SOFTWARE PACKAGE FOR MODELING AND PROCESSING OF THE DATA ON REMOTE SENSING OF THE ATMOSPHERIC GAS COMPOSITION BY SPECTROPHOTOMETRIC METHODS

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The software package PARSEG for modeling and processing of the data on remote sensing of the atmospheric gas composition by spectrophotometric methods is described. Some methods for spectrometry of directly transmitted and scattered solar radiation are considered. Expressions are derived that can be used to determine the total content of atmospheric gases and errors of it reconstruction. The flowchart of the software package is also presented.

1. INTRODUCTION

Methods for determining the total content (TC) of atmospheric gases and aerosols based on the interpretation of the data of measurements of directly transmitted and scattered solar radiation as well as of radiation emitted by the atmosphere or underlying surface have long been in use for atmospheric studies.[1–6] They are characterized by high selectivity, accuracy, and sensitivity as well as advanced opto-electronic devices. The feasibility of obtaining the data on spatiotemporal variations of the atmospheric composition on a global scale has stimulated the development and wide application of the spectrophotometric sensing methods.

Based on the employed physical principles, the spectrophotometric methods can be subdivided into three classes: 1) methods for measuring the atmospheric transparency with the use of extra-atmospheric light sources, namely, the Sun, the Moon, or star; 2) methods for measuring the solar radiation scattered by the atmosphere or reflected by the underlying surface; 3) methods for measuring the thermal radiation emitted by the atmosphere or underlying surface. By the geometry of the experiment (position of a measuring device), they can be classified as: 1) ground-based, 2) airborne and balloonborne, and 3) satellite. By the number of spectral channels, measuring devices can be subdivided into single-channel, dual-channel, and multichannel ones. The measurable parameters are: 1) column (total) content (TC) of gases; 2) vertical profiles of gas concentration, temperature, and pressure; and, 3) aerosol and molecular components (their optical thicknesses and vertical profiles of their extinction coefficients).

An important stage of engineering design is preliminary modeling of the potentialities of measuring systems and choice of optimal spectral channels. In the present paper, the first version of the software package PARSEG for modeling of remote sensing of the atmospheric gases by passive methods is described. In this first version, we restricted ourselves to only two methods, namely, the method for measuring the transparency and the ground-based method for measuring the scattered solar radiation.[7]

2. PROBLEM FORMULATION

The radiative transfer equation provides a mathematical basis for modeling of sensing of atmospheric gases. Let us write down main relations for the above-enumerated methods.

a) Transparency method

Two-wavelength method. A recorded signal is related to the gas transmittance T_g by the expression

$$I_\lambda = J_{0\lambda}\, C_\lambda\, T_{AM}(\lambda,m) \int\limits_{\Delta\lambda} G(\lambda - \lambda') \times$$

$$\times\, T_g(\lambda', m)\, T_f(\lambda', m)\, d\lambda' , \qquad (1)$$

where $J_{0\lambda}$ is the solar constant, in $W/m^2{\cdot}\mu m{\cdot}sr$; C_λ is the instrument constant, $C_\lambda = A\Omega\, q_\lambda\, \eta_{\lambda'}(1 - q_l)$; A is the area of a receiving aperture; $\Omega = \pi\, \varphi^2/4$; φ is the total linear field-of-view angle of a receiving telescope; q_λ is the total efficiency of the entire optical train; η_λ is the quantum yield of a photodetector; g_l is the additional loss factor; $G(\lambda - \lambda')$ is the instrumental function of the device; $T_{AM}(\lambda,m)$ is the transmittance of the aerosol-gaseous atmosphere in the direction toward the Sun; $m = 1/\cos\theta$, θ is the zenith viewing angle; $T_g(\lambda,m)$ is the transmittance of the examined gas; and, $T_f(\lambda,m)$ is the transmittance of the foreign gases.

The expression $T_g(\lambda,m)$ can be written as

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$$T_g(\lambda, m) = \exp\left\{ - m\int\limits_0^H K(\lambda, z)\, p(z)\, dz \right\}, \tag{2}$$

where $p(z)$ is the concentration of the examined gas, $K(\lambda, z)$ is the coefficient of absorption by the gas of unit concentration, and H is the height of the atmosphere top.

To interpret the data of solar spectrum measurements, the total transmittance of gases is approximated by the product of transmittances of corresponding gaseous components, that is,

$$I_\lambda = J_{0\lambda}\, C_\lambda\, T_{AM}(\lambda, m)\, T_g(\lambda, m)\, T_f(\lambda, m) , \tag{3}$$

where T_g and T_f are the total transmittances of the examined and foreign gases.

In the two-wavelength approximation, the conditions $J_{0\lambda_1} = J_{0\lambda_2}$; $T_{AM}(\lambda_1, m) = T_{AM}(\lambda_2, m)$; $T_f(\lambda_1, m) = T_f(\lambda_2, m)$ are valid. Then the ratio of signals recorded at two wavelengths depends on the desired parameter $W = \int\limits_0^H p(z)\, dz$.

$$I_{\lambda_1} / I_{\lambda_2} = F(W, m) , \tag{4}$$

where W is the total gas content.

b) Method of scattering

In the UV and visible ranges, the spectra of most gases are nonselective for typical spectral resolution of 0.1–1 nm of spectrophotometers in the real atmosphere. Therefore, the instrumental function can be neglected. Then in the single scattering approximation the recorded signal has the form[8]

$$I_\lambda = J_{0\lambda}\, \tilde{C}_\lambda \exp[- K_\lambda\, W - \tau_{AMf}(\lambda,H)]\, J_s(\lambda,\theta) ; \tag{5}$$

$$J_s(\lambda,\theta) = \int\limits_0^H d_\lambda(z,\theta) \times$$

$$\times \exp\left\{ \int\limits_z^H \alpha_\Sigma(z',\lambda)[1 - B_\lambda(z,z',\theta)]\, dz' \right\} dz , \tag{6}$$

where K_λ is the absorption coefficient of the examined gas; $\tilde{C}_\lambda$ is the calibration factor; $\tau_{AMf}(\lambda, H)$ is the total optical density of aerosol, molecular component, and foreign gases; $d_\lambda(z, \theta)$ is the scattering coefficient of the aerosol and air molecules; α_Σ is the total extinction coefficient; $\alpha_\Sigma = \alpha_A + \alpha_M + \alpha_g + \alpha_f$; α_A and α_M are the volume aerosol extinction and molecular scattering coefficients, respectively; α_g and α_f are the volume absorption coefficients of the examined gas and foreign gases, respectively; $B_\lambda(z, z', \theta)$ is the function of the propagation path,

$$B_\lambda(z,z',\theta) = \frac{(R + z')\, n(z')}{\sqrt{(R + z')^2\, n_\lambda^2(z') - (R + z)^2\, n^2(z)\, \sin^2\theta}} ,$$

$n_\lambda(z)$ is the refractive index of the air; and, R is the Earth's radius.

For the two-wavelength method, the following expression was derived for the total gas content:

$$W = \frac{1}{\Delta K} \left\{ \ln\left[\frac{J_0^{1,2}\, C^{1,2}}{I^{1,2}}\right] - [\Delta\tau_A + \Delta\tau_M + \Delta\tau_f] + \ln J_s^{1,2} \right\}, \tag{7}$$

where

$\Delta K = K(\lambda_1) - K(\lambda_2)$;

$\Delta\tau_j = \tau_j(\lambda_1) - \tau_j(\lambda_2)$; j = A, M, f;

$J_0^{1,2} = \dfrac{J_0(\lambda_1)}{J_0(\lambda_2)}$; $I^{1,2} = I(\lambda_1) / I(\lambda_2)$; $J_s^{1,2} = \dfrac{J_s(\lambda_1)}{J_s(\lambda_2)}$.

The corresponding expressions can be easy obtained for four-wavelength method of determining the TC (see Refs. 4 and 8).

3. MODEL OF ATMOSPHERIC TRANSMITTANCE

To derive the expression analogous to Eq. (4) in the problem of determining the TC of the examined gas from the measured solar radiation spectra, the transmittance T_g is represented as

$$T_g = \exp \{- \beta_\lambda\, [\, mW]^{N_\lambda}\} , \tag{8}$$

where the adjustable parameters β_λ and N_λ are determined by fitting to laboratory measured or calculated data. In the present paper, the data calculated by the line-by-line method of calculation of the atmospheric transmittance were used as reference values of T_g. Calculations were done for various meteorological conditions and optical air masses. In this case, the meteorological conditions were varied to define the applicability limits of model (8) and air mass m was varied to determine the parameters β_λ and N_λ. In Table I, the values of the parameters β_λ and N_λ are given for two gases and two recording channels as an example.

TABLE I.

Gas	H_2O		CO_2
λ, μm	2.06	2.18	2.06
β_λ	0.93	0.74	8.4
N_λ	0.78	0.68	0.64

4. ERRORS IN DETERMINING THE TOTAL CONTENT OF GASES

a) Transparency method

Equation (4) for determining the total gas content W can be written in the following form:

$$F(W) = \frac{I_1}{I_2}\, b\, g\, h = \frac{T_g(\lambda_1, W)}{T_g(\lambda_2, W)}\,, \tag{9}$$

where

$$b = \frac{C_2}{C_1}\,;\quad g = T_{AM}(\lambda_2)/T_{AM}(\lambda_1)\,;\; h = T_f(\lambda_2)/T_f(\lambda_1)\,.$$

The parameters b, g, and h are often set equal to unity to determine the TC of the gas. This introduces the systematic error. Invoking model representations of b, g, and h, we may reduce this error. However, it cannot be eliminated completely.

We now estimate the total error in determining W for model (8) of the transmittance T_g. Let $\delta_{\beta_1} = \delta_{\beta_2} = \delta_\beta$ be the relative error in determining the parameters β_1 and β_2, $\delta_{N_1} = \delta_{N_2} = \delta_N$ be the relative error in determining the parameters N_1 and N_2, $\Delta T_g(\lambda_1) = \Delta T_g(\lambda_2) = \Delta T_g$ be the error of the transmittance model,

$$A = N_1\, \beta_1\, a^{N_1} - N_2\, \beta_2\, a^{N_2}\,;\quad a = m\, W\,; \tag{10}$$

$$P = A \ln a\,; \tag{11}$$

$$R^2 = \beta_1^2 a^{2N_1} + \beta_2^2 a^{2N_2}\,; \tag{12}$$

$$V^2 = T_g^{-2}(\lambda_1) + T_g^{-2}(\lambda_2)\,; \tag{13}$$

$$\gamma_i^2 = \frac{1}{\Delta t\, f\, I_i^2}\{\delta^2\,(I_i + I_b)^2 + NEP^2\, \eta^2\, f\} \tag{14}$$

be the signal recording error, $i = 1, 2$, Δt be the time of signal accumulation, f be the sampling frequency, NEP be the equivalent noise power of a detector, δ be the relative error in measuring the signal, and I_b be the background signal.

The formula for the relative error in determining W has the form

$$\delta_W = \frac{1}{A}\{\gamma_1^2 + \gamma_2^2 + \Delta b^2 + \Delta g^2 + \Delta h^2 + \delta_\beta^2 R^2 + \delta_N^2 P^2 + \Delta T_g^2 V^2\}^{1/2}. \tag{15}$$

Here, the first two terms represent the random errors in measuring signals and Δb^2, Δg^2, and Δh^2 specify the errors of model interpretation of data.

b) Method of scattering

The model of the data interpretation in the single scattering approximation used in this method is much more complicated than that in the transparency method. In this connection, we abandoned the analytical formulas for the error in the form of Eqs. (10)–(15).

The total error in determining the TC of the gas was determined from the following formulas[8]:

$$\delta_W = \left\{\sum_{i=1}^{n} \delta_W^2(i)\right\}^{1/2},\quad \delta_W(i) = \frac{\Delta W_i}{W_i}\,, \tag{16}$$

where $\delta_W(i)$ is the relative error in determining the TC due to error Δy_i in determining the ith argument of the function $W(y_1, \dots, y_n)$

$$\Delta W_i = W(y_1, \dots, y_i + \Delta y_i, y_{i+1}, \dots, y_n) - W(y_1, \dots, y_i, y_{i+1}, \dots, y_n), \tag{17}$$

n is the number of arguments whose errors are considered. Thus, the error is calculated by variation of all the arguments specified with errors. Let us list all error sources. Among them are the relative error of assignment of the absorption coefficient of the examined gas, δK_g; the relative error in measuring the signal ratio for two wavelengths, $\delta I^{1,2}$; the relative error of assignment of the solar constant ratio, $\delta J_0^{1,2}$; the absolute error in determining the solar zenith angle, $\Delta\theta$; the relative error of assignment of the optical thicknesses of aerosol, molecular scattering, and foreign gases, $\Delta\tau_{AMf}$; and, the absolute error in the calibration of the spectrophotometer according to wavelengths, $\Delta\lambda$.

5. SOFTWARE PACKAGE

The flowchart of the software package PARSEG (Passive Remote Sensing of Atmospheric Gases) is shown in Fig. 1. It comprises four blocks: 1) input data, 2) modes of operation, 3) archive, and 4) output data with a control block (“enclosureB). The block of the input data specifies 1) parameters of the measuring system (in the regime of modeling), 2) errors of assigning these parameters; 3) serial number of the examined gas, and 4) method of sensing. The software package can operate in regimes of modeling and real data processing. The archive METEO comprises information on vertical distribution of the temperature, pressure, and concentration of 11 gases (H_2O, CO_2, O_3, N_2O, CO, CH_4, NO, SO_2, NO_2, NH_3, and HNO_3) for five models of the atmosphere[9,10] for the tropics, mid-latitudes in summer (winter), and polar latitudes in summer (winter). It also comprises information about the optical parameters of the aerosol[11] (extinction and scattering coefficients), spectral dependence of the solar constant,[12] coefficients of absorption of the above-enumerated gases,[13–16] and models of the atmospheric transmittance.

The output parameters of the software package are the total content of the examined gas and the errors of its determination (in the regime of data processing) or optimal pairs of wavelengths and predicted errors of determination of the TC of gases (in the regime of modeling).

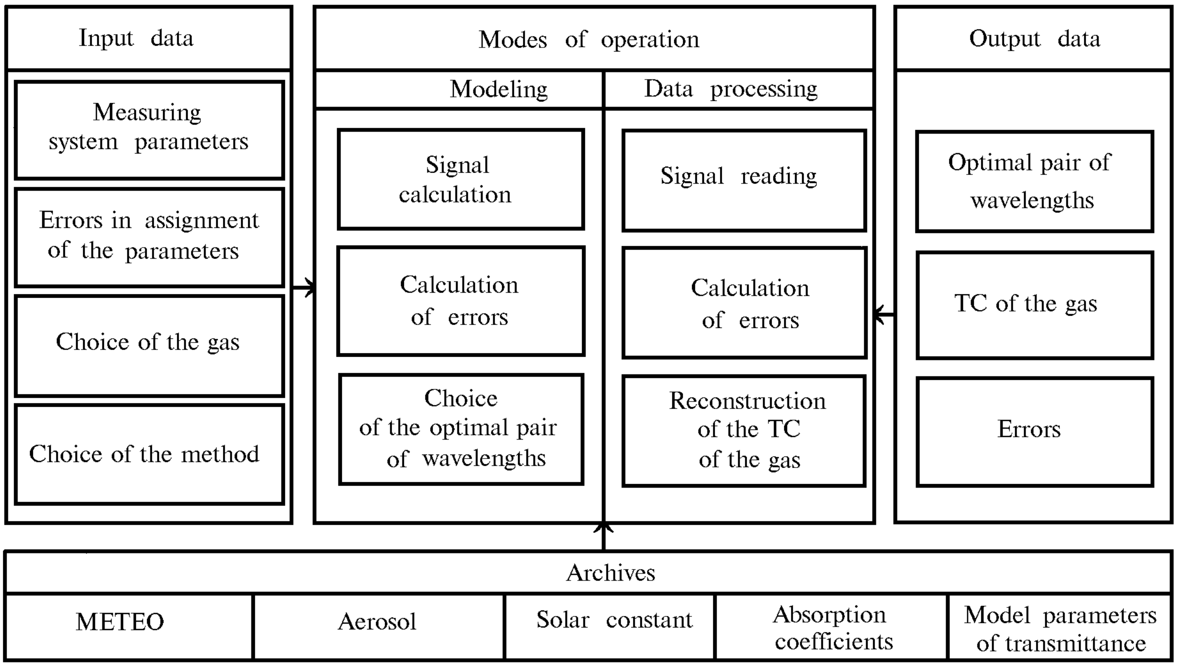

FIG. 1.

The software package envisages display of the input data and calculated results on a screen in tabular or graphics mode as well as their printing.

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