1. Introduction

The accuracy of determination of gas and aerosol constituents in the Earth's atmosphere by optical remote sensing depends on the design of an experiment, measurement errors, the retrieval algorithm, and the accuracy of the forward model; the latter depends strongly on the choice of a radiative transfer model. Adequate description of the radiation field in the atmosphere requires a solution of the transfer equation for the unknown vector of the Stokes parameters; the latter characterize the radiance intensity and the degree, plane, and ellipticity of the radiance polarization [1]. A simplified treatment of light as being characterized by the scalar radiance intensity only has a limited range of applicability. Indeed, the light that comes from the Sun being originally unpolarized is then scattered by air molecules or aerosol particles and becomes partially polarized. It produces different source functions of the components in two perpendicular polarization directions for the second-order scattering, which the scalar theory neglects. Several studies, beginning from [1] as well as more recent papers [2–8], compared solutions of the vector and the scalar radiative transfer equations for various observational geometries. They showed that scalar calculations of the radiance intensity are in error by up to 5–10% for many cases, depending on aerosol loading and surface albedo.

To escape the above-mentioned error of scalar modeling, recent, more precise versions of retrieval algorithms of ground-based and satellite experiments apply vector models even if they exploit polarization non-sensitive instruments such as Dobson [9], TOMS [10] and OMI [11]. Several satellite instruments are polarization-sensitive, because use the grating spectrometers, which have different efficiency to light polarized parallel and perpendicular to the grating grooves. In this case, measured quantity is a composition of the intensity and the degree of polarization and, therefore, requires correction based on vector radiative transfer modeling together with broadband polarization measurements, if it is available, (GOME [12] and SCIAMACHY [13]) or alone (OSIRIS [7] and GOMOS [14]).

To extend information on properties of the atmosphere and surface, which may be gathered from scattered solar radiation, measurements of the polarization in addition to the intensity are performed. Thus, the satellite instruments POLDER and POLDER-2 have begun to provide global systematic measurements of polarization of backscattered radiation [15,16]. Similar instruments with improved characteristics, PARASOL scheduled for lunch in 2004 [17] and APS [18,19], were proposed to continue the polarimetric measurements of the backscattered radiation. A new instrument, DARE [20], which can measure polarization not only in several nadir but also in limb directions, is designed. Furthermore, recent studies have found new opportunities to derive more detailed information on the atmosphere based on polarimetric observations [21–24]. Retrieval of atmosphere and land properties from this polarized radiance requires the vector radiative transfer model.

Several radiative transfer models including the polarization were developed [4,10,11,13,15,24–26]. Few of them can also accurately treat sphericity of an atmosphere. That are a family of Monte Carlo models of Mikhailov et al. [27,2,28], a model of Gauss–Seidel iterations [3], a Monte Carlo model SIRO [7], an iterative model of Odin/OSIRIS project [29], and Monte Carlo model MCC++ [30]. However, experience of treatment of optical remote sensing data manifests that calculation of Stokes vector in itself is not enough for efficient application of radiative model, because other characteristics of radiance requiring extensive calculation are also used in remote sensing [31,32]. There are three typical problems in remote sensing, which requires additional characteristics of radiance field.

First, modern instruments for determination of the gas contents are spectral ones, and therefore forward model of experiment is in need of calculations for large arrays of slightly differing wavelengths. To accelerate spectral calculations, instead of multiple runs of a radiative model one can estimate radiance $i(\lambda)$ for a set of wavelengths $\lambda = \lambda_0 + \Delta\lambda$ around some wavelength λ_0 using approximate expansion

$$i(\lambda) \approx i(\lambda_0) + \frac{\partial i(\lambda_0)}{\partial \lambda}\Delta\lambda \quad \text{for } \Delta\lambda \to 0,\ \ \lambda = \lambda_0 + \Delta\lambda, \tag{1}$$

if radiative model provides not only radiance $i(\lambda_0)$ but also derivative of radiance with respect to wavelength $\partial i(\lambda_0)/\partial\lambda$.

The second problem in remote sensing, which requires additional characteristics of radiance, is analysis of errors of retrieval of atmosphere and surface properties $\mathbf{x} = (x_1\ x_2\ \ldots\ x_n)$. Routine error propagation analysis, relating to remote sensing measurement i_m,

$$i_m = i(\mathbf{x}) + \boldsymbol{\gamma}, \tag{2}$$

distorted by noise $\boldsymbol{\gamma}$, is based on linearization of both a forward model $i(\cdot)$ and a retrieval operator $\mathbf{R}(\cdot)$ near the retrieved vector of properties $\hat{\mathbf{x}} = \mathbf{R}(i_m)$ [33]. Thus, it needs a radiative model capable to calculate derivatives $\partial i(\hat{\mathbf{x}})/\partial x_j$ with respect to retrieved properties $\mathbf{x}$.

Third, for interpretation of remote sensing measurement i_m (2) it is most convenient to linearize forward model $i(\cdot)$,

$$i(\mathbf{x}) \approx i(\mathbf{x}_0) + \sum_j \frac{\partial i(\mathbf{x}_0)}{\partial x_j}\Delta x_j \quad \text{for } \Delta x_j \to 0,\ \ x_j = x_{0_j} + \Delta x_j \tag{3}$$

near some a priori vector $\mathbf{x}_0 = (x_{0_1}\ x_{0_2}\ \ldots\ x_{0_n})$ and to solve the raising linear retrieval problem [33,34]. There are also alternative iterative algorithms for solution of non-linear problem (2), such as Newton, Gauss–Newton, Levenberg-Marquart et al. [33]. However, all of them use the same radiance derivatives for solution.

Note that derivatives with respect to wavelength λ needed for forward simulation of spectral measurements by formula (1) can be calculated using derivatives with respect to $\mathbf{x}$:

$$\frac{\partial i(\lambda_0)}{\partial \lambda} = \sum_j \frac{\partial i(\mathbf{x}_0)}{\partial x_j}\frac{\partial x_j(\lambda_0)}{\partial \lambda}, \quad \mathbf{x}_0 = \mathbf{x}(\lambda_0). \tag{4}$$

Therefore, for application to remote sensing a model is needed which supplies radiance derivatives with respect to atmospheric and surface properties in addition to radiance. A model, which solves equation in derivatives of radiance simultaneously with transfer equation in radiance, is termed linearized. Gained experience proved that a simultaneous solution of these equations can be greatly faster than the traditional algorithm of the finite difference approach based on multiple runs of a radiative model with perturbed optical properties (on the traditional algorithm see, for example, [29]).

Five linearized radiative transfer models have been developed, two of them are Monte Carlo models and three are non-statistical ones. Marchuk et al. [2] first proposed a general approach to linearization of Monte Carlo radiative transfer models by differentiation of the Monte Carlo weighted estimation of the intensity. It was applied to a double local estimation method for calculation of derivatives with respect to the aerosol scattering coefficient and was implemented in a scalar version of a spherical Monte Carlo model [2]. A Monte Carlo estimation of derivatives with respect to extinction (gas concentration) in scalar model was deduced in paper [35]. This algorithm was used for linearization of the model MCC++ simulating transfer in a spherical-shell atmosphere.

The first non-statistical linearized model was the radiative model GOMETRAN/CPI of Rozanov et al. [32,36], based on the finite difference method. Later, the theory of linearization was extended to the discrete ordinate model LIDORT of Spurr et al. [37] and the Gauss–Seidel model LIRA of Landgraf et al. [38]. A study [38] pointed out that linearization of all three methods can be carried out based on a general approach proposed by Marchuk [31] and Box [39] to evaluation of derivatives by the perturbation theory. All three models may calculate derivatives with respect to extinction (or gas concentration) in the scalar case and use pseudospherical approximation of geometry of an atmosphere. The LIRA model estimates also derivatives with respect to surface properties [40]. A plane-parallel version of the LIRA model was the only model extended to the vector model [41].

This paper presents linearization of the Monte Carlo MCC++ model in the vector case with respect to atmosphere extinction (or with respect to gas concentrations). The model solves the transfer equation in spherically symmetrical (spherical shell) atmosphere taking into account gases, aerosol and molecular scattering. Section 2 reminds basic conceptions related to polarization and Monte Carlo simulation. Monte Carlo estimation of the derivative of the Stokes vector of radiance is deduced in Section 3. Section 4 presents examples of calculations of derivatives, and Section 5 overviews validation of the MCC++ model.

2. Basic conceptions

2.1. Characterization of polarized radiance

A vector of four parameters introduced by Stokes can characterize the polarized light in an atmosphere [1]

$$\mathbf{I} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}. \tag{5}$$

The first element I of the Stokes vector describes the intensity measured by a polarization non-sensitive instrument, and the others define the plane and ellipticity of polarization. The elements of a Stokes vector are constrained by inequality

$$I^2 \geqslant Q^2 + U^2 + V^2. \tag{6}$$

The effect of a rotation of the axes through an angle i is to subject to the linear transformation $\mathbf{I}' = \mathbf{L}(i)\mathbf{I}$ of the Stokes vector $\mathbf{I}$ with the rotation matrix [28]

$$\mathbf{L}(i) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2i & \sin 2i & 0 \\ 0 & -\sin 2i & \cos 2i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{7}$$

So the Stokes parameters I, V, and a composition $\sqrt{Q^2 + U^2}$ are invariant under a rotation of axes, while the elements Q and U are defined with respect to a certain reference plane.