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DEVELOPMENT OF PROGRAMS FOR COMPUTING CHARACTERISTICS OF ULTRAVIOLET RADIATION

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16. Abstracts

The purpose of this study was to develop efficient programs for computing all four characteristics of the radiation scattered by a plane-parallel, turbid, terrestrial atmospheric model. They are developed (FORTRAN IV) and tested on the IBM/360 computers with 2314 direct access storage facility. The storage requirement varies between 200K and 750K bytes depending upon the task.

The scattering phase matrix (or function) is expanded in a Fourier series whose number of terms depend upon the zenith angles of the incident and scattered radiations, as well as on the nature of aerosols. A Gauss-Seidel procedure is used for obtaining the numerical solution of the transfer equation.

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PREFACE

The purpose of this final report prepared under NASA Contract NAS 5-21680 is to summarize the work carried out during the term of this contract. Two sets of programs were developed for computing characteristics of the scattered radiation emerging at selected levels of a plane-parallel, nonhomogeneous atmosphere containing an arbitrary vertical distribution of ozone concentration and/or aerosol (spherical particles of known refractive index) number-density, and bounded at the lower end by a Lambert ground of known reflectivity. The atmosphere is assumed to be illuminated at the top by unidirectional, unpolarized, monochromatic radiation.

In the first set of programs referred to as a scalar case, polarization characteristics of the scattered radiation are neglected during evaluation of the contribution to the emergent radiation from higher orders of scattering. Consequently, this first set of programs enables the user to compute, with moderate amount of computer time and storage requirements, variations of the scattered intensity as a function of several parameters such as, zenith angle, azimuth angle, Lambert ground reflectivity, sun's position, wavelength, and atmospheric parameters. The second set (referred to as a vector case) of programs can be used to compute all four characteristics (intensity, as well as degree, direction and ellipticity of polarization) of the scattered radiation for the various parameters listed above.

Each set consists of four separate programs. The first two programs are used for evaluating needed scattering properties of a unit volume containing a known size distribution of spherical particles made of a material whose refractive index with respect to air is given. The remaining two programs are for evaluating various characteristics of the scattered radiation by using a modified Fourier series method combined with the Gauss-Seidel iterative procedure.

TABLE OF CONTENTS

I. INTRODUCTION

The analysis of data acquired with the Backscatter Ultraviolet (BUV) experiment aboard the Nimbus IV satellite requires knowledge of the respective contributions to the outgoing radiation due to scattering by molecules and aerosols, as well as due to reflection by the surface underlying the atmosphere. The objective of NASA Contract No. NAS 5-21680 is to develop and to test programs aimed at computing various characteristics of the radiation emerging at selected levels of a plane-parallel, nonhomogeneous atmosphere containing an arbitrary vertical distribution of ozone and/or aerosol number-density, and bounded at the lower end by a Lambert ground of known reflectivity. The scattering aerosols are assumed to be spherical particles made up of a material whose refractive index with respect to air is known. It is further assumed that this refractive index and the size-distribution function are independent of height. The atmosphere is assumed to be illuminated at the top by unidirectional, unpolarized, monochromatic radiation. Various characteristics of the scattered radiation emerging at selected levels of a given atmospheric model are evaluated by using a modified Fourier series method (Dave and Gazdag, 1970, Dave, 1970A and 1970B) combined with the Gauss-Seidel iterative procedure (Hildebrand, 1956, Chapter 10).

The computer requirements for evaluating scattered-radiation characteristics depend upon several factors such as optical properties of the model, wavelength to be investigated, desired accuracy, and the number of cases for which output is required for a meaningful analysis of a given problem. The total computer requirement for a given study can heavily tax some of the most modern computing facilities available to typical research group associated with a large organization. Hence, we have developed, and tested, two sets of programs which are described below.

In the first set of programs referred to as a scalar case, polarization characteristics of the scattered radiation are neglected during evaluation of the contribution to the emergent radiation from the radiation which is scattered more than once in the atmosphere. Consequently, this first set of programs enables the user to evaluate, with moderate amounts of computer time and storage requirements, variations of the scattered intensity as a function of several parameters such as zenith (or nadir) angle, azimuth angle, Lambert ground reflectivity, sun's position, wavelength, and atmospheric parameters. It is known that the values of intensities obtained with such a scalar treatment of the transfer problem can differ significantly (~ 10 to 30%) from those obtained with a full vector treatment, i.e., when polarization of the scattered radiation is properly accounted for (e.g., Chandrasekhar, 1950, Sec. 70.4; Adams and Kattawar, 1970; Dave and Gazdag, 1970). The magnitude of the difference depends upon the optical thickness of the atmosphere, zenith angle of the sun and direction of observation, location of the observer within the atmosphere, and nature of the scattering phase function. However, because of the excessive computer requirements, some investigators not concerned with polarization aspects of the scattered radiation work with numerical results obtained with such a scalar program. A plausible reason advanced for justifying the validity of the ultimate findings of such an investigation is that of biasing of all numerical results by the same amount. The second set of programs can be used to compute all four characteristics (intensity, as well as degree, direction and ellipticity of polarization) of the scattered radiation for the various parameters listed above.

Each set of the programs described above consists of four different programs. A description of the purpose, computational procedure, FORTRAN listing, and the results of test runs obtained with each of these eight programs are given in the following eight reports prepared for this contract:

Title of the Report	Date Submitted	No. of Pages
Technical Report - Scalar Case, Program I	20 Jan. 1972	43
Technical Report - Scalar Case, Program II	24 Feb. 1972	38
Technical Report - Scalar Case, Program III	06 Mar. 1972	50
Technical Report - Scalar Case, Program IV	04 May 1972	106
Technical Report - Vector Case, Program I	10 Feb. 1972	50
Technical Report - Vector Case, Program II	18 May 1972	46
Technical Report - Vector Case, Program III	08 June 1972	70
Technical Report - Vector Case, Program IV	03 August 1972	138

A brief description of the basic radiative transfer equation used for this work, and the function of each of the eight programs listed above are given in the sections which follow.

II. DEFINITION OF THE BASIC QUANTITIES

In this section we shall give brief definitions of various quantities required for writing down the equation of radiative transfer for a plane-parallel, nonhomogeneous atmosphere.

2.1 Directional parameters (μ, φ): The direction of propagation is denoted by the zenith angle $\theta\,(=\cos^{-1}|\mu|)$ which the direction makes with local zenith, and the azimuth angle φ which the meridian plane containing the direction of propagation makes with an arbitrarily chosen meridian plane. A negative (positive) sign before μ will imply the radiation traveling along the downward (upward) direction. A subscript "o" for μ and φ will imply the direction of propagation of the incident solar radiation.

2.2 Normal Rayleigh-scattering optical depth $\tau^{(s,r)}$: This optical depth of a level situated at a height of h km above the ground is given by

$$\tau^{(s,r)} = \int_h^\infty k^{(s)}\, \rho(h)\, dh \quad , \tag{1}$$

where

$k^{(s)}$ = mass scattering coefficient of air at wavelength λ ,

and

$\rho(h)$ = density of air at height h .

2.3 Normal Mie-scattering optical depth $\tau^{(s,m)}$: The attenuation suffered by a beam of radiation travelling along the vertical due to scattering by atmospheric aerosols is determined after making the following assumptions: (a) aerosol particles are spherical in shape, (b) all particles are made of one material whose refractive index with respect to air is $m(=n_1 - i n_2)$, and (c) the size-distribution function, i.e., n(r) = number of particles per cc in 1 micron interval at radius r, is independent of height. Accordingly, we have,

$$\tau^{(s,m)} = \beta_s \, N(h)/N_o \tag{2}$$

where

β_s = volume scattering coefficient per cm [Eq. (3)],

N(h) = total number of particles in one sq. cm column above the level located at a height of h km above the ground, and

N_o = total number of particles per cc [Eq. (4)] .

The explicit expression for β_s is

$$\beta_s = \pi \int_{r_{min}}^{r_{max}} Q_s(x,m) \, r^2 \, n(r) \, dr \quad , \tag{3}$$

where

$Q_s(x,m)$ = efficiency factor for scattering for a particle with size parameter $x = 2\pi r/\lambda$; r is the radius of the particle (Van de Hulst, 1957, Sec. 9.3.2).

The quantity N_o is given by

$$N_o = \int_{r_{min}}^{r_{max}} n(r)\ dr \quad . \tag{4}$$

2.4 Normal Mie absorption optical depth $\tau^{(a,m)}$: Following the procedure given in Sec. 2.3, the Mie absorption optical depth of a level is given by

$$\tau^{(a,m)} = \beta_a\ N(h)/N_o \tag{5}$$

where the explicit expression for β_a is obtained after replacing s with a in Eq. (4); $Q_a(x,m)$ is the efficiency factor for absorption.

2.5 Normal ozone-absorption optical depth $\tau^{(a)}$: This quantity is given by

$$\tau^{(a)} = \alpha\, x(h) \quad , \tag{6}$$

where

α = absorption coefficient (to the base e, e.g., Handbook of Geophysics, Revised Edition, U.S. Air Force, Macmillan Company, 1961, pp. 16-23 to 16-25) of one cm-atm of ozone at NTP, for the wavelength λ, and

$x(h)$ = total amount of ozone in cm-atm above the level.

2.6 Normal total optical depth τ : The attenuation suffered by a beam of radiation travelling (in a direction making an angle θ with local zenith) from the top of the atmosphere to a level located at a height h km above the ground is $\exp(-\tau/\mu)$. The quantity τ is given by

$$\tau = \tau^{(r)} + \tau^{(m)} \quad , \tag{7}$$

where the attenuation optical depth due to gases is given by

$$\tau^{(r)} = \tau^{(s,r)} + \tau^{(a)} \quad , \tag{8}$$

and the attenuation optical depth due to aerosols is given by

$$\tau^{(m)} = \tau^{(s,m)} + \tau^{(a,m)} \quad . \tag{9}$$

2.7 Albedo of single scattering $\omega(\tau)$: This quantity defines the relationship between absorption and scattering characteristics of the materials located at the level τ . It is given by

$$\omega(\tau) = \frac{\Delta\tau^{(s,m)} + \Delta\tau^{(s,r)}}{\Delta\tau^{(m)} + \Delta\tau^{(r)}} \quad , \tag{10}$$

where $\Delta\tau^{(j)}$ represents a change in the $\tau^{(j)}$ -th optical depth.

2.8 Turbidity factor $T(\tau)$: This quantity defines the relationship between the scattering characteristics of molecules and aerosols located at the level τ . It is defined as follows:

$$T(\tau) = \Delta\tau^{(s,m)} / [\Delta\tau^{(s,m)} + \Delta\tau^{(s,r)}] \quad . \tag{11}$$

2.9 Stokes parameters $\underline{I}(\tau;\mu,\varphi)$: Since we are interested in all aspects of scattering, it is necessary to treat a beam of monochromatic radiation of wavelength λ as a vector or as a one-column matrix with four elements. In the Stokes representation (Chandrasekhar, 1950, Sec. 15), the intensity matrix is represented by

$$\underline{I}(\tau;\mu,\varphi) = \begin{bmatrix} I_e(\tau;\mu,\varphi) \\ I_r(\tau;\mu,\varphi) \\ I_u(\tau;\mu.\varphi) \\ I_v(\tau;\mu,\varphi) \end{bmatrix} \quad . \tag{12}$$

The first two elements $[I_e(\tau;\mu,\varphi)$ and $I_r(\tau;\mu,\varphi)]$ of this matrix represent the specific intensities (or for short, intensities) of the beam in two directions, e and r , respectively. These two directions are mutually at right angles to each other, such that the e - r plane is perpendicular to the direction of propagation of energy. The intensity of the beam, i.e., the amount of energy per unit wavelength interval at λ flowing per unit time in a cone of unit solid angle with axis in the direction μ,φ , is given by

$$I(\tau;\mu,\varphi) = I_e(\tau;\mu,\varphi) + I_r(\tau;\mu,\varphi) \quad . \tag{13}$$

The degree of polarization of the beam is given by

$$P = [\,Q^2(\tau;\mu,\varphi) + I_u^2(\tau;\mu,\varphi) + I_v^2(\tau;\mu,\varphi)\,]^{1/2} \,/\, I(\tau;\mu,\varphi) \quad , \tag{14}$$

where

$$Q(\tau;\mu,\varphi) = I_e(\tau;\mu,\varphi) - I_r(\tau;\mu,\varphi) \quad . \tag{15}$$

The angle (χ) which the direction of maximum vibration makes with the e-direction, i.e., the deviation of the plane of polarization, or alternately the direction of polarization, is given by

$$\tan 2\chi = I_u(\tau;\mu,\varphi) / Q(\tau;\mu,\varphi) \quad . \tag{16}$$

The ellipticity of polarization defined as the ratio of minor to the major axis of the ellipse traced by the electric vector, is given by

$$\tan \beta = -I_v(\tau;\mu,\varphi) / \; [\,Q^2(\tau;\mu,\varphi) + I_u^2(\tau;\mu,\varphi) + I_v^2(\tau;\mu,\varphi)]^{1/2} + [\,Q^2(\tau;\mu,\varphi) + I_u^2(\tau;\mu,\varphi)]^{1/2} \quad . \tag{17}$$

It may be noted that the quantities P, χ, and β given by Eqs. (14), (16), and (17) as well as the intensity $I(\tau;\mu,\varphi)$ given by Eq. (13) are functions of τ, μ, φ, directional parameters $(-\mu_o, \varphi_o)$ of the incident radiation, and various optical properties of the atmosphere and underlying surface.

2.10 Normalized scattering phase matrix $\underset{\sim}{P}(\tau;\mu,\varphi;\mu',\varphi')$:
This four-by-four matrix gives, on a relative scale, the Stokes parameters of the radiation scattered by a unit volume at the level τ in the direction μ,φ when the volume is illuminated by an incident beam of known Stokes characteristics from the direction μ',φ' . For a volume containing both aerosols and molecules, this matrix has the following form:

$$\underset{\sim}{P}(\tau;\mu,\varphi;\mu',\varphi') = T(\tau)\ \underset{\sim}{M}(\mu,\varphi;\mu',\varphi') + [1 - T(\tau)]\ \underset{\sim}{R}(\mu,\varphi;\mu',\varphi') \tag{18}$$

where $T(\tau)$ is the turbidity factor defined above. The quantities $\underset{\sim}{M}(\mu,\varphi;\mu',\varphi')$ and $\underset{\sim}{R}(\mu,\varphi;\mu',\varphi')$ are four-by-four normalized matrixes for a unit volume of aerosol (Mie scattering) and air (Rayleigh scattering), respectively. Their ij-th elements are either even or odd functions of $\varphi' - \varphi$ depending upon the value of the subscript ij (Dave, 1970A). The azimuth dependence is given by:

$$M_{ij}(\mu,\varphi;\mu',\varphi') = \sum_{n=1}^{N(\mu,\mu')} M_{ij}^{(n)}(\mu,\mu')\ f_{n-1}(\varphi' - \varphi) \quad , \tag{19}$$

and

$$R_{ij}(\mu,\varphi;\mu',\varphi') = \sum_{n=1}^{3} R_{ij}^{(n)}(\mu,\mu')\ f_{n-1}(\varphi' - \varphi) \quad , \tag{20}$$

where for $ij = 11, 12, 21, 22, 33, 34, 43$, and 44, these elements are even functions, i.e.,

$$f_{n-1}(\varphi' - \varphi) = \cos[(n-1)(\varphi' - \varphi)] \quad , \tag{21}$$

and for $ij = 13, 14, 23, 24, 31, 32, 41$, and 42, these elements are odd functions, i.e.,

$$f_{n-1}(\varphi' - \varphi) = \sin[(n-1)(\varphi' - \varphi)] \quad . \tag{22}$$

The explicit expressions for $M_{ij}^{(n)}(\mu,\mu')$ and $R_{ij}^{(n)}(\mu,\mu')$ can be found in Technical Reports - Vector Case, Programs III and IV respectively. With the Fourier series form of the Mie and Rayleigh phase matrices given above, the ij-th element of the matrix $\underset{\sim}{P}(\tau;\mu,\varphi;\mu',\varphi')$ can be written as

$$P_{ij}(\tau;\mu,\varphi;\mu',\varphi') = \sum_{n=1}^{N(\mu,\mu')} P_{ij}^{(n)}(\tau;\mu,\mu')\, f_{n-1}(\varphi' - \varphi) \quad , \tag{23}$$

where

$$P_{ij}^{(n)}(\tau;\mu,\mu') = T(\tau)\, M_{ij}^{(n)}(\mu,\mu') + [1 - T(\tau)]\, R_{ij}^{(n)}(\mu,\mu') \quad . \tag{24}$$

Evidently, $R_{ij}^{(n)}(\mu,\mu') \equiv 0$ for $n > 3$. The series given by Eq. (23) is even or odd depending upon the value of subscript ij .

III. EQUATION OF RADIATIVE TRANSFER

The basic transfer equation for a plane-parallel atmosphere of infinite extent and homogeneous along the horizontal, but of finite extent and nonhomogeneous in the vertical has the following form.

$$\mu \frac{d\,\mathbf{I}(\tau;\mu,\varphi)}{d\tau} = \mathbf{I}(\tau;\mu,\varphi) - \varpi(\tau)\,\mathbf{J}(\tau;\mu,\varphi) \quad , \tag{25}$$

where the source matrix $\mathbf{J}(\tau;\mu,\varphi)$ is given by

$$\mathbf{J}(\tau;\mu,\varphi) = \frac{1}{4}\, e^{-\tau/\mu_o}\, \mathbf{P}(\tau;\mu,\varphi;-\mu_o,\varphi_o)\cdot \mathbf{F} + \frac{1}{4\pi}\int_{-1}^{+1}\int_{0}^{2\pi} \mathbf{P}(\tau;\mu,\varphi;\mu',\varphi')\cdot \mathbf{I}(\tau;\mu',\varphi')\, d\mu'\, d\varphi' \quad . \tag{26}$$

The boundary conditions are given by

$$\mathbf{I}(0;-\mu,\varphi) \equiv 0 \, , \quad \text{and} \quad \mathbf{I}(\tau_b;+\mu,\varphi) \equiv 0 \quad , \tag{27}$$

where τ_b is the total normal optical thickness of the atmosphere. In arriving at Eq. (26) for the source matrix, it is assumed that the atmosphere is illuminated by unidirectional $(-\mu_o, \varphi_o)$ solar radiation with a net flux of πF per unit area normal to the direction of propagation. The Stokes parameters of the incident solar radiation are represented by a one-column matrix given by

$$\pi \underset{\sim}{F} = \pi \begin{bmatrix} F_e \\ F_r \\ F_u \\ F_v \end{bmatrix} . \tag{28}$$

The net flux $\pi F = \pi(F_e + F_r)$. For our calculations we have assumed that $F_e = F_r = 1/2$, and $F_u = F_v = 0$, i.e., the incident solar is unpolarized, and has a net flux π per unit area normal to its direction of propagation. All the quantities appearing in Eqs. (25) to (27) are defined in Sec. 2. It may be noted that this transfer equation is, strictly speaking, valid only for a monochromatic radiation. However, one may use the same program for computing various characteristics of the emergent radiation integrated over a specified wavelength interval provided he feels justified in using average values of various input parameters described in Secs. 2.2 to 2.5.

The form of the normalized phase matrix for a unit volume [Eq. (23)] suggests that we expand the elements of $\underset{\sim}{I}(\tau;\mu,\varphi)$ and $\underset{\sim}{J}(\tau;\mu,\varphi)$ in similar forms. After substituting the Fourier series expressions for $\underset{\sim}{I}(\tau;\mu,\varphi)$, $\underset{\sim}{J}(\tau;\mu,\varphi)$ and $\underset{\sim}{P}(\tau;\mu,\varphi;\mu',\varphi')$ in Eqs. (25) and (26), we can carry out the integration over azimuth angle (φ') analytically by making use of the well-known orthogonality relations obeyed by the trigonometric functions. It can be shown that (Technical Report - Vector Case, Program IV, Sec. 2.2) Eq. (25) reduces to the following system of uncoupled integro-differential equations:

$$\mu \frac{d\underset{\sim}{I}^{(n)}(\tau;\mu)}{d\tau} = \underset{\sim}{I}^{(n)}(\tau;\mu) - \text{[illegible]}(\tau)\,\underset{\sim}{J}^{(n)}(\tau;\mu) \quad , \tag{29}$$

where the superscript n increases from 1 to $N(\mu_o)$. The magnitude of this upper limit depends upon the nature of aerosols in the atmospheric model under investigation, and also on the zenith angle of the sun (Dave and Gazdag, 1970). The n-th term of the Fourier series for the source matrix has the following form:

$$\underset{\sim}{J}^{(n)}(\tau;\mu) = \frac{1}{4}\,\underset{\sim}{P}^{(n)}(\tau;\mu,-\mu_o)\cdot \underset{\sim}{F}\, e^{-\tau/\mu_o}$$

$$+ \frac{1+\delta_{1n}}{4}\int_{-1}^{+1} \underset{\sim}{P}^{(n)}(\tau;\mu,\mu')\cdot \underset{\sim}{I}^{(n)}(\tau;\mu')\,d\mu' \tag{30}$$

where δ_{1n} is the Kronecker delta function given by $\delta_{1n} = 1$ when $n = 1$ and otherwise zero. The boundary conditions for the n-th term of Eq. (29) are given by

$$\left.\begin{array}{l} \underset{\sim}{I}^{(n)}(0;-\mu) \equiv 0 \\ \text{and} \\ \underset{\sim}{I}^{(n)}(\tau_b;+\mu) \equiv 0 \end{array}\right\} \quad . \tag{31}$$

Identical equations for the scalar case are arrived at by treating the quantities $\underset{\sim}{I}(\tau;\mu,\varphi)$, $\underset{\sim}{J}(\tau;\mu,\varphi)$, $\underset{\sim}{P}(\tau;\mu,\varphi;\mu',\varphi')$, $\underset{\sim}{I}^{(n)}(\tau;\mu)$, $\underset{\sim}{J}^{(n)}(\tau;\mu)$, $\underset{\sim}{J}^{(n)}(\tau;\mu)$, and $\underset{\sim}{P}^{(n)}(\tau;\mu,\varphi)$ as scalar quantities (Technical Report - Scalar Case, Program IV, Sec. 2.2).

In order to evaluate the contribution to $\underset{\sim}{I}(\tau;\mu,\phi)$ due to the presence of an idealized Lambert ground located underneath the atmosphere, we can write equations similar to Eqs. (25) to (27) but with an isotropic source illuminating the model from below. In this case, we can easily carry out reductions similar to the one used for arriving at Eqs. (29) through (31). When this is done (Technical Report - Vector Case, Program IV, Sec. 2.3, or Technical Report - Scalar Case, Program IV, Sec. 2.3), we find that because of the nature of the illuminating source, this contribution to $\underset{\sim}{I}(\tau;\mu,\phi)$ is azimuth independent.

IV. FUNCTION OF VARIOUS PROGRAMS

The job of evaluating characteristics of the scattered radiation emerging at selected levels of a nonhomogeneous, plane-parallel atmosphere can be divided into the following two main tasks: (a) Computations of the elements of the phase matrix $\underset{\sim}{P}^{(n)}(\tau;\mu,\mu')$ given by Eq. (24), and (b) numerical solution of the transfer equation given by Eqs. (29) through (31) for the required number of terms of the Fourier series. As mentioned in Sec. I of this report, we have provided two sets of programs; one set of four programs for the scalar case, and another set again consisting of four programs for the vector case. In what follows, we will describe the functions of four programs for the vector case. The i-th program for the scalar case performs functions identical to the one performed by the i-th program for the vector case, but by treating related vector quantities as scalars.

The function of the first program is to enable the user to compute values of coefficients of the Legendre series for four different scattering functions which can be used for evaluating the intensity as well as the degree, direction, and ellipticity of polarization of the radiation scattered by a sphere of known refractive index. Values of efficiency factors for extinction, scattering, and absorption for the sphere under investigation are also computed. This program enables the user to compute, and to store on a magnetic tape for further use with the second program, values of these quantities for hundreds of discrete but equally spaced values of the size parameter of the sphere.

The function of the second program is to enable the user to compute coefficients of the Legendre series representing four scattering functions of the normalized scattering phase matrix of a unit volume containing a known size distribution of spherical particles made of the same material. Values of the volume extinction and volume scattering coefficients are also obtained during execution of this program. Values of these quantities are stored in punched-card form for use with the third program.

The function of the third program is to enable the user to compute the Fourier coefficients $M_{ij}^{(n)}(\mu',\mu)$ [appearing in Eqs. (19) and (24)] of series representing elements of a normalized four-by-four scattering phase matrix of a unit volume containing an arbitrary distribution of spherical particles. These coefficients are computed for the values of $\theta'(=\cos^{-1}|\mu'|)$ and $\theta(=\cos^{-1}|\mu|)$ given by $\theta' = 0^{\circ}(2^{\circ})180^{\circ}$, and $\theta = 0^{\circ}(2^{\circ})90^{\circ}$. This program also prepares a table of the upper limit $N(\mu',\mu)$ of the Fourier series [Eq. (19)]. For further use with the fourth program, values of $M_{ij}^{(n)}(\mu,\mu')$ for all values of n, i, j, θ', and θ are stored on a magnetic tape, and those of $N(\mu',\mu)$ are stored in punched-card form.

The function of the fourth program is to enable the user to compute the intensity (I), the degree of polarization (P), the direction of polarization (χ), and the ellipticity of polarization $(\tan\beta)$ of the scattered radiation emerging at selected levels of the atmospheric model under investigation. After completing computations for all required Fourier components of the intensity [Eq. (29)] values of I, P, χ, and $\tan\beta$ of the scattered radiation emerging at selected levels of atmospheric models are computed and printed out for the desired values of Lambert ground reflectivities, and azimuth as well as zenith angles of the directions of the scattered radiation.

V. RELIABILITY OF NUMERICAL RESULTS

Because of the nature of the computations and also because of the unavailability of accurate numerical results in published form, it is not possible to make a definite statement about the absolute accuracy of the numerical values obtained using these programs. However, based on various considerations and direct as well as indirect comparison with published and unpublished results of higher quality, we make the following statements:

Various Legendre coefficients as well as values of the efficiency factors for absorption and scattering obtained using the first program for the vector (or scalar) case, are expected to be correct to the first ten significant figures in most cases.

The reliability of the normalized Legendre coefficients and of the scattering and absorption volume coefficients of a unit volume containing a known size distribution (analytic function) of spherical particles (second program for the Vector or the Scalar Case), is primarily determined by the value of the integration increment (Δx) used for the computations. For typical atmospheric aerosol distributions, the choice of Δx is governed to a considerable extent by the economics of computations. For such cases, a value of about 0.1 for Δx is generally considered fine enough to provide results of about four significant figure reliability.

Values of the Fourier coefficients of a series representing elements of a normalized four-by-four scattering phase matrix (or of a series representing phase function for the scalar case) of a unit volume as obtained using the third program are expected to be as accurate as values of the normalized Legendre coefficients used as input.

The reliability of the values of the intensity for the scalar case and of all four parameters for the vector case is primarily determined by the value of the integration increment ($\Delta\theta$) used for evaluating the contribution to the source term by atmospheric radiation [e.g., the second term in Eq. (30)]. A provision is made in the fourth program to enable the user to work with a value of 2°, 6°, or 10° for $\Delta\theta$. The reliability of this output also depends to some extent on the nature of the scattering phase matrix used in the model. Thus, for a given $\Delta\theta$, the numerical results for an aerosol model with a very strong forward peak (~ 300 or more terms in Legendre representation) are bound to be less accurate than those for a model with a less strong forward peak.

Other input parameters which determine the accuracy of the numerical output of the fourth program are the number of layers into which the basic atmospheric model is divided, the nature of vertical nonhomogeneities, and the value of the albedo of single scattering. A provision is made in the fourth program for permitting the user to divide his basic atmospheric model into 160/n number of layers where the integer n can assume anyone of the following values: 1, 2, 4, 5, 8, or 10. The results obtained with finer division of the atmosphere can be expected to be more accurate than those obtained with the coarser ones. However, the value of the parameter n and that of $\Delta\theta$ described in the preceding paragraph should be compatible. It is recommended that for $\Delta\theta = 2^{\circ}$, the atmosphere be divided into a sufficient number of layers so that the total scattering optical thickness of any one layer does not exceed 0.02. The discussion given above applies to a homogeneous atmospheric model, or to a model in which the nonhomogeneity varies slowly with height. If not numerical results for a basic nonhomogeneous model divided into $160/n_1$ and $160/n_2$ number of layers may be found to differ significantly from each other as the division procedure used does not provide exactly identical models in both cases.

The output for a non-absorbing, Rayleigh atmosphere ($\tau_b^{(s,r)} = 0.1$ and 1.0, $\theta_o = 0^{\circ}$ and 60°, R = 0.0, 0.06941 and 0.25) was checked for several values of θ and φ with that obtained using Chandrasekhar's X- and Y-function method by the author, and also by the Technical Officer of this contract, Dr. R.S. Fraser. A value of 2° was used for the parameter $\Delta\theta$ in all cases. Values of the intensity of the radiation emerging at the top and at the bottom of the atmosphere were found to agree, on the average, within ± 3 units in the fourth place after the decimal point ($\sim 0.2\%$ accuracy) when the models with $\tau_b^{(s,r)} = 0.1$ and 1.0 were divided into 16 and 40 layers, respectively. Values of the degree of polarization were found to agree within ± 1 units in the third place after the decimal points, and those of the direction of polarization were found to agree within $\pm 0.1^{\circ}$.

Computations were also performed for a nonhomogeneous, Rayleigh case ($\lambda = 0.3125\mu$, $\tau_b^{(s,r)} = 1.025$, $\theta_o = 60^{\circ}$, total ozone = 0.341 cm - atm) for which numerical results of good quality are available in published form (Dave and Furukawa, 1966). For this run, the basic atmospheric model was divided into 80 layers, and a value of 2° was taken for the input parameter $\Delta\theta$. Values of intensities obtained using the fourth vector program were found to agree, on the average, within $\pm 2\%$ with those of Dave and Furukawa: and the values of degree of polarization within $\pm$ 4 units in the third place after the decimal point. The results of this comparison are considered as satisfactory especially when one notes that Dave and Furukawa divided their model into 366 layers. However, they used a value of 1,000 mb for their surface pressure (versus 1,013 mb in our case), and they approximated the contribution from higher-than-seventh-order scattered radiation by a geometric series.

VI. COMPUTER REQUIREMENTS

In Table I we have listed some computing facilities required during test executions of the various programs. It may be added that a 9-track, 1600 BPI tape was used as an input or output tape during execution of each of the eight programs. The computer facility used for the test run was an IBM System/360 Model 91 computer located at the NASA Goddard Space Flight Center.

During the execution of the first program, values of the Legendre coefficients and efficiency factors needed to fully describe the scattering properties of a single spherical particle were computed for the discrete values of the size parameter x given by $x = 0.1(0.2)169.9$. A value of $1.5 - 0.03i$ was used for the refractive index of the material of the particle. The CPU time needed for all computations for a given value of x increases with x; e.g., CPU time for the vector case and for $x = 1.1$, 10.1, 100.1, and 169.9 was 0.02, 0.08, 13.98, and 57.73 seconds, respectively. For the scalar case, the corresponding timings were smaller by about 20%.

During the execution of the second program, values of the normalized Legendre coefficients and absorption as well as scattering volume coefficients for a unit volume containing an arbitrary size distribution (Haze C; $r_{min} = 0.03\mu$, $r_{max} = 10.0\mu$, change of slope at 0.1μ, $m = 1.5 - 0.03i$) of spherical aerosols, were computed for monochromatic radiation of 0.55μ wavelength. The value of the parameter x corresponding to the largest particle is 114, and accordingly we required 267 terms in the Legendre series.

Table I

Compiler, storage in kilobytes, use (or non-use) of 2314 direct access facility, and Central Processing Unit (CPU) time in minutes during test runs of various programs.

Program	Compiler	Storage in kilobytes	2314 direct access facility	CPU time in min.
Scalar I	G	200	NO	184
Vector I	G	200	NO	224
Scalar II	G	200	NO	0.4
Vector II	G	200	NO	0.5
Scalar III	H,OPT=2	220	YES	14
Vector III	H,OPT=2	748	NO	20
Scalar IV	H,OPT=2	500	YES	5
Vector IV	H,OPT=2	750	YES	31

It may be pointed out that the first two programs require less than 200K bytes of storage space during execution. A region of 200K bytes was asked for because the system used assigned a minimum of 200K bytes all the time.

During the execution of the third program, values of the Fourier coefficients were computed for $\theta' = 0^\circ(2^\circ)180^\circ$ and $\theta = 0^\circ(2^\circ)90^\circ$ for the case for which punched card output was obtained after execution of the second program. Because of the use of a less strict criterion, this Fourier series output could be terminated after 225 terms instead of 267.

For the test runs for the fourth program, values used for several input parameters of interest are as follows: $\theta_o = 40^\circ$, $\Delta\theta = 2^\circ$, Number of layers = 40, $\lambda = 0.55\mu$, $\tau_b^{(s,r)} = 0.098$, $\tau_b^{(s,m)} = 0.242$, $\tau_b^{(a,m)} = 0.060$, no ozone, and a typical atmospheric aerosol number density versus height curve with Haze C for the size distribution function. Because of the use of the modified Fourier series method [see discussion following Eq. (29)], the number of terms of the series to be evaluated depends upon the nature of the aerosols and value of θ_o . For this particular case, we required 147 terms instead of 225. The CPU time and the number of iterations required for evaluation of some selected terms of the Fourier series are given in Table II for the vector and scalar cases.

Finally, it should be pointed out that this CPU time for the fourth program depends upon the number of layers into which the basic atmospheric model is divided. The above timings will be approximately

Table II

CPU time and number of iterations required for evaluation of some selected terms of the Fourier series during multiple-scattering calculations in a plane-parallel atmosphere (for details of the model, please see the text).

Term of the series	CPU time in secs. Scalar	Vector	Number of iterations Scalar	Vector
Lambert ground	13.5	108.9	5	5
n = 1	15.4	123.3	6	6
n = 10	7.3	53.2	4	4
n = 50	1.4	6.8	3	3
n = 100	0.8	2.3	2	2
n = 147	0.5	1.6	2	2

twice as much when calculations are repeated for an 80-layer model. On the other hand, these timings also depend very strongly on the value of the input parameter $\Delta\theta$. The timings given above were found to decrease by a factor of about 8 and 20 when calculations for the above case were repeated for $\Delta\theta = 6^\circ$ and 10°, respectively.

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