MODELING OF THE OPTICAL CHARACTERISTICS OF NEAR–GROUND AEROSOL IN THE REGION OF MEXICO IN DRY AND MOIST SEASONS

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Model calculations of the characteristics of light scattering in the ground atmospheric layer in the region of Mexico in dry and moist seasons have been carried out for visible range. The results of numerical modeling have shown the importance of correct account of the transformation of not only particle size spectrum but also particle microstructure, i.e., nonsphericity and especially heterogeneous chemical composition.

An attempt to create adequate models of aerosol structure applicable to a calculation of aerosol optical characteristics have been undertaken on the basis of the available data on aerosol microstructure in the ground layer in the region of Mexico for dry and moist seasons.

A basic data array was obtained by means of a TSI–2000 electrostatic spectrometer of aerosol particles. In addition, the data of the electron microscope analysis, which allowed definite conclusions about particle origin and shape, were used. Unfortunately, the data of an AZ–5 photoelectric counter were not included in the created models, since these measurements started in late 1991.

The particle size distribution functions $f(R)$ for corresponding seasons are shown in Figs. 1*a* and *b*. The averaged tabular data for dry and moist seasons were used in the range of the particle size 0.003–0.3 μm. These data were experimentally measured with the photoelectric counter as well as smoothed (curves were processed instead of histograms) and extrapolated in the range of the particle size 0.3–10 μm for the purpose of calculations. Extrapolation was made by the law $f(R) = AR^{-4}$, where $A = 0.613186$ for dry season and 0.471033 for moist season, and R is the radius of homogeneous spherical particles.

The optical characteristics were calculated for the wavelength range $\lambda = 0.35–1.0$ μm with a step of 0.05 μm.

In particular, we investigated the effect of inhomogeneity and nonsphericity of scattering particles on the following optical characteristics: the extinction, scattering, absorption, and backscattering coefficients (K_{ext}, K_{sca}, K_{abs}, k_{back}), scattering phase function $I(\Theta)$, the asymmetry coefficient of the scattering phase function

$$\gamma = \frac{\int_0^{\pi/2} I(\theta)\sin\theta\, d\theta}{\int_{\pi/2}^{\pi} I(\theta)\sin\theta\, d\theta},$$

and the degree of linear polarization

$$Pol = \frac{I_{\perp}(\theta) - I_{||}(\theta)}{I_{\perp}(\theta) + I_{||}(\theta)}.$$

The following models were considered for moist season: model I employed in studying the effect of two–layer particles (microstructural inhomogeneity) and model II employed in studying the effect of particle nonsphericity.

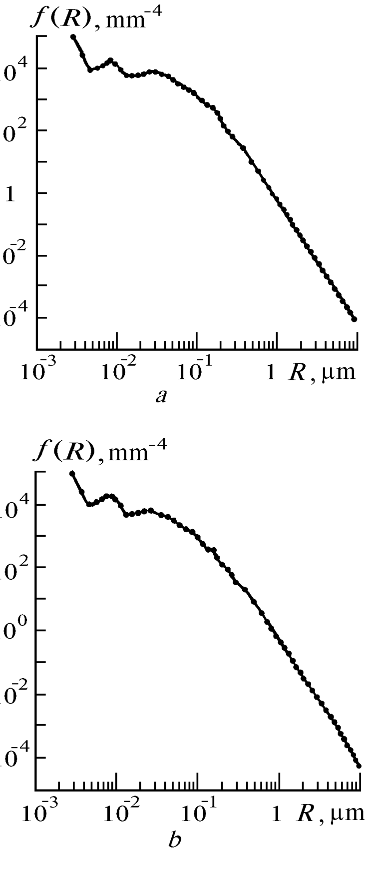

FIG. 1. Model particle size distribution functions f(R) for the visible range in dry (a) and moist (b) seasons in the region of Mexico.

A mixture of homogeneous and two–layer particles in different ranges of particle size was included in model I. The following models were employed:

I.1. Homogeneous spheres with radii 0.003–0.01 mm and two–layer spheres with radii of the core $r = R - d$, where d = 0.001 μm is the constant thickness of coating.

I.2. Homogeneous spheres with radii 0.003–0.01 μm and two–layer spheres with radii 0.01–10 μm and d = 0.002 μm.

I.3. Homogeneous spheres with radii 0.003–0.01 μm, two–layer spheres with radii 0.01–0.05 μm and d_1 = 0.001 μm, and two–layer spheres with radii 0.05–10 μm and d_2 = 0.01 μm.

I.4. Homogeneous spheres with radii 0.003–0.01 μm, two–layer spheres with radii 0.01–0.05 μm and d_1 = 0.002 μm, and two–layer spheres with radii 0.05–10 μm and d_2 = 0.01 μm.

The results of calculation of the optical characteristics for these models were compared with those for the model of homogeneous spheres. The refractive index of these spheres was taken $\tilde{m} = (1.47 - i\ 0.003)$ (see Refs. 1–3), and for two–layer spheres the refractive index of the material of the core was $m_c = (1.65 - i\ 0.005)$ in accordance with the model refractive index of soil aerosols, and $m_{cov} = (1.33 - i\ 0.0)$ corresponded to the refractive index of water.

Model II was employed for studying the effect of nonsphericity on the optical scattering characteristics. A mixture of homogeneous spheres and cylinders was taken so as to fit approximately the results of electron microscope analysis of samples. The light scattering characteristics of cylinders were calculated by the formulas of light scattering on infinite cylinders, since for the ratio of the length of a cylinder to its radius $l/r > 5$ the finite–size cylinder can be considered infinite.

The cylinder radius was calculated from the equality of the volumes of cylinder and sphere: $V_{cyl} = V_{sp}$ for $l/r = 5$ and 10. The cylinders with different orientations relative to the incident radiation direction ($\alpha = 0°$ and 89°) were considered, where α is the angle between the incident radiation direction and the perpendicular to the cylinder axis.

A mixture of spherical and cylindrical particles was considered for the moist season: for $0.003 \le R \le 0.1$ homogeneous spheres constituted 100% of particles, for $0.1 < R \le 10$ μm homogeneous spheres constituted 95% of particles, and cylinders constituted 5%. The refractive index of the cylinders $m_{cyl} = (1.65 - i{\cdot}0.005)$ and the refractive index of the spheres $m_{sp} = (1.47 - i{\cdot}0.003)$.

Model III was considered for dry season. It represented a mixture of homogeneous spheres with the refractive index $m_1 = (1.55 - i{\cdot}0.003)$ and soot particle with $m_2(\lambda)$ presented in Table I.

The following particle composition was assumed in model III: for $R = 0.003 - 0.1$ μm the model incorporated 10% of soot particles with $\tilde{m} = m_2$ and 90% of particles with $\tilde{m} = m_1$, and for $R = 0.1 - 10$ μm it incorporated 100% of particles with $\tilde{m} = m_1$.

The calculated results are presented in the tables and shown in the figures. The relative errors in the scattering coefficients $\delta^i = (K^i_{mixt} - K^i_{hom})/K^i_{hom}$ for models I.1–I.4 at the wavelengths λ = 0.35, 0.55, and 1.0 μm are presented in Table II.

It follows from the data in Table II that the appearance of the two–layer particles, i.e., the change of their inner structure, results in the sharp increase in the relative error of the absorption and backscattering coefficients and is experimentally significant for these coefficients.

TABLE I.

λ, μm	m_2
0.35	1.80 – i·0.74
0.40	1.80 – i·0.74
0.45	1.81 – i·0.74
0.50	1.82 – i·0.74
0.55	1.83 – i·0.74
0.60	1.84 – i·0.74
0.65	1.84 – i·0.73
0.70	1.85 – i·0.72
0.75	1.85 – i·0.71
0.80	1.86 – i·0.70
0.85	1.87 – i·0.69
0.90	1.88 – i·0.69
0.95	1.89 – i·0.68
1.00	1.90 – i·0.68

TABLE II.

Error	Model											
	I.1			I.2			I.3			I.4		
λ, μm	0.35	0.55	1.00	0.35	0.55	1.00	0.35	0.55	1.00	0.35	0.55	1.00
δ_{ext}	14.58	25.6	28.5	13.9	24.5	27.9	8.90	18.7	22.7	8.85	18.7	22.7
δ_{sca}	12.55	23.9	27.0	11.4	23.1	26.3	6.90	17.1	21.2	6.94	17.1	21.2
δ_{abs}	64.40	72.3	77.0	63.1	71.9	76.1	55.9	63.4	67.5	55.8	63.4	67.5
δ_{back}	270	284	299	266	282	297	269	192.8	244	244	269	192.8

The scattering phase functions $I(\Theta) = I(\Theta)/I(0°)$ are shown in Fig. 2*a* for the model of homogeneous particles (curve *1*) and mixture of homogeneous and two–layer particles for models I.1–I.4 (curves *2*, *3*, and *4*) at λ = 0.55 μm.

The analysis of the curves allows us to conclude that the effect of two–layer particles becomes pronounced for $\Theta > 40°$: the shape of the scattering phase function changes and at $\Theta = 130°$ the ratio $I_{mixt}/I_{hom} = 2$ while at $\Theta = 180°$, $I_{mixt}/I_{hom} = 4$.

The degree of linear polarization $Pol(\Theta)$ is shown in Fig. 2*b* for the homogeneous model (curve *1*) and mixture of homogeneous and two–layer particles for models I.1–I.4 (curves *2*, *3*, and *4*).

The effect of the particle inhomogeneity on the degree of linear polarization is very significant:

the shapes of the curves change,
the maxima shift to the left,
and additional maxima and minima appear.

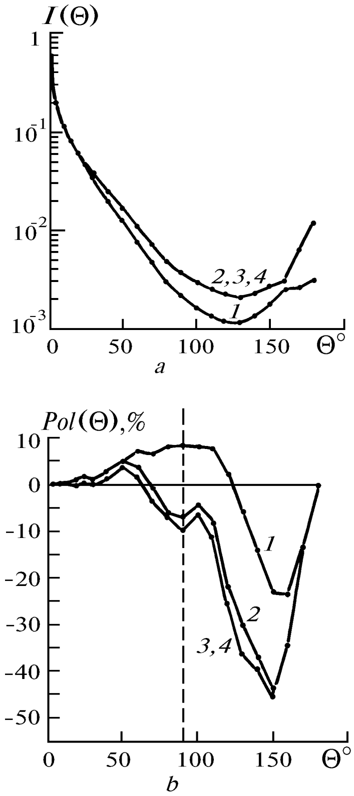

FIG. 2. Angular scattering characteristics for the moist season in the region of Mexico at λ = 0.55 μm: a) scattering phase functions I(Θ), b) degree of linear polarization Pol(Θ), % (curve 1 is for the model of homogeneous spheres and curves 2, 3, and 4 are for models I.1–I.4).

The asymmetry of the scattering phase function γ is presented in Table III for the model of homogeneous spheres and mixture.

TABLE III.

λ, μm	Homogeneous model	Mixture
0.35	1.42	1.11
0.40	1.27	0.98
0.45	1.10	0.89
0.50	1.13	0.83
0.55	1.09	0.79
0.60	1.07	0.76
0.65	1.05	0.75
0.70	1.03	0.73
0.75	1.04	0.71
0.80	1.035	0.70
0.85	1.03	0.70
0.90	1.03	0.70
0.95	1.04	0.71
1.00	1.006	0.703

The two–layer microstructure of spherical particles results in the change of the asymmetry of the scattering phase function by a factor of 0.8–0.6. Therefore, we can conclude that the appearance of two–layer particles (particulary, their moistening) significantly changes the optical scattering characteristics. The change in the shape of the scattering phase function and the shift of the minimum in the parameter *Pol* can be good indicators of the appearance of moistened aerosol particles.

The fraction of nonspherical particles, which was experimentally revealed in the atmosphere of Mexico, does not essentially change the properties of the near–ground aerosols.

The analysis of the results of model calculations for the dry season (model III) shows that addition of 10% of soot particles with radii $0.003 \le R \le 0.1$ μm results only in the change of the absorption coefficient by 19–25% (relative error δ), but the angular characteristics remain practically unchanged.

An increase of the scattering coefficient in the dry season may be noted from a comparison of the optical scattering characteristics for moist and dry seasons.

These conclusions are illustrated by Table IV and Figs. 3*a* and *b* in which the values of $K(\lambda)$ for dry and moist seasons as well as the scattering phase functions and the degree of linear polarization for polydispersed systems of homogeneous spherical particles in dry and moist seasons are given in the range of particle size $0.003 \le R \le 10$ μm.

TABLE IV.

λ	$K_{ext}\cdot10^{-3}$ km^{-1}		$K_{abs}\cdot10^{-3}$ km^{-1}		$K_{back}\cdot10^{-3}$ km^{-1}	
	Season					
	Dry	Moist	Dry	Moist	Dry	Moist
0.35	52.2	32.3	1.84	1.26	35.0	10.20
0.40	49.1	30.1	1.66	1.11	32.5	7.60
0.45	45.8	28.1	1.48	1.02	22.8	8.60
0.50	42.8	26.1	1.35	1.93	22.7	8.30
0.55	39.3	24.1	1.23	1.86	21.3	7.60
0.60	36.3	22.7	1.12	1.79	18.6	6.90
0.65	34.1	21.3	1.03	1.74	16.8	7.10
0.70	31.7	20.1	0.98	0.68	15.9	6.20
0.75	29.9	19.11	0.91	0.64	15.2	6.10
0.80	28.2	18.1	0.84	0.60	13.7	5.60
0.85	26.7	17.1	0.82	0.56	14.5	5.10
0.90	25.2	16.1	0.77	0.53	13.5	5.03
0.95	23.8	15.4	0.71	0.51	11.2	5.50

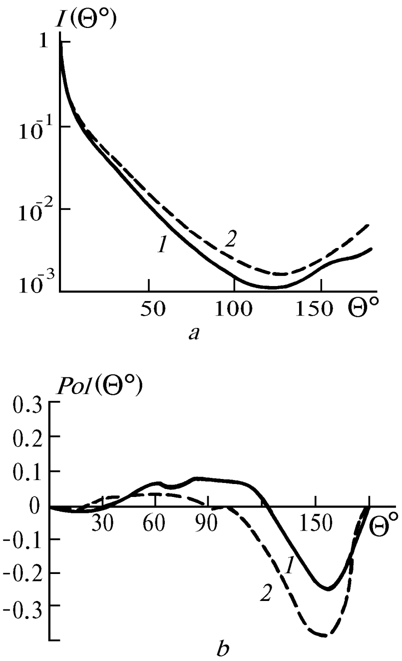

FIG. 3. Angular scattering characteristics at λ = 0.55 μm for moist (curve 1) and dry (curve 2) seasons in the region of Mexico: a) scattering phase functions I(Θ) and b) degree of linear polarization Pol(Θ).

A comparison of the results of calculation of the extinction, absorption, and backscattering coefficients and the well–known data on these characteristics obtained in Refs. 2 and 3 for the urban atmosphere demonstrates extremely underestimated values of these characteristics from the data of electrostatic counter. Possible reasons for this underestimation are evident. They are: (1) incorrect extrapolation of data for large particles and (2) very pure air in the region of measurements.

As noted above, the data of the photoelectric counter were not included in our calculations since these measurements started only in late 1991.

We note that for giant particles ($R > 1.0$ μm) their concentration is overestimated in comparison with the values obtained by the Junge formula $f(R) = A\,R^{-4}$. This significantly affects the real values of the aerosol extinction and scattering coefficients. Investigations of this sort are scheduled by us with allowance for the data obtained in 1992–1993. In addition, it should be emphasized that the measurement region was on the outskirts of Mehico within the purest zone (in the University campus), and the measurements were performed in very clear days.

Thus the results of numerical modeling of the optical characteristics of atmospheric aerosols in Mexico for dry and moist seasons are evidence of the importance of taking into account not only the transformation of the particle size spectra but also their microstructure, i.e., nonsphericity and inhomogeneous composition, especially the latter characteristic. A more comprehensive integrated study of microstructural and optical properties of the aerosols in Mexico is required for modeling of the aerosol optical characteristics.

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REFERENCES.

1. L.S. Ivlev and S.D. Andreev, *Optical Properties of Atmospheric Aerosols* (State University Publishing House, Leningrad, 1986), 358 pp.
2. K.Ya.Kondrat'ev, N.I. Moskalenko, and D.V. Pozdnyakov, *Atmospheric Aerosol* (Gidrometeoizdat, Leningrad, 1983), 224 pp.
3. V.E. Zuev and G.M. Krekov, *Optical Models of the Atmosphere* (Gidrometeoizdat, Leningrad, 1986), 256 pp.