Development of the software for calculations of aerosol extinction of optical radiation in the surface layer of marine and coastal atmosphere

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Description of the program module MaexPro intended for estimating signal energy in the surface layer of marine and coastal atmosphere is presented. The key input parameter for the module is the fetch. The program makes it possible to estimate aerosol extinction as a function of standard, readily measured meteorological parameters, microphysical composition of aerosol, detector's spectral range, and observation path geometry.

Introduction

It is well known that the atmospheric aerosol scattering and absorption in the atmosphere is a main cause of the optical radiation extinction in the visible and IR ranges in the marine surface layer. The extinction affects the spectral transmission function of both natural and artificial light, which is of interest for many problems, in particular, for radiation problems, studying the peculiarities of climate formation, and for some applications connected with prediction for signal energy potentiality in coastal conditions, when estimating characteristics of optical electronic devices and systems.

According to present-day knowledge of the surface layer aerosol in marine and coastal atmosphere, its microphysical and optical characteristics determining the coefficient of aerosol extinction $\alpha(\lambda)$, significantly depend on the type of air masses and wind regime, namely, on velocity and direction of the wind, which govern the humidity and dimension of the wave tide area. These characteristics have a pronounced height profile, especially in the height range 0–30 m.[1–6]

Aerosol and its effects on processes in the boundary layer of marine and coastal atmosphere have been investigated during last 10–15 years by numerous research groups, united by several long-term international programs. Most known among them are the RED (Rough Evaporation Duct),[7] EOPACE (Electro Optical Propagation Assessment in Coastal Environment),[8–10] ASE-1, -2 (Aerosol Characterization Experiment),[11] MAPTIP Experiment (Marine Aerosol Properties and Thermal Imager Performance),[12] PARFORCE (New Particle Formation and Fate in the Coastal Environment).[13]

One of the goals of the programs is to develop efficient coastal aerosol models, in which the easily measured meteorological parameters are used as input data. Simultaneously, numerous computer versions of models, packages, or codes, where aerosol extinction spectra are main calculation characteristics, are under development.

In this paper we describe the last version of the program module MaexPro (**M**arine **a**erosol **ex**tinction **Pro**file) intended to calculate spectral and vertical profiles of the aerosol extinction coefficient $\alpha(\lambda)$, size distribution function, number concentration, scattering cross section, volume distribution, and spectral profiles of individual modes.

1. Contents of the MaexPro module

If aerosol particles have a spherical form, the size distribution function and refractive index of which are known, then, using the Mie theory, calculation coefficients of aerosol scattering and extinction are used in the form[14–18]:

$$\alpha(\lambda) = \int_0^\infty K_p(\rho,m)\frac{\mathrm{d}N}{\mathrm{d}r}\pi r^2 \mathrm{d}r; \qquad (1)$$

$$\varepsilon(\lambda) = \int_0^\infty K(\rho,m)\frac{\mathrm{d}N}{\mathrm{d}r}\pi r^2 \mathrm{d}r, \qquad (2)$$

where $\mathrm{d}N/\mathrm{d}r$ is the aerosol size distribution function, $\mathrm{cm}^{-3}\cdot\mu\mathrm{m}^{-1}$; $K_p(\rho, m)$, $K(\rho, m)$ are the Mie coefficients (of scattering and extinction efficiency, respectively); $\rho = 2\pi r/\lambda$ is the relative particle size; m is the complex refractive index; r is the radius of aerosol particles, μm.

1.1. Microphysical model MaexPro

The derivative $\mathrm{d}N/\mathrm{d}r$ was calculated by the last version of the similar microphysical model MaexPro.[19–25] The model is characterized by a 4-modal particle size distribution function and is written as a sum of four lognormal functions:

$$\frac{\mathrm{d}N}{\mathrm{d}r} = \sum_{i=1}^{4}\frac{A_i}{\mathrm{f}}\exp\left\{-C_i\left[\ln(r/\mathrm{f}r_{0i})\right]^2\right\}, \qquad (3)$$

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where A_i, C_i are the amplitude and width of the ith mode, respectively; r_{0i} is the modal radius of the ith mode, μm ($r_{01} = 0.03$; $r_{02} = 0.24$; $r_{03} = 2$; $r_{04} = 10$ μm); $\mathrm{f} = \left[(2 - S)/6(1 - S)\right]^{1/3}$ is the function (factor) of growth, depending on humidity; $S \equiv f/100$ is the saturation index; f is the relative humidity of air, %. At $f = 80\%$ $\mathrm{f} = 1$.

A feature of the model is that the amplitude and the width of different modes are parameterized as functions of the fetch (the distance along open water from the windward side (wind tide area)), X, and the wind velocity U.[26]

The applicability domain of the model is as follows:

– the model MaexPro is designed for a particle size spectrum between 0.001 and 100 μm by the radius r and at present is developed for the range of heights H from 0 to 25 m, where the most significant changes in the microphysical composition occur;

– the wind velocity U varies from 3 to 18 m/s;

– dimensions of the wave tide area X vary from 3 to 120 km;

– relative humidity f varies from 40 to 98%.

1.2. Optical model MaexPro

In the MaexPro model, the real and imaginary parts of the complex refractive index for components of aerosol matter were taken from the experimental graphed data[27–30] and extrapolated to a wavelength range from 0.2 to 40 μm with the step $\Delta\lambda = 0.0001$ μm. The aerosol matter is represented as 4 combinations of dry substance, sea salt, and water.

Table 1. Components of aerosol matter

Mode	Matter	Dimension of the mode, μm	Reference
1	Unsolvable	0.03	[27]
2	Solvable	0.24	[28, 29]
3	salt + water	2	[27]
4	salt + water	10	[30]

Besides, the aerosol extinction coefficient $\alpha(\lambda)$ was calculated with the following extrapolation connected with the vertical profile of the growth function f [Refs. 31–34]:

$$\left(\frac{\alpha_H}{\alpha_{0\,\mathrm{m}}}\right) = \left(\frac{0.037}{1.017 - \mathrm{f}_H/100}\right)^{0.84}, \qquad (4)$$

where $\alpha_{0\,\mathrm{m}}$ is the coefficient of aerosol extinction at the height $H_0 = 0$, km^{-1}; f_H is the growth function at the height H.

The vertical profiles of f were calculated under the following conditions:

– at $20\ \mathrm{m} \le H \le 25\ \mathrm{m}$ $\mathrm{f} = \mathrm{f}_{25\,\mathrm{m}}$;

– at $H \le 20$ m and $\mathrm{f} \le \mathrm{f}_{25\,\mathrm{m}}$ $\mathrm{f} = \mathrm{f}_{25\,\mathrm{m}}$;

– otherwise: at $H \le 20$ m $\mathrm{f} = (\mathrm{f}_{25\,\mathrm{m}} + 7)H^{-0.03}$. Here $\mathrm{f}_{25\,\mathrm{m}}$ is the growth function at a height of 25 m. The extrapolation is valid for f ranging from 40 to 98%.

2. Operation of the MaexPro module: main stages

To realize the module MaexPro 5.0, the Borland Delphi 2005 was chosen as a programming environment. This choice was caused by the presence of highly efficient applications, which made it possible to develop a maximally convenient and functional user interface.

The structure diagram of the module is presented in Fig. 1.

The MaexPro module can calculate:

– spectral and vertical profiles of $\alpha(\lambda)$ according to Eqs. (1)–(4);

– particle size distribution functions, scattering cross sections, volume distributions;

– spectral profiles of individual modes;

– extrapolation of complex refractive indices of the aerosol particulate matter.

The following values are input data for the MaexPro module:

– $X(70)$ – the fetch, km;

– $f(80)$ – the relative humidity, %;

– $U(3.5)$ – the wind velocity at a height of 10 m, m/s;

– $H(10)$ – the height above the sea surface, m;

– $\Delta H(1)$ – the height step, m;

– $r_{\min}(0.001)$, $r_{\max}(100)$, $\Delta r(0.001)$ – minimal and maximal radii and the radius step, μm;

– $\lambda_{\min}(0.2)$, $\lambda_{\max}(40)$, $\Delta\lambda(0.0001)$ – minimal and maximal radiation wavelengths and the wavelength step, respectively, μm.

The most typical values of input parameters are written in the parentheses as specified by default and can be varied by the user within the scope of the model applicability.

The aerosol extinction spectra are calculated in the following sequence. First, the input parameters with values from the domain of the model applicability, i.e., data on microphysical aerosol composition, spectral range, and necessary meteorological conditions are entered. Then the kind and model of calculation are chosen. The possible options are as follows: calculation of spectral extinction (full and module variants), calculation of spectral extinction from the measured distribution (depending on this, dN/dr is calculated either by Eq. (3) or by data from the measured distribution), representation of output files in the form convenient to enter MODTRAN/LOWTRAN, calculation of spectral extinction (program variant). The full regime of calculations is basic, therefore it is taken by default. The model is chosen from the following options: MaexPro 5.0, MaexPro 2.0, and NAM6.

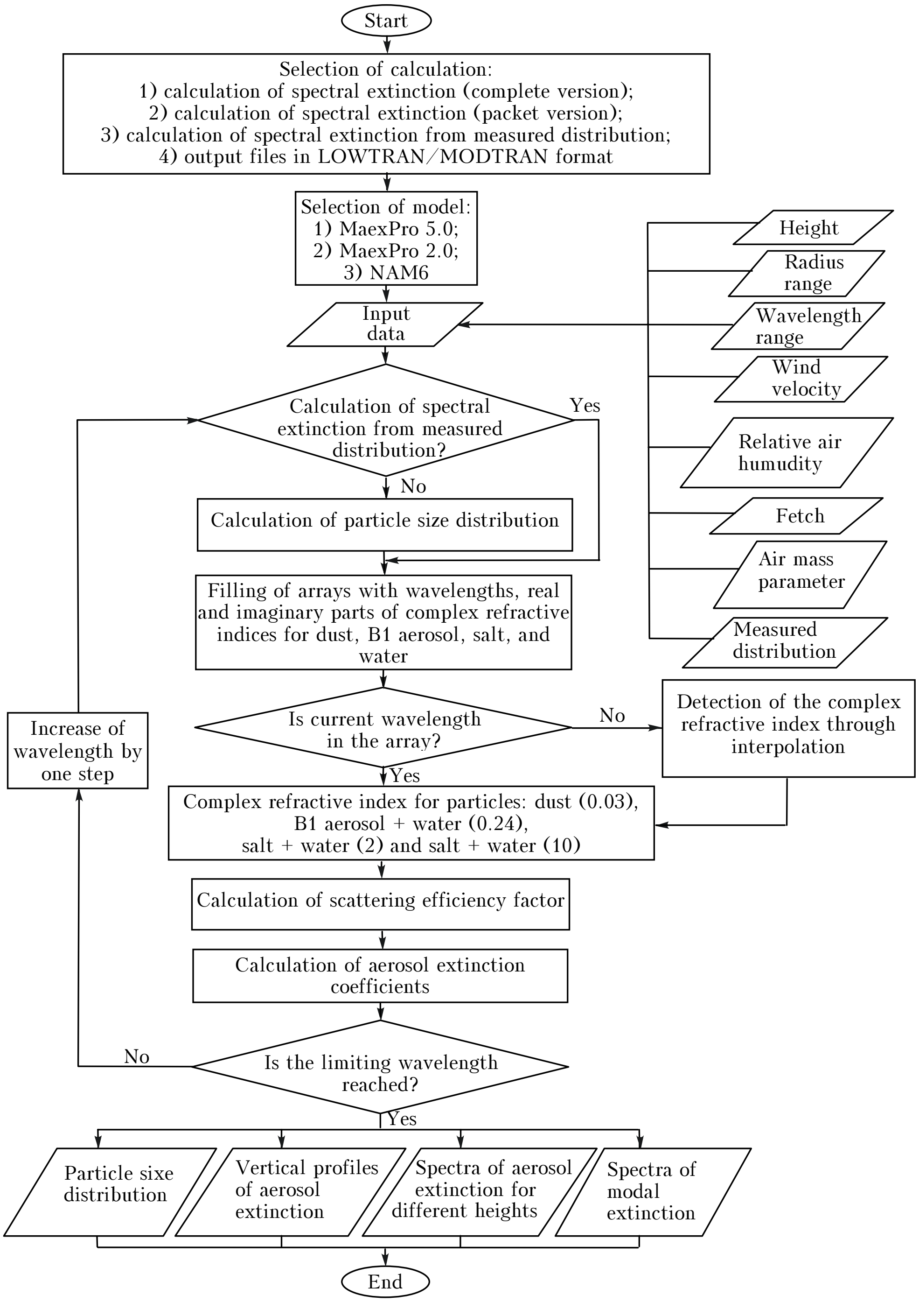


Fig. 1. Structure diagram of the MaexPro module.

This is followed by the main cycle of the program, where the current parameter is the wavelength. The derivative dN/dr is calculated depending on the chosen model for each mode, then, after summation, the general distribution is constructed. The dynamic arrays are filled with values of wavelengths and corresponding real and imaginary parts of the complex refractive index. The index is calculated for a current wavelength, which is searched in the array, and if is not found in the array, the real and imaginary parts of the complex refractive index are calculated by interpolation. Then the efficiency factors of extinction and scattering are calculated in accordance with the Mie theory using the subroutine MieCalc.[35] The series are calculated by the method of inverse recursion.

Coefficients of aerosol extinction and scattering are calculated through integration by the trapezoid method over the given radius of particles. The input parameter of the step over the radius range is taken as the integration step. If the wavelength limit value is reached, the basic cycle of the program is completed and the following output data are displayed: the particles size distribution, vertical profiles of aerosol extinction, spectra of aerosol extinction for different heights, and spectra of mode extinction. These data are used for further visualization in tables and plots. If the limit value of the wave-length is not reached, the basic cycle of the program is continued.

3. Control for the MaexPro module

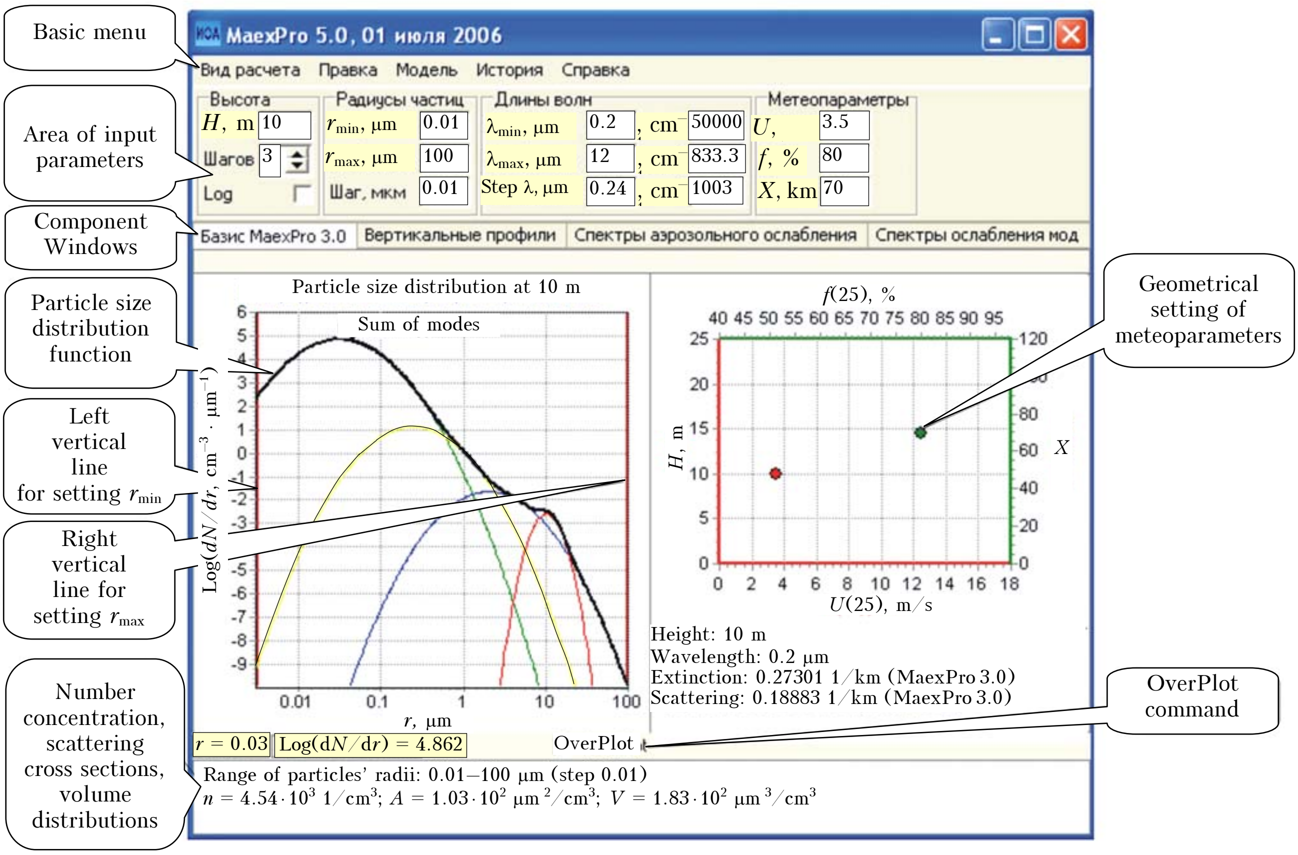
The window of the MaexPro 5.0 module is presented in Fig. 2 and consists of three parts: menu string (Type of calculation, Edit, Model, History, and Help), area of input parameters, and component windows.

The structure of the obtained results consists of four groups which are presented in corresponding windows: base, vertical profiles, spectra of aerosol extinction, and spectra of mode extinction. The obtained results are displayed in the corresponding windows as plots, numerical values, and tables. The area of input parameters does not change when switching from one window to another.

In Fig. 2 the Base window is active. It presents the function dN/dr, which can be changed by a double click to the functions of scattering cross sections and volume distribution. The bottom information area presents their numerical values.

The user can vary the aerosol particle size spectrum by moving corresponding vertical lines. An additional window to the right permits setting meteorological parameters by the movement of circles. Besides, several service commands are included: the OverPlot function for superposition or change of plots, interpolation of profiles $\alpha(\lambda)$ by height, scaling and tracing, various copy functions, representation of data in tables, representation of data in the form, convenient for entering into the MODTRAN code, etc.

Figure 3 presents the Spectra of aerosol extinction window illustrating optical activity of aerosol in the surface layer of marine and coastal atmosphere the most typical values of input meteorological parameters and geometry of measurements. The spectra $\alpha(\lambda)$ were obtained by the service command "OverPlot switch" and calculated based on dN/dr for 8 particle size spectra, including dN/dr, which can be obtained by the use of the aerosol counter AZ-5 (with the measurement radius range Δr = 0.4–10 μm) and the dust counter OMPN-10.0 (OPTEK, Saint-Petersburg), controlling fractions according to the standards RM-10.0; RM-2.5, and RM-1.



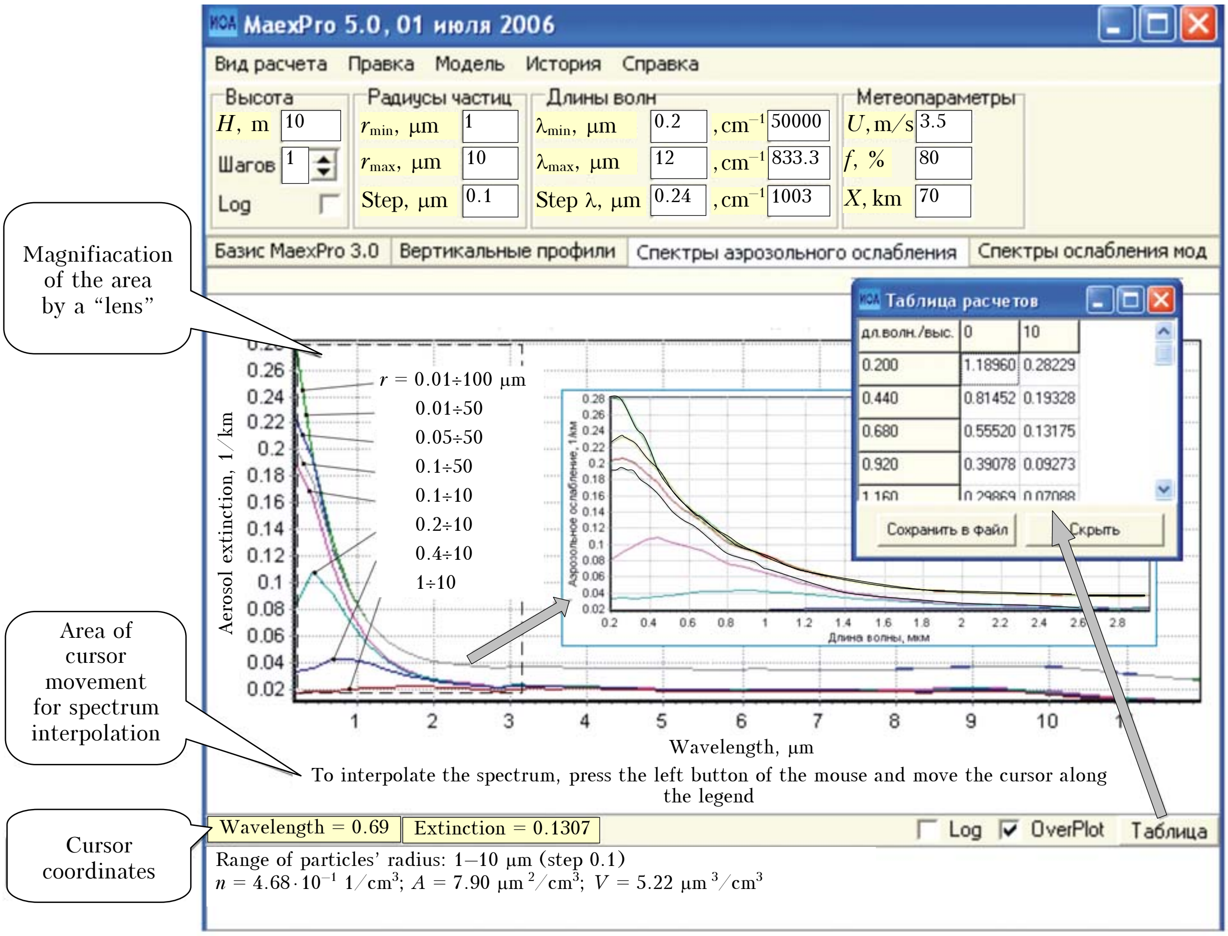
H, m 10
Шагов 3
r_{min}, μm 0.01
r_{max}, μm 100
Шаг, мкм 0.01
λ_{min}, μm 0.2, cm⁻¹ 50000
λ_{max}, μm 12, cm⁻¹ 833.3
Step λ, μm 0.24, cm⁻¹ 1003
U, 3.5
f, % 80
X, km 70

Height: 10 m
Wavelength: 0.2 μm
Extinction: 0.27301 1/km (MaexPro 3.0)
Scattering: 0.18883 1/km (MaexPro 3.0)

r = 0.03 Log(dN/dr) = 4.862

Range of particles' radii: 0.01–100 μm (step 0.01)
$n = 4.54 \cdot 10^3$ 1/cm³; $A = 1.03 \cdot 10^2$ μm²/cm³; $V = 1.83 \cdot 10^2$ μm³/cm³

Fig. 2. Interface of the MaexPro module.



H, m 10
Шагов 1
$r_{\min}$, μm 1
$r_{\max}$, μm 10
Step, μm 0.1
$\lambda_{\min}$, μm 0.2 , cm^{-1} 50000
$\lambda_{\max}$, μm 12 , cm^{-1} 833.3
Step λ, μm 0.24 , cm^{-1} 1003
U, m/s 3.5
f, % 80
X, km 70

дл.волн./выс.	0	10
0.200	1.18960	0.28229
0.440	0.81452	0.19328
0.680	0.55520	0.13175
0.920	0.39078	0.09273
1.160	0.29869	0.07088

To interpolate the spectrum, press the left button of the mouse and move the cursor along the legend

Wavelength = 0.69 Extinction = 0.1307

Range of particles' radius: 1–10 μm (step 0.1)
$n = 4.68 \cdot 10^{-1}$ 1/cm^3; $A = 7.90$ μm^2/cm^3; $V = 5.22$ μm^3/cm^3

Fig. 3. MaexPro module: "Spectra of aerosol extinction" window.

Table 2 presents the values of the number concentration N, scattering cross section A, and distribution of volumes V at varying the spectrum of particle sizes by Δr from 0.01–100 to 1–10 μm for $H = 10$ m, $U = 3.5$ m/s, $f = 80\%$, $X = 70$ km.

Table 2. Countable concentration, scattering cross section, and volume distribution in varying the spectrum of particles' size

Δr, μm	N, 1/cm^3	A, μm^2/cm^3	V, μm^3/cm^3
0.01–100	4540	103	183
0.01–50	4540	103	183
0.05–50	2210	94.5	182
0.1–50	663	69.9	180
0.1–10	663	63.8	69.8
0.2–10	90.4	31.4	63.5
0.4–10	7.26	14.2	57.2
1–10	0.468	7.90	52.2

Analysis of the calculation results (see Fig. 3 and Table 2) demonstrates that the data of $\alpha(\lambda)$ obtained on the base of dN/dr for the full spectrum of aerosol particle sizes $\Delta r = 0.01$–100 μm are appropriate to calculations, connected with estimation of optical signal energy in the spectral range $\Delta\lambda = 0.2$–12 μm. Note that for chosen values of input meteorological parameters and the geometry of measurements, the $\alpha(\lambda)$ values calculated on the base of dN/dr for the full spectrum of aerosol particle size $\Delta r = 0.01$–100 μm coincide with those for the partial spectrum $\Delta r = 0.01$–50 μm. For incomplete spectra, which can be obtained by the use of counters AZ-5 and OMPN-10.0, the calculated values of $\alpha(\lambda)$ in the range $\Delta\lambda = 2$–12 μm differ approximately by the factor of two, and in the range $\Delta\lambda = 0.2$–2 μm the differences in $\alpha(\lambda)$ reach 50 [Ref. 36]. Similarly significant differences (see Table 2) are observed in numerical values of the number concentration, scattering cross sections, and volume distributions, which are displayed in the bottom of the corresponding window. At the same time, calculations demonstrate that the use of the partial spectrum $\Delta r = 0.05$–50 μm and even $\Delta r = 0.1$–50 μm does not lead to considerable errors in $\alpha(\lambda)$ in the range $\Delta\lambda = 0.4$–12 μm.

At present, there is no common aerosol counter to obtain dN/dr both for the full and partial spectra of aerosol particle sizes. Therefore, a combination of aerosol counters is required. In particular, taking into account a high cost of aerosol counters, incomplete spectra can be obtained by the use of the following devices: differential analyzer of mobility RDMA (produced by Particle Measuring Systems Inc., Boulder, Co.) for the spectrum of aerosol particle sizes with $\Delta r = 0.01–0.3$ μm; laser aerosol counter OPC (produced by TSI Inc.) for Δr = 0.1–7 μm and laser aerosol counter of FSSP type (produced by Particle Measuring Systems Inc., Boulder, Co.) for Δr = 0.3–20 μm or 0.5–50 μm.

The MaexPro module was tested by comparing calculated and measured dN/dr and $\alpha(\lambda)$. The tests have shown that the model demonstrates a good agreement in 70% of cases, a satisfactory agreement in 23% of cases, and in 7% of cases the results do not coincide.[37–41]

Conclusions

1. The MaexPro module calculates spectral and height profiles of $\alpha(\lambda)$ as functions of standard meteorological parameters, microphysical composition of aerosol and permits one to take into account both wind regime and the air mass parameter indirectly through the fetch parameter.

2. The module realistically describes the influence of meteorological parameters, geometry, wind regime, the known phenomena and regularities on spectral and vertical profiles of $\alpha(\lambda)$.

3. The spectral profiles of $\alpha(\lambda)$ can be represented both by plots and tables. All possible service applications are provided: OverPlot commands to overlap or change plots, profile interpolation, scaling and tracing, copying, data representation in the form, convenient to enter into the MODTRAN code, and so on.

4. The user interface of the MaexPro package is fully point-and-click controllable and operates in the Windows system. The time for calculation of a spectral profile depends on necessary resolution by wavelength, particle radius, and height; at high resolution, it does not exceed tens of seconds. Other characteristics, such as the function of particle size distribution, scattering section, distribution of volumes, spectral profiles of individual modes are calculated almost instantly.

5. MaexPro package is a permanently upgraded computer program, which can be used for estimating signal energy at the site of signal receiving, depending on the standard and easily measured meteorological parameters, microphysical composition of aerosol, spectral range of the receiver, and geometry of the observation path.

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