Synthesis of corrected multi-wavelength spectrometers for atmospheric trace gases

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The method for synthesis of corrected three-wavelengths spectrometers for trace gas components of atmosphere on the basis of development of mathematical model has been suggested. The classification table for possible structures of corrected spectrometers is considered. The synthesis allows to reveal some new variants for development of three-wavelength spectrometers for trace gas components of atmosphere. For experimental checkup of achieved theoretical results, a laboratory pattern of three-wavelength spectrometer is developed and tested.

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The carrying out of spectral measurements in ultraviolet (UV) band is one of the high-priority fields of atmospheric researches, because the results of these measurements may be used both for assessment of some trace components of atmosphere (aerosol, ozone, etc.) and the level of effect of harmful spectral part of solar UV radiation. The basic method in this area is two-wavelength method of Dobson, which till now is used in modern spectrometers for measurements of total amount of ozone content[1−3]. Recently proposed three-wavelength method of measurements[4,5] differs from the Dobson method in principle and is featured with its wide functional possibilities for measurements and carrying out of different corrections. Despite the sufficient number of publications on this theme, the synthesis of possible variants for the construction of three-wavelength spectrometers and the classification of such instruments, embracing various forms of correction of measurement error, are not considered. In this letter, we carry out the synthesis of all possible variants for the construction of three-wavelength spectrometers and develop a classification table of synthesis on the basis of revealed classification signs.

It should be noted that the three-wavelength measurement method is based on the Bouguer's law, which in common case may be formulated as

$$I_1 = I_0 \, \mathrm{e}^{-\, [\alpha_\lambda \mu X + \beta_\lambda m_1 + \delta_\lambda m_2]}, \qquad (1)$$

where I_1 is the intensity of solar radiation at the ground level in $\mathrm{W}/(\mathrm{m}^2 \cdot \mathrm{n\,m})$; I_0 is the solar constant in $\mathrm{W}/(\mathrm{m}^2 \cdot \mathrm{n\,m})$; α_λ is the ozone's absorption index in cm^{-1}; X is the total amount of ozone in atmosphere in $\mathrm{atm} \cdot \mathrm{cm}$; β_λ and δ_λ are appropriate optical thicknesses of Rayleigh scattering and aerosol, which are dimensionless; m_1, m_2, and μ are appropriate optical air masses of Rayleigh scattering, aerosol, and ozone respectively, which are also dimensionless, and m_1 equals the ratio of optical thickness of Rayleigh scattering of non-

perpendicular light beam to that of perpendicular light beam.

From the view points of meteorology and accuracy characteristics of remote atmospheric measurements, the most unstable component of atmosphere is aerosol. It should be noted that the atmospheric aerosol is characterized by a bimodal distribution function describing the dependence of volume depth on particle sizes[6−9], which is physically explained with the presence of strictly discernible fine and coarse fractions of aerosol in atmosphere. These fractions have different sources. The correlation existing between them is so weak that it is impossible to reveal any deviation of Ångström parameter of fine aerosol fraction in dependence from the same parameter of coarse fraction[10]. Such a situation allows to describe the optical thickness of atmospheric aerosol δ_λ as a linear sum of two non-correlated components:

$$\delta_\lambda = \delta_{\lambda\mathrm{f}} + \delta_{\lambda\mathrm{c}}, \qquad (2)$$

where $\delta_{\lambda\mathrm{f}}$ is the optical depth of fine fraction of aerosol, and $\delta_{\lambda\mathrm{c}}$ is the optical depth of coarse fraction of aerosol. Thus, to increase the accuracy of atmospheric measurements, consideration of correlation dependences may be limited only by considering the correlations between internal parts of fractions for each selected fraction. The practical benefit from aforesaid physical feature of atmospheric aerosol is the possibility to separate statistical compensation of effect of aerosol to the accuracy of measurements. It is obvious that in order to reach mathematical conditions of compensation, the individual weight coefficients of compensation for measuring channels involved in joint measurements should be applied.

The conceptual chart diagram of multi-channel corrected atmospheric measurement device is shown in Fig. 1, which consists of the unit of optoelectronic meters $f_i(\lambda_i)$ carrying out measurements at the wavelength λ_i, the unit of correcting devices, the unit of intermediate transformation, and the unit of controlling and computing output parameters. In factual realization of

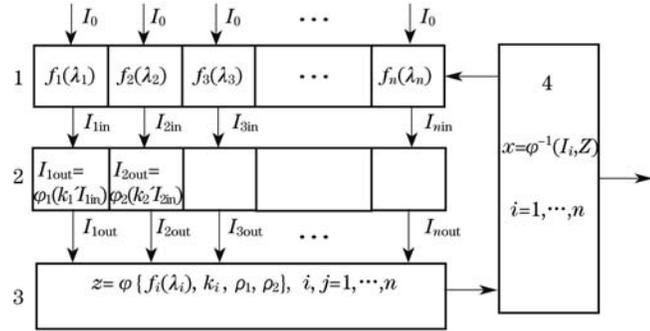the conceptual chart diagram, the functions of correction

Fig. 1. Block diagram of multichannel corrected atmospheric measurement device. 1: Optoelectronic meter unit, 2: correcting device unit, 3: intermediate transformation unit, 4: controlling and computing unit.

and transformation are carried out by the controlling and computing unit.

The relevant mathematical model of multichannel compensated spectrometer consists of three equations. The first one is the equation of transformation of the single measurement channel:

$$
\begin{aligned}
I_i = \quad & f_i \left[I_0(\lambda_i),\, X,\, \mu, m,\, m_1, \delta_f(\lambda_i), \right. \\
& \left. \delta_c(\lambda_i),\, \beta(\lambda_i), \alpha(\lambda_i) \right],\, i = 1, \cdots, n. \quad (3)
\end{aligned}
$$

The second one is the equation of intermediate transformation of output signals of channels:

$$
\begin{aligned}
z = \quad & \varphi\{ f_i(\lambda_i),\, k_i, \rho_1 \left[\delta_f(\lambda_i), \delta_f(\lambda_j) \right], \\
& \rho_2 \left[\delta_c(\lambda_i),\, \delta_c(\lambda_j) \right] \},\, i,\, j = 1, \cdots n, \quad (4)
\end{aligned}
$$

where ρ is the coefficient of correlation between the relevant parameters.

The third one is the equation for computing X:

$$
X = \varphi^{-1}(I_i, z),\ \ i = 1, \cdots n. \quad (5)
$$

Equations (3) – (5) represent the mathematical model of corrected spectrometer for trace gas components of atmosphere in UV band. It should be noted that all points of the mathematical model are to be carried out using appropriate software.

As an example of realization of three-wavelength spectrometer, we consider the construction variants, where the intermediate transformation is

$$
z = \frac{I_1^{k_1} \cdot I_3^{k_2}}{I_2}. \quad (6)
$$

As it will be shown later, such an equation makes it possible to carry out separate compensation of both parts of aerosol optical depth.

Taking into consideration Eqs. (1), (2), and (6), we can obtain

$$
\begin{aligned}
k_1 \delta_{\lambda_1,c} + k_2 \delta_{\lambda_2,c} &= \delta_{\lambda_2,c}, \\
k_1 \delta_{\lambda_1,f} + k_3 \delta_{\lambda_3,f} &= \delta_{\lambda_2,f}, \quad (7)
\end{aligned}
$$

characterizing the conditions of separate compensation of fine and coarse fractions.

Solution to Eq. (7) regarding k_1 and k_2 allows to find out factual values of correcting coefficients, making it possible to carry out full separate compensation of two fractions of atmospheric aerosol.

Now we consider another possible method for synthesis of corrected three-wavelength spectrometers based on identification of major classification signs of correction and composing of classification table. Major classification signs are as follows. 1) Realization of correction: multi-component correction; mono-component correction.

2) Types of mono-component interfractional correction: separate correction of effect of fractions; absence of separate correction of effect of fractions.

3) Quantity of used parameters of correction: mono-parameter correction; multi-parameter correction.

Aforesaid classification parameters allow to develop the classification table and therefore to carry out table type synthesis of all possible variants for the development of three-wavelength spectrometers, as shown in Table 1.

Now we can characterize the possible models for the construction of corrected three-wavelength spectrometers, according to models M1-M6. It should be noted that models M4 and M6 are described in detail in Ref. [4]. The model M2 is considered above. The model M3 possesses surplus elements and is impractical. The models M1 and M5 are valuable for further research.

The conditions for full correction of effect of separate components may be obtained as those for M2. The model M5 is of special interest, where only one correcting parameter is used and the separate correction on fractions is envisaged. But the research of possibility of technical realization of these models in detail is out of purpose of this letter.

For experimental checkup of the achieved theoretical results, a laboratory pattern of three-wavelength spectrometer was developed and tested. This spectrometer was designated for measuring the total content of ozone in atmosphere. The diagram of the device is shown in Fig. 2.

Table 1. Classification Table for Synthesis of Three-Wavelength Spectrometers

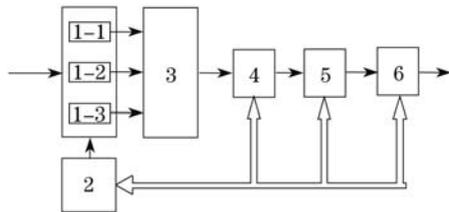| Sign 3. Amount of Correcting Parameters	Sign 1. Realization of Correction		
	Multi-Component Correction	Sign 2. Mono-Component Interfractional Compensation	
		Separate Compensation on Fractions	Non Compensation on Fractions
Multiple	M1	M2	M3
Single	M4	M5	M6

Fig. 2. Diagram of three-wavelength spectrometer. 1: Interference filters with central pass wavelengths of 300, 312.5, and 325 nm; 2: rotation motor for the disk containing interference filters; 3: photosensor; 4: amplifier with regulated coefficient of amplification; 5: analog-digital convertor; 6: control processor.

For approximate determination of the coefficients k_1 and k_2, we use the Ångström's formula[11,12], according to which the optical depth of aerosol δ_{aer} may be determined as

$$\delta_{\text{aer}} = A\lambda^{-b}, \qquad (8)$$

where A is the optical depth of aerosol at the wavelength $\lambda = 1\,\mu m$, b is the Ångström coefficient.

From Eqs. (7) and (8), we have

$$\begin{aligned} k_1\lambda_1^{-b_\text{c}} + k_2\lambda_3^{-b_\text{c}} &= \lambda_2^{-b_\text{c}}, \\ k_1\lambda_1^{-b_\text{f}} + k_2\lambda_3^{-b_\text{f}} &= \lambda_2^{-b_\text{f}}. \end{aligned} \qquad (9)$$

For further calculations, we should know the most characteristic values of b_c and b_f, for our region – Azerbaijani coastal area of the Caspian Sea, which has a geographic location similar to Persian Gulf. Therefore, in first approximation we can use the most characteristic values of b_c and b_f for Persian Gulf, $b_\text{c} \approx 1$, $b_\text{f} \approx 0.5$[10].

In this case, solution to Eq. (9) gives us $k_1 = 0.434$ and $k_2 = 0.562$. Therefore, it is shown that the coefficients k_1 and k_2 may be calculated separately for the determined models of aerosols and kept in the data storage unit.

The improvement of measurement accuracy was tested as follows. Indicators of three-wavelength ozonometer directed to the Sun were registered and deviation data were derived by half hour interval during sunny time periods within one weak. Each day we changed the value of k_1 while kept k_2 unchanged. In experiments, it was revealed that the standard deviation of analog output signal of three-wavelength ozonometer had a characteristic minimum on k_1. The dependence of standard deviation σ on k_1 is given in Fig. 3. This result may be used to indirectly prove the existence of an optimal pair of k_1 and k_2, upon which the effect of aerosol on measurement results is minimal.

In conclusion, the mathematical model and the method for synthesis of multi-wavelength spectrometers with multi-parameter corrections are suggested. A table
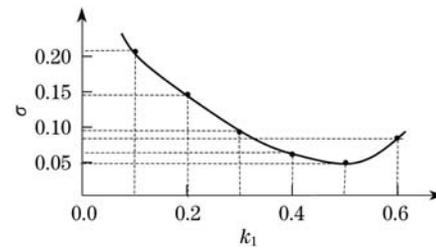

Fig. 3. Standard deviation σ of spectrometer's indicator versus k_1 for a fixed value of k_2 of 0.562.

synthesis of variants for designing multi-wavelength multiparameter spectrometers is carried out. It is shown that upon the use of Ångström's formula, the parameters k_1 and k_2 may be calculated separately for various aerosol models. The experimental research of developed laboratory pattern of three-wavelength two-parameter ozonometer shows the presence of an optimal pair of k_1 and k_2, which confirms the idea of two-parameter correction of aerosol error.

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