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Spherical Radiative Transfer Model with Computation of Layer Air Mass Factors and Some of Its Applications

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Abstract—A radiative transfer model was designed for use in inverse problems of atmospheric optics. The model calculates intensities and their derivatives with respect to absorption. In other notations, these derivatives are known as weighting functions or layer air mass factors. Multiple scattering radiation in the model is evaluated by the Monte Carlo method. Radiative transfer is simulated for a spherical shell atmosphere taking into account polarization, Rayleigh and aerosol scattering, gas and aerosol absorption, and Lambert surface albedo. The speed of intensity computations accurate to 1% is approximately the same as in other authors' pseudospherical models used for comparison. The time required for simultaneous computation of intensities and their derivatives is only 1.2–1.8 times as much as the time required for the computation of intensities alone. The model was compared with other spherical and pseudospherical models for geometries in which the sphericity of the atmosphere is important: twilight observations from the ground and limb scatter observations from space. The layer air mass factors calculated by different models were also compared. The influence of approximate (single scattering) computation of weighting functions on the accuracy of ozone profile retrievals was investigated for the Umkehr method used as an example. It was shown that the single scattering approximation gives additional large retrieval errors.

INTRODUCTION

Passive remote sensing in the UV and visible spectral ranges is used to determine the gas composition and aerosol characteristics of the atmosphere from the ground, satellites, and aircraft. Remote sensing based on simpler schemes (such as ozone, nitrogen dioxide, and aerosol retrieval from direct sunlight measurements with ground-based ([1–7], etc.) and satellite photometers (SAM, SAGE, SAGE II [8], SMF-2 [9]), zenith sky observations for ozone content determination ([1, 10, 11], etc.), nadir sounding of ozone from satellites (the instruments TOMS, SBUV, SBUV/2 [12], BUFS [13])) have promoted the development of more advanced measurement models and have provided a better understanding of the approaches to the solution of inverse problems. On the one hand, this resulted in the transition from multiwave to spectral sounding techniques for the atmosphere (Ozone-M/Mir [14], GOME, [15], and subsequent instruments), which made it possible to increase the number of observed gases due to routine or occasional measurements of O_2, O_4, NO, NO_3, OClO, ClO, BrO, IO, HCHO, SO_2, H_2O, HNO_3, HO_2, and $ClONO_2$ contents. On the other hand, limb-viewing geometry (more difficult to interpret) has been used as a major or additional observation geometry (the instruments OSIRIS [16], SAGE III [17], SCIAMACHY [18], GOMOS [19], OMPS [20]). This allows one to increase the coverage of satellite measurements, while preserving the high high-altitude resolution typical of direct sunlight observations, and subsequently pass to solving two- and three-dimensional tomography problems. In ground-based optical sounding, the interest of researchers has also shifted toward spectral techniques and more informative geometry—twilight observations. Twilight measurements make it possible to enhance the sensitivity of optical sounding and, in some cases, to determine not only the total content but also the vertical distribution of atmospheric constituents ([21–25], etc.).

The model of optical measurements is based on the theory of radiation transfer in the atmosphere. The problem of simulating spectral measurements required the development of efficient methods for calculating scattered radiation for large arrays of slightly differing wavelengths. In most cases, this is associated with bulky computations for small variations in the parameters of the atmospheric state, which can be effectively implemented through the calculation of radiative transfer characteristics for a single wavelength—the linearization point for the radiative transfer equation—and the derivatives of these characteristics with respect to a varying parameter of the atmospheric state. The radiative transfer characteristics and, simultaneously, their derivatives with respect to optical parameters are also required for solving inverse problems in atmospheric optics. The derivatives calculated are used to linearize the transfer operator, followed by the consideration of a linear measurement scheme, or they are used in iterative algorithms for solving an inverse problem. For this reason, a radiative transfer model designed for remote sensing must not only compute the radiative transfer characteristics but also involve an efficient algorithm for computing their derivatives with respect to the parameters of the atmospheric state. An accurate interpretation of the most informative limb scattered and twilight measurements must be based on a model with a spherical atmosphere.

In the foreign literature dealing with inverse problems in atmospheric optics, the derivatives with respect to optical characteristics are frequently referred to as weighting functions, following Rodgers' terminology [26]. We also consider the concept of the effective air mass factor of an atmospheric layer, which is related to the derivative. Introduced for scattered radiation, the concept of the effective air mass factor of a layer has an illustrative physical meaning similar to its counterpart for direct radiation.

A general approach to the design of radiative transfer models with computation of weighting functions is based on perturbation theory and was first proposed in [27]. The evaluation of derivatives by the Monte Carlo method was originated in [28]. The first efficient algorithm for calculating weighting functions for radiation transfer was first designed for the model described in [29]. That algorithm was implemented in spherical geometry for computing the derivatives with respect to the aerosol scattering factor in double local Monte Carlo estimation. The idea of [29] on the computation of derivatives was further developed in [57]. Other models with computation of weighting functions have been developed in recent years: the GOMETRAN finite-difference model [30], the LIDORT discrete ordinate model [31], the LIRA Gauss–Seidel iteration model [32], and the CDI model based on a combined integro-differential approach [33; A. Rozanov, personal communication]. These models do not take into account polarization and were designed for a plane-parallel atmosphere, but, as a rule, they have pseudospherical modifications. In pseudospherical models, only single scattering is treated in spherical geometry, while scattering of a higher order is treated for a plane-parallel atmosphere. Some questions related to the linearization of the transfer equation with respect to aerosol characteristics with allowance for multiple scattering were also considered in [34–36].

A radiative transfer model designed for use in inverse problems of atmospheric optics is presented in this paper. The principles of the model construction are described, and the results of its comparison with other radiative transfer models are briefly outlined. The possibility of improving retrieval results by replacing weighting functions computed in the single scattering approximation with weighting functions taking into account multiple scattering is considered.

METHOD FOR CALCULATING DERIVATIVES, WEIGHTING FUNCTIONS, AND LAYER AIR MASS FACTORS

The application of the Monte Carlo method to atmospheric optics is based on the fact that light propagation can be treated as a random Markov chain of collisions between photons and atmospheric molecules, which result in either scattering or absorption of photons. The Monte Carlo method simulates random paths of this chain on a computer and calculates its characteristics, which are estimates of the desired quantities [29, 37–39]. Importantly, a probability estimate of the accuracy of the results obtained can be simultaneously calculated in Monte Carlo simulation. Specialized simulation techniques have been developed to minimize CPU time for various observation conditions. These techniques use modified algorithms simulating photon passage through the atmosphere and take into account the symmetry of problems.

Let us consider the theoretical substantiation of the method for calculating derivatives used in the model under consideration. Light propagation through the atmosphere is described by an integral transfer equation for the photon collision density $\rho = \rho(\mathbf{x})$ in the phase space X:

$$\rho = \mathbf{K}\rho + \psi, \tag{1}$$

where $\psi = \psi(\mathbf{x})$ is the density of initial collisions, $\mathbf{x} = (r, \omega) \in X$, r is the radius vector of a point, ω is a unit direction vector, and $\mathbf{K}$ is an integral operator whose kernel $k(\mathbf{x}', \mathbf{x})$ is the transition density of a photon from $\mathbf{x}'$ to $\mathbf{x}$:

$$\int_X k(\mathbf{x}', \mathbf{x}) d\mathbf{x} = \frac{\sigma_S(r')}{\sigma(r')} \le 1.$$

When the photon does not reach the Earth's surface, the kernel is given by

$$K(\mathbf{x}', \mathbf{x}) = \frac{\sigma_S(r')}{\sigma(r')} \frac{g(\mu, r') e^{-\tau(r', r)} \sigma(r)}{2\pi \|r - r'\|^2} \delta(\omega - s),$$
$$\mu = (s, \omega'), \quad s = \frac{1}{\|r - r'\|}(r - r'), \tag{2}$$