapes. Finally, in the spring of 1980, the Air Force selected the Eastern Test Range facility. A new software system was required for the data translation effort, however, since the Eastern Test Range used a different computer system than the Western Test Range. The Air Force and its contractors constructed that necessary software system in the following months.

To date, we have not received all of the digital-data tapes from the first year. (A few tapes have been received from the second and third year, but these amount to only a few dozen orbits from these years.) In all, we have received approximately 3,000 10-inch magnetic data tapes for the first year's data, each with small records of PAM-II data. The sheer number of tapes required us to first concatenate the data records, a one-year endeavor in itself. At present, eleven months of data have been packed into 32 data tapes to allow for the orderly analysis of PAM-II data.

II. Determination of Ephemeris:

In order to perform the inversions of full-sun extinction data, it is necessary not only to have the radiometric data but also to know the geometry whereby the measurements were made, that is, the geometry determining where the individual rays pass through the atmosphere. This requires a detailed knowledge of the orbit geometry during which the radiometric measurements were made. While the University of Wyoming specified the need for such detailed geometry in its proposal to NASA, early analysis clearly showed the tracking data of the Air Force were not sufficiently precise: Preliminary inversions performed on the data yielded results impossible to obtain in the inversion process.

In hopes of being able to determine the position of the satellite, we began to examine in detail how light is refracted by the earth's upper atmosphere. In this study, we found that the location of the spacecraft could be determined as a function of time by making use of the refracted rays that the PAM-II experiment observed. In fact, we could determine with very high accuracy where the rays went through the atmosphere.

A summary of this study, which was performed using perturbation techniques, is shown in Figure 1. This graph shows the accuracy of determining the tangential altitude for rays that traverse the atmosphere as a function of reference altitudes used in the refraction fitting procedures that we developed. Four curves are illustrated: two for the 430 nm wavelength and two for the 1000 nm wavelengths. The upper curves for each spectral region refer to the perturbations that would be expected if the

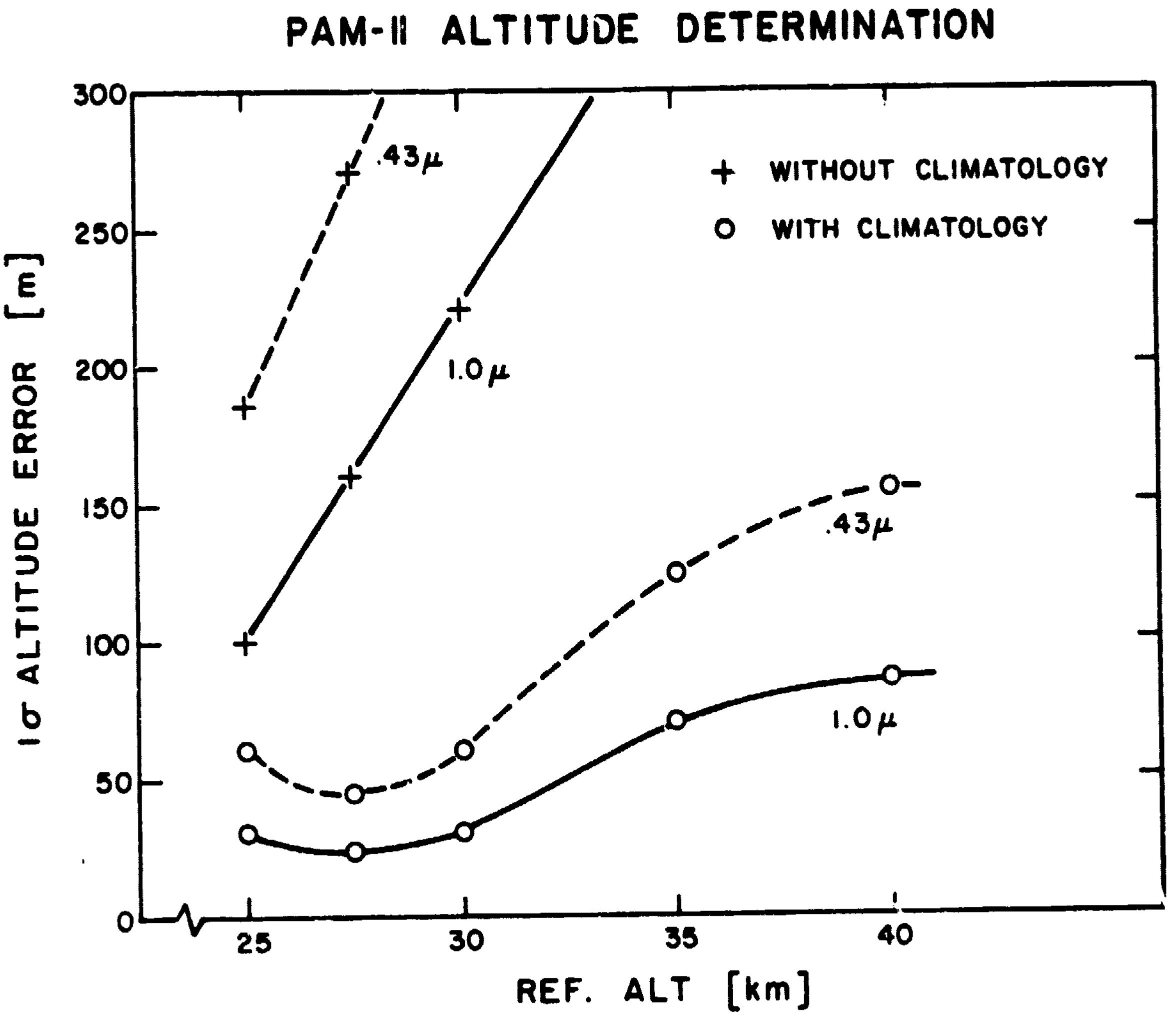

Figure 1. PAM-II altitude determination.

extreme values of summer to winter temperature variations in the stratosphere were assumed. The lower curves illustrate the expected two-sigma altitude errors when the atmospheric temperature is known (from the NOAA temperature profiles interpolated for the expected positions for the PAM-II measurements). We have found that using the ray altitudes, determined by the 1000 nm extinction data derived from NOAA climatology reports, provides inversions which are consistent with other measurements (as will be discussed in a later section of this report).

The mathematical ray traces required to perform the refraction calculations that led to these altitude determining routines have been summarized in a paper to be published in the November 1982 issue of the Journal of the Optical Society of America (Thompson, Pepin, and Simon, 1982; see Appendix A for a preprint of this paper).

III. Inversion of the Full-Sun Data:

The inversion algorithms necessary to invert the full-sun measured extinction data are essentially those based on the theoretical presentation of inversions described previously (Pepin, 1977). These algorithms assume a spherically symmetrical, refracting atmosphere and make use of the double inversion technique. The measurements of the solar flux from the full solar disk during the sunrise or sunset events are used to determine the vertical profile of the volume extinction coefficient for each of the PAM-II wavelength regions.

The first of these inversion processes inverts the intensity as a function of time to determine the transmission function of the atmosphere as a function of altitude. Making use of the results of the first inversion, the second of these processes inverts for the volume extinction coefficient as a function of altitude. The linear inversion employed to obtain the solutions for both the transmission and extinction coefficients makes use of smoothing constraints: The solution is constrained so that the second derivative of the function is minimized; additional constraints are applied which allow for the smoothing of the solution as a function of altitude. These smoothing constraints are in fact determined by examining the significant variations observed in the primary data set.

COMPARISON OF SAGE AND PAM-II RETRIVALS FOR OZONE

The potential observations of the SAGE and PAM-II satellites coincided several times during the summer of 1979. Unfortunately, of the four possible coincidences, SAGE and PAM-II were operating simultaneously only once, on June 3, 1979. The other three sets of overlapping data were not available for various reasons: Air Force priorities for observation precluded making PAM-II observations during the first possible comparison; during the other two possible comparisons, battery problems on board SAGE precluded the collection of data. Furthermore, the full potential range of the PAM-II observations could not be made during the one documented coincidence because of the time-sharing constraints among the instruments on the P78-1 satellite. Figure 2 shows the latitudes and longitudes of the tangent points for the events measured by PAM-II and SAGE on June 3, 1979.

The documented coincidence of PAM-II and SAGE observations occurred for the northern polar latitudes. Data reduction of PAM-II data was achieved with the two inversion algorithms which use refraction-determined altitudes. Data reduction of the SAGE data released in September of 1982 was achieved using the NASA Langley standard reduction (Chu and McCormick, 1979).

Figure 3 shows the average value of extinction measured by SAGE in the ozone band for June 3, 1979, and also indicates the ± one-sigma SAGE variations. Both aerosol and Rayleigh extinction have been subtracted from this result. Figure 4 shows the average ozone extinction profile as measured by PAM-II. For the PAM-II result, only the Rayleigh component has been removed. The contribution due to aerosol, which is only present below 25 km altitude, has not yet been removed.

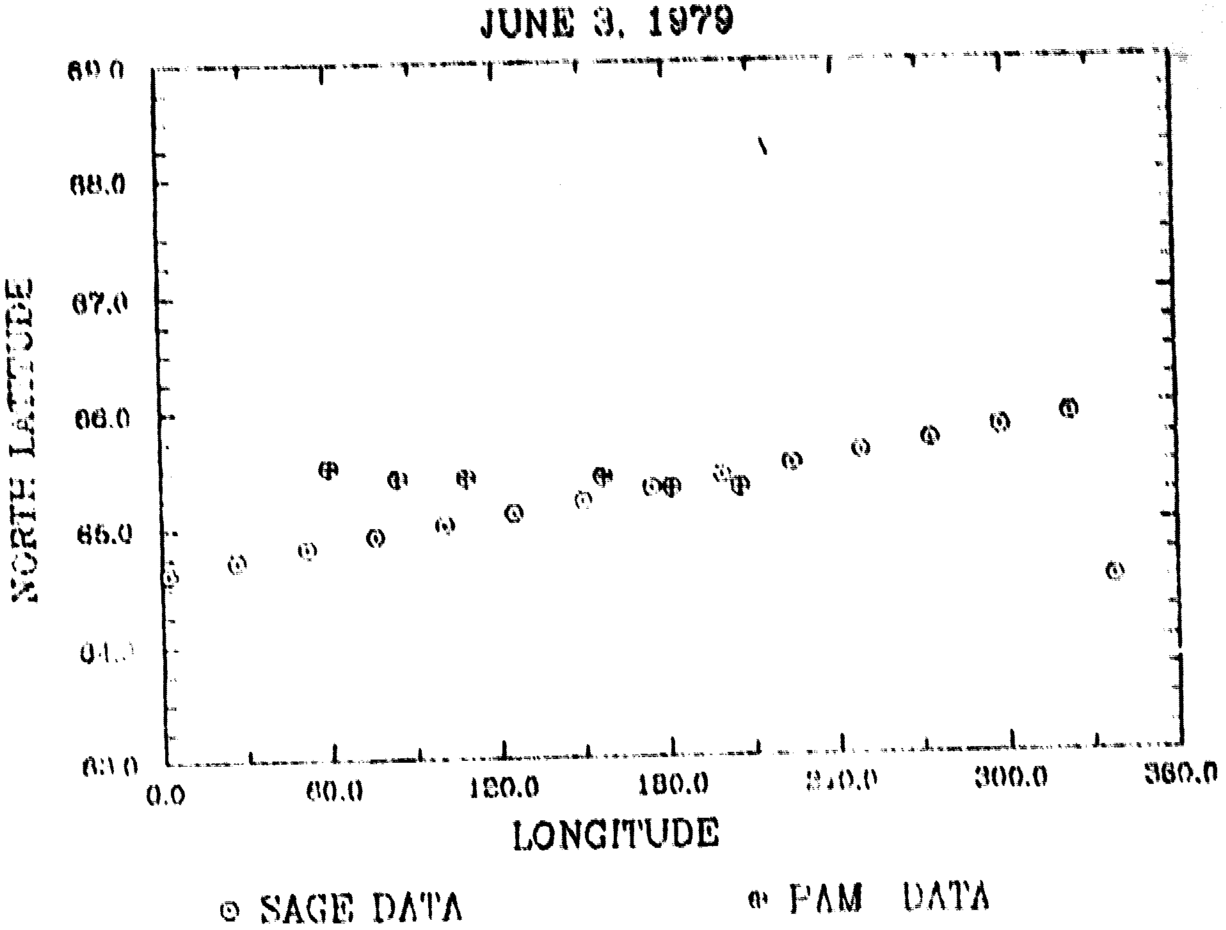

Figure 2. Tangent points for the events on June 3, 1979.

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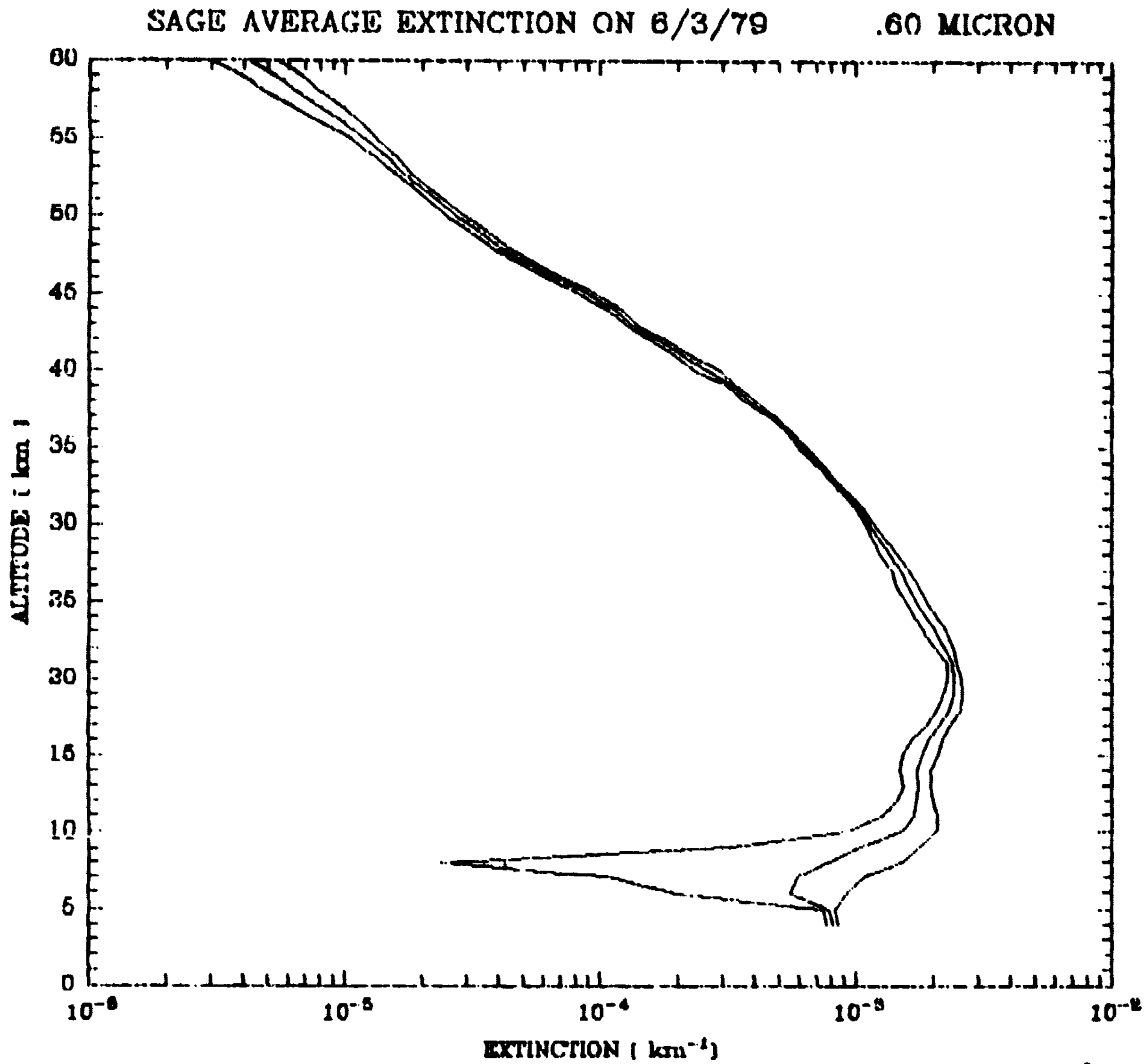

Figure 3. SAGE average extinction on June 3, 1979.

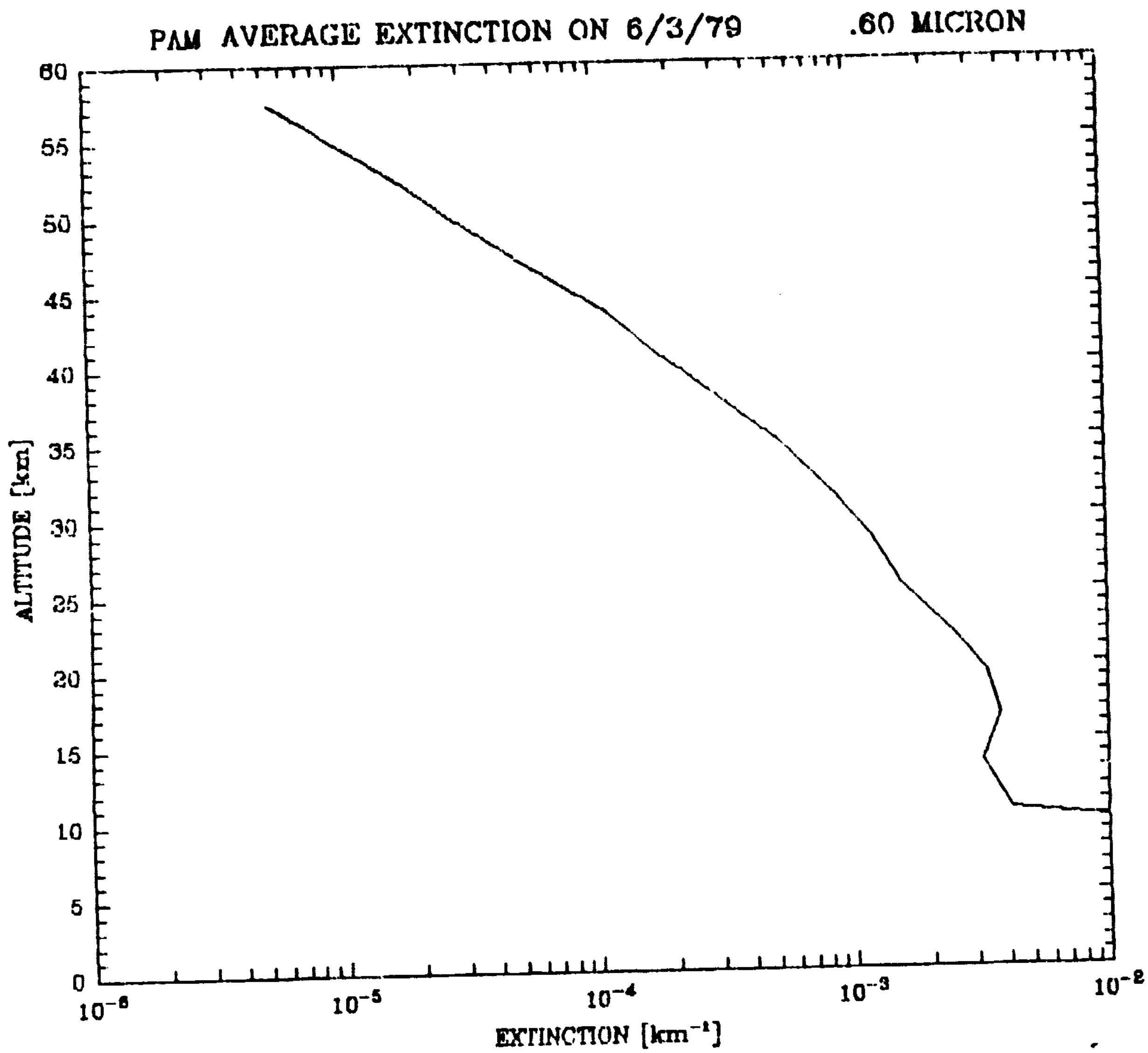

Figure 4. PAM-II average extinction on June 3, 1979.

CONCLUSIONS

As a result of this NASA grant, a working software system for the reduction of the PAM-II full-sun extinction data has been constructed and tested. The form of the data products allows comparisons of PAM-II data with SAM-II and SAGE data. The development of this system has provided additional insight into the solution of the refraction problem, in particular, the removal of the numerical instabilities that are naturally contained within the equations describing the refraction.

We are continuing to use the algorithms set up to invert the PAM-II data. In particular, we are concentrating on data reduction which will allow for the detailed study of ozone profiles in the polar latitudes. Since a good portion of the PAM-II data has been collected near the time of solar maximum, this information will make it possible to investigate the modulation of the ozone in the polar regions at times of solar activity.

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Thompson, Dennis A.; Pepin, Theodore J.; and Simon Frances W.: Ray Tracing in a Refracting Spherically Symmetric Atmosphere. Accepted for pub., J. Opt. Soc., Nov. 1982 (72).

APPENDIX A

A Preprint of

RAY TRACING IN A
REFRACTING, SPHERICALLY SYMMETRIC ATMOSPHERE

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Ray tracing in a refracting spherically symmetric atmosphere

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ABSTRACT

Satellite- and balloon-borne instruments may be used to measure the total transmission of electromagnetic radiation along a slant path trajectory traversing the earth's atmosphere. Inversions of this type of measurement data to determine the altitude and wavelength dependent atmospheric extinction require accurate ray tracing techniques. The ray tracing equations used in our inversion procedures are derived. These equations describe the refraction angle and generate the path length matrix for such radiation traversing a refracting, spherically symmetric atmosphere. Furthermore, they are presented in forms suitable for numerical integration.

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INTRODUCTION

Satellite- and high altitude balloon-borne instrumentation has long been used to study the optical properties of the earth's atmosphere. One of the primary methods of conducting such studies is that of solar occultation, utilizing the relative motion of the satellite, balloon or sun with respect to the earth to vertically scan the atmosphere, measuring the total transmission through it. Such an approach requires accurate techniques of ray tracing through the atmosphere to permit the necessary inversions. One therefore needs an accurate determination of the angle of refraction through the atmosphere and the appropriate path length matrix. The method described here is one we have been and are using to analyze our PAM, SAM-II, and SAGE satellite based experiments and will use for our forthcoming SAGE-II and POAM experiments.[1-5]

The basic assumptions are that the atmosphere is a refracting and spherically symmetric one with individual ray paths as indicated in Figure 1. It is necessary to calculate the ray path lengths in each onion skin layer and the refraction angle of the ray traversing the atmosphere. Accordingly, this paper first reviews the derivation of the necessary refraction angle and path length equations and then derives a set of equations which lend themselves to numerical evaluation.

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As represented in Figure 1, the instrument is carried outside the atmosphere and satellite motion provides the basic scanning effect. For high altitude balloon-borne experiments, the instrument is essentially stationary and located within the atmosphere. Sunrise or sunset provides the primary scanning motion. The following discussion can be modified to allow for this different geometry, although not done so here.

DISCUSSION

Denote the altitude dependent refractive index by n and call r the distance from the center of the earth to a point along the ray's path and θ the local zenith angle of the wave front traversing the atmosphere. Further, specify the ray path tangent point by the refractive index, n_t, and distance, r_t, at that point. This completely defines the coordinate system and Snell's Law for spherical geometry states that

$$nr \sin\theta = k = n_t r_t . \tag{1}$$

Trigonometry and division yield

$$\tan\theta = \frac{k}{[(nr)^2 - k^2]^{\frac{1}{2}}} . \tag{2}$$

Define ϕ to be the angle of refraction from the proj[illegible]ion of the ray outside the atmosphere to the local horizontal at the ray tangent point (Figure 2). For any given point along the ray,

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$$\frac{dn}{n} + \cot\theta \; d\theta = 0 \tag{3}$$

as described by McLeod.[6] Note that

$$\phi = \int_{\theta_t}^{\theta_i} d\theta = -\Delta\theta \tag{4}$$

the total change in local zenith angle, and $\theta_i + \Delta\theta = \pi/2$, where θ_i is the initial zenith angle of the light ray before the refractive effects of the atmosphere are felt. This gives

$$\phi = -\int_{n_t}^{1} \frac{\tan\theta}{n} \, dn \tag{5}$$

or

$$\phi = \int_{1}^{n_t} \frac{k}{n[(nr)^2 - k^2]^{\frac{1}{2}}} \, dn. \tag{6}$$

Doubling this yields the total refraction angle, ω, of a light ray traversing the atmosphere. The path length in each atmospheric layer (Figure 1) can be calculated as

$$P_{tj} = 2\int_{r_j}^{r_{j-1}} \frac{dr}{\cos\theta}. \tag{7}$$

This by substitution becomes

$$P_{tj} = 2 \int_{r_j}^{r_{j-1}} \frac{nr}{[(nr)^2 - k^2]^{1/2}} dr, \tag{8}$$

where both r_{j-1} and r_j are arbitrary and $r_{j-1} > r_j \geq r_t$. These expressions for ϕ and P_{tj} are to be numerically integrated to yield the total refraction half-angle and the path length matrix for light rays traversing the atmosphere.

Equations of the form of (6) and (8) and still other integrals dealing with atmospheric refraction and other phenomena have long been known as have approaches to their evaluation.[6-10] Further problems in evaluation present themselves in this case because the index of refraction is not necessarily a well-defined function of altitude. A specific functional dependence cannot be included in the above equations.

The index of refraction in these calculations is taken to be of the form

$$n = 1 + \mu\rho \tag{9}$$

where μ is a function of wavelength at standard atmospheric conditions and ρ is the ratio of the local atmospheric density to the density of an atmosphere at standard conditions. Calculating the index of refraction requires complete temperature and pressure profiles of the atmosphere. The density ratio can then be determined by use of the ideal gas law and these temperature and pressure data. The refractivity, μ, used is of the form devised by

Edlen[11] and tabulated by Penndorf.[12] However, the specific expression we use has been updated and corrected by Edlen to give greater accuracy.[13] Owens discusses and amplifies this formulation in his paper.[14]

Equations (6) and (8) are fundamental equations describing the ray path of electromagnetic radiation traversing the earth's atmosphere for the given coordinate system. However, the integrands in both equations exhibit singularities at the tangent point and the integrals cannot be directly numerically evaluated. This problem is eliminated by removing the effects of these singularities and then calculating the resulting refraction and path integrals. Pearce's method of eliminating singularities for a different coordinate system suggested the following approach to the problem.[15]

First, consider the refraction half-angle integral, equation (6). Subtract from both sides of the equation the term

$$\delta = \int_1^{n_t} \frac{k}{n[k^2 - (nr_t)^2]^{\frac{1}{2}}}\, dn, \tag{10}$$

which can be simplified and evaluated as

$$\delta = \ln\,[n_t + (n_t{}^2 - 1)^{\frac{1}{2}}]. \tag{11}$$

Note that the integrand has a form similar to that in equation (6). The resulting equation has the form

$$\phi - \delta = \int_{1}^{n_t} \frac{k}{n} \left\{ \frac{1}{[(nr)^2 - k^2]^{\frac{1}{2}}} - \frac{1}{[k^2 - (nr_t)^2]^{\frac{1}{2}}} \right\} dn. \tag{12}$$

Since this equation still has the singularity problem associated with it, make the change of variable $y = (n_t - n)^{\frac{1}{2}}$. After some manipulation equation (12) becomes

$$\phi = \int_{0}^{(n_t - 1)^{\frac{1}{2}}} \frac{2\,k}{(n_t - y^2)} \left\{ \frac{1}{r\left\{\left(\frac{r-r_t}{r}\right) \frac{n_t}{y^2} - 1\right\}^{\frac{1}{2}} \left\{\left(\frac{r+r_t}{r}\right) n_t - y^2\right\}^{\frac{1}{2}}} \right.$$

$$\left. - \frac{1}{r_t(2n_t - y^2)^{\frac{1}{2}}} \right\} dy + \ln\,[n_t + (n_t^2 - 1)^{\frac{1}{2}}], \tag{13}$$

which has the singularity removed from the integrand. It may be advisable to express this equation in a form which is less sensitive to possible computer dependent truncation errors in the calculation. Thus, further manipulation yields the expression

$$\phi = \int_{1}^{(n_t-1)^{\frac{1}{2}}} \frac{2n_t}{(n_t - y^2)DE} \left\{ \left(1 + \frac{r_t^2}{r^2}\right)(2n_t - y^2) - \left(\frac{r + r_t}{r}\right) \left(\frac{r - r_t}{r}\right)\frac{n_t^2}{y^2} \right\} dy$$

$$+ \ln\,[n_t + (n_t^2 - 1)^{\frac{1}{2}}], \tag{14}$$

where

$$D = \frac{r_t}{r}\,(2n_t - y^2)^{1/2} + \left\{\left(\frac{r - r_t}{r}\right)\frac{n_t}{y^2} - 1\right\}^{1/2}\left\{\left(\frac{r + r_t}{r}\right)n_t - y^2\right\}^{1/2} \tag{15}$$

and

$$E = (2n_t - y^2)^{1/2}\left\{\left(\frac{r - r_t}{r}\right)\frac{n_t}{y^2} - 1\right\}^{1/2}\left\{\left(\frac{r + r_t}{r}\right)n_t - y^2\right\}^{1/2}, \tag{16}$$

to minimize these possible errors.

A similar approach may be used in the path lengths integral, equation (8). Here subtract an expression of the form

$$\gamma_{tj} = 2\int_{r_j}^{r_{j-1}} \frac{n_t r}{[(n_t r)^2 - k^2]^{1/2}}\,dr \tag{17}$$

which can be evaluated, after simplification, as

$$\gamma_{tj} = 2[(r_{j-1}^2 - r_t^2)^{1/2} - (r_j^2 - r_t^2)^{1/2}]\,. \tag{18}$$

This results in the equation

$$F_{tj} - \gamma_{tj} = 2\int_{r_j}^{r_{j-1}} \left\{\frac{nr}{[(nr)^2 - k^2]^{1/2}} - \frac{n_t r}{[(n_t r)^2 - k^2]^{1/2}}\right\} dr, \tag{19}$$

which, upon making the change of variable $x = (r - r_t)^{1/2}$ and some manipulation, becomes

$$P_{tj} = 2\int_{(r_j - r_t)^{1/2}}^{(r_{j-1} - r_t)^{1/2}} 2(x^2 + r_t) \left\{ \frac{1}{\left(1 - \left(\frac{n - n_t}{n}\right) \frac{r_t}{x^2}\right)^{1/2} \left(x^2 - \left(\frac{n + n_t}{n}\right) r_t\right)^{1/2}} \right.$$

$$\left. - \frac{1}{(x^2 + 2r_t)^{1/2}} \right\} dx + 2[(r_{j-1}{}^2 - r_t{}^2)^{1/2} - (r_j{}^2 - r_t{}^2)^{1/2}] \qquad (20)$$

with the singularity removed.

Again truncation may be a problem for machines with short word lengths. Further manipulation yields an equation of the form

$$P_{tj} = 2\int_{(r_j - r_t)^{1/2}}^{(r_{j-1} - r_t)^{1/2}} 2r_t{}^2 \left(\frac{n_t + n}{n}\right)\left(\frac{n_t - n}{n}\right) \frac{(x^2 + r_t)}{x^2\ FG}\, dx$$

$$+ 2[(r_{j-1}{}^2 - r_t{}^2)^{1/2} - (r_j^2 - r_t{}^2)^{1/2}], \qquad (21)$$

where

$$F = (x^2 + 2r_t)^{1/2} + \left\{1 + \left(\frac{n - n_t}{n}\right) \frac{r_t}{x^2}\right\}^{1/2} \left\{x^2 + \left(\frac{n + n_t}{n}\right) r_t\right\}^{1/2} \qquad (22)$$

and

$$G = (x^2 + 2r_t)^{1/2} \left\{1 + \left(\frac{n - n_t}{n}\right) \frac{r_t}{x^2}\right\}^{1/2} \left\{x^2 + \left(\frac{n + n_t}{n}\right) r_t\right\}^{1/2}. \qquad (23)$$

and thus these errors may be minimized.

For our calculations, utilizing a CDC Cyber 760, truncation errors have not been found to be a problem. High order Gaussian Quadratures integration has also not been necessary for all computations. Our numerical integration calculations for the refraction half-angle integral over the entire region of interest use a 32nd order Gaussian Quadratures routine. For the path length matrix generation with one or two kilometer layer thicknesses, a 4th order Gaussian Quadratures routine gives the same results as a 32nd order calculation. In this case the sums of all path lengths through the entire refracting atmosphere with a sea level tangent point are the same to within one meter.

CONCLUSIONS

The method outlined here is based only on the assumption of a spherically symmetric refracting atmosphere. Other conditions, such as specifying the layer thicknesses in our limits of integration, are present only for convenience in developing the inversion algorithms. The refraction half-angle calculations may easily be made for limits other than those specified. For instance, it is a straightforward process to subtract off the refractive effects along a ray path above any specified altitude and determine only the refraction occurring before reaching a measuring instrument within the atmosphere, as is the case for high altitude balloon-borne payloads. The path length matrix calculations can be similarly modified. There is also no need to restrict the calculations to specific altitude layer spacings.

It should be noted that the above expressions for the refraction half-angle, as well as the path length matrix elements, are obviously wavelength dependent. Hence, evaluations of these integrals at different wavelengths will provide for the staightforward determination of atmospheric dispersion. Furthermore, if instead one knows the total atmospheric refraction, the refraction equations discussed above may be inverted to yield equations of similar form which give the index of refraction, and hence the atmospheric density, as a function of altitude.[16] These equations would also have the same singularity problem and may be numerically computed through an approach exactly analogous to the one described here.

The approach outlined is more general than indicated in the previous paragraph and may be used on other equations of this form. The real utility of this approach when compared to others is its ease of implimentation in computer algorithms for numerical evaluation. Minimal changes of variables are required and maximal use is made of the tabulated data input. Approximations to, or assumptions of, other analytic forms within the integrand are kept to a minimum.

Note that this discussion deals only with tracing the path of electromagnetic radiation traversing the earth's atmosphere. Other phenomena, such as absorption and scattering into and out of the ray path, do not contribute to this problem, as formulated. The next, and non-trivial, step is to generalize these equations to allow for horizontal inhomogeneities in the atmosphere.

ACKNOWLEDGMENTS

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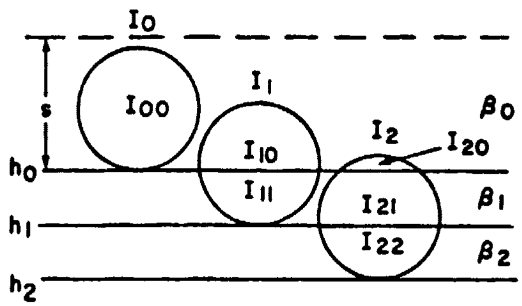
FIGURE 1. The onion-skin model of a spherical atmosphere. Path lengths in each atmospheric layer are noted. The first subscript denotes the appropriate tangent layer and the second defines the layer traversed by the path segment under consideration. For simplicity the refraction effects of the atmosphere are not specifically represented.

FIGURE 2. Geometry of a light ray traversing a refracting atmosphere. Notation is defined in the text.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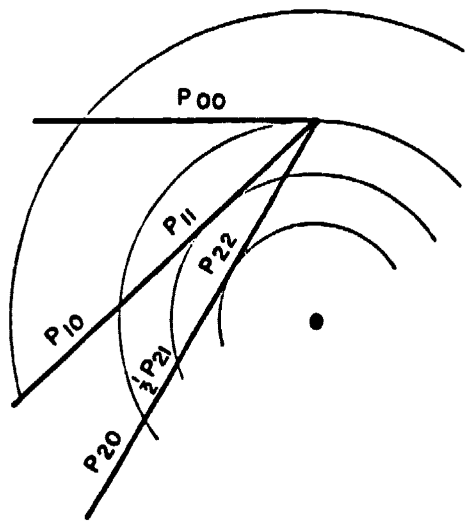
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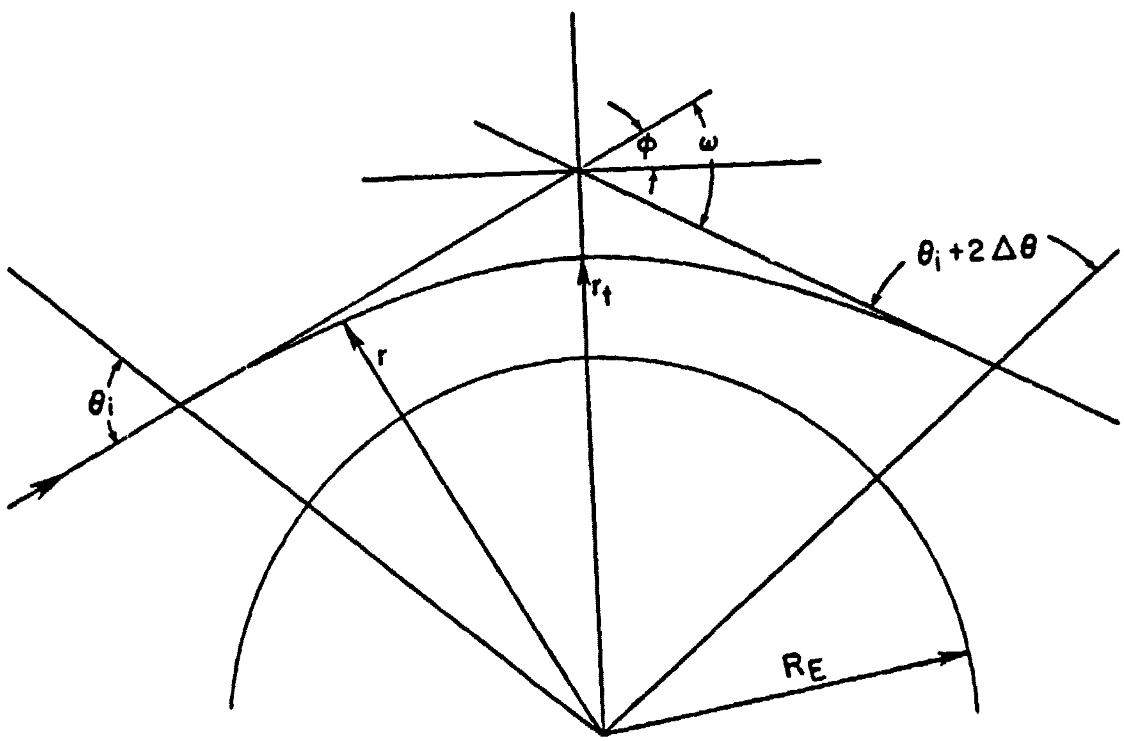
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