Linearization of vector radiative transfer with respect to aerosol properties and its use in satellite remote sensing

Otto P. Hasekamp and Jochen Landgraf
SRON National Institute for Space Research, Utrecht, Netherlands

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[1] We present a plane parallel radiative transfer model for polarized light that provides the intensity vector field as well as analytical derivatives of the four Stokes parameters at the top of the atmosphere with respect to physical properties of spherical aerosols. The linearization consists of two steps: (1) calculation of the derivatives of the four Stokes parameters at the top of the atmosphere with respect to scattering coefficient, extinction coefficient, and expansion coefficients of the scattering phase matrix. These derivatives are calculated employing the forward-adjoint perturbation theory. General expressions are presented that can be applied for the linearization of any vector radiative transfer model that calculates the internal radiation field in the model atmosphere. (2) The second step is calculation of the derivatives of the scattering coefficient, extinction coefficient, and the expansion coefficients of the scattering phase matrix, with respect to the real and imaginary part of the refractive index, and parameters describing the size distribution (e.g., effective radius, effective variance). These derivatives are analytically calculated following Mie theory. The use of the developed linearized radiative transfer model for the retrieval of aerosol properties is demonstrated using synthetic measurements of intensity and polarization of the Global Ozone Monitoring Experiment-2 (GOME-2). Here it is shown that an iterative retrieval approach based on the linearized radiative transfer model is suited to solve the nonlinear aerosol retrieval problem, and additionally allows a solid error analysis.


1. Introduction

[2] Tropospheric aerosols are believed to have a significant effect on the Earth's climate. The direct effect of aerosols on climate is caused by scattering and absorption of solar radiation (cooling effect), and absorption of long-wave radiation emitted by the Earth (warming effect). Aerosols also indirectly affect the climate by changing the microphysical properties of clouds. The magnitude and even the sign of the total aerosol effect are unknown and represent some of the largest uncertainties in climate research. To reduce these uncertainties accurate measurements are needed of various aerosol properties, such as size distribution, refractive index, and optical thickness. The only realistic way to obtain these measurements at a global scale is by means of satellite remote sensing.

[3] Satellite instruments that may be used for tropospheric aerosol retrieval can roughly be divided in four categories: (1) instruments that perform multispectral measurements of the intensity in one viewing direction. Among these instruments are the Advanced Very High Resolution Radiometer (AVHRR), the Total Ozone Mapping Spectrometer (TOMS), the Moderate Resolution Imaging Spectroradiometer (MODIS) and the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY). (2) Instruments that perform multispectral measurements of the intensity and observe the same ground pixel under different viewing geometries. Among these instruments are the Multiangle Imaging Spectroradiometer (MISR), the Along Track Scanning Radiometer-2 (ATSR-2), and the Advanced Along Track Scanning Radiometer (AATSR). (3) Instruments that perform multispectral measurements of the intensity and the polarization in one viewing direction. The Global Ozone Monitoring Experiment-2 (GOME-2) will be the first instrument in this category. (4) Instruments that perform multispectral measurements of the intensity and the polarization and observe the same ground pixel under different viewing geometries. Among these instruments are the Polarization and Directionality of the Earth’s Reflectances (POLDER)-1 and -2, which both were active for about 8 months in 1996/97 and 2003, respectively.

[4] Aerosol retrievals from radiance only measurements suffer from a severe uniqueness problem, because several combinations of aerosol parameters fit the measured radiance spectrum within the measurement noise [Mishchenko and Travis, 1997a, 1997b; Chowdhary et al., 2001, 2002]. Thus, the number of aerosol parameters that can be retrieved from the measurement is limited. For example, MODIS
retrievals have difficulties in distinguishing between mono-modal and bimodal size distributions, despite the broad spectral range of MODIS [Tanré et al., 1997]. The limited information content of intensity measurements with respect to aerosol properties means that many aerosol properties need to be assumed a priori in the retrieval. Obviously, errors in the a priori assumptions will result in errors in the retrieved parameters. The uniqueness problem of intensity only retrievals can be significantly reduced if polarization measurements are additionally included in the retrieval [Mishchenko and Travis, 1997a, 1997b; Chowdhary et al., 2001, 2002].

The retrieval of aerosol parameters from satellite measurements requires a forward model \( F \) that describes how the measured data depend on the aerosol parameters:

\[
y = F(x) + \epsilon_y.
\]

Here \( y \) is the measurement vector containing the measured data, e.g., intensity and/or polarization measurements at different wavelengths and/or different viewing angles, and \( \epsilon_y \) is the corresponding error vector. \( x \) is the state vector containing the aerosol parameters to be retrieved, e.g., the refractive index, aerosol loading, and parameters describing the size distribution. The forward model consists of two parts. The first part relates the physical aerosol properties (size distribution, refractive index) to their optical properties (scattering and extinction coefficient, phase matrix). This relation can be described by Mie theory for spherical particles [van de Hulst, 1957] or alternative theories for particles with other shapes [Wiscombe and Grans, 1988; Koepke and Hess, 1988; Mishchenko and Travis, 1994; Mishchenko et al., 1995]. The second part of the forward model is an atmospheric radiative transfer model that simulates the intensity vector at the top of the atmosphere for given optical input parameters.

The task of an inversion algorithm for aerosol retrieval is to determine the set of aerosol parameters \( \hat{x} \) for which a certain cost function is minimized at least contains the difference between forward model and measurement in some metric. Since the forward model is not linear in \( \hat{x} \) this minimum has to be found iteratively. By far most methods to solve nonlinear inverse problems replace the forward model \( F \) in (1) by its linear approximation

\[
y \approx F(\hat{x}_{\text{itr}}) + K \Delta x + \epsilon_y, \tag{2}
\]

for each iteration step. Here \( \Delta x = x - \hat{x}_{\text{itr}} \) where \( \hat{x}_{\text{itr}} \) is the state vector for the current iteration step, and \( K \) is the Jacobian matrix containing the derivatives of the forward model with respect to the elements of \( x \), where element \( K_{ij} \) of \( K \) is defined by

\[
K_{ij} = \frac{\partial F_i}{\partial x_j}(\hat{x}_{\text{itr}}). \tag{3}
\]

The inversion of (2) yields the state vector for the next iteration step, where the iteration is started by a certain first guess state vector. Once the minimum has been reached the Jacobian matrix \( K \) can be used to calculate the mapping of the measurement errors \( \epsilon_y \) to errors on the retrieved aerosol parameters \( \epsilon_x \), in linear approximation. Thus, the Jacobian matrix \( K \) plays an important role in the retrieval process, both for finding the minimum of the inversion problem and for a solid error analysis. Therefore, in the most general case of aerosol retrieval from intensity and polarization measurements, a linearized vector radiative transfer is needed that simulates the intensity vector at the top of the model atmosphere and additionally calculates the derivatives of the Stokes parameters with respect to the aerosol properties to be retrieved.

For scalar radiative transfer a general linearization approach was proposed by Marchuk [1964], who employed the forward-adjoint perturbation theory approach, known from neutron transport theory [see, e.g., Bell and Glasstone, 1970], to atmospheric scalar radiative transfer. This approach has been used, among others, by Ustinov [1991], Rozanov et al. [1998], and Landgraf et al. [2002] for the linearization of scalar radiative transfer with respect to atmospheric absorption properties, by Landgraf et al. [2001] for the linearization with respect to surface properties, and, for example, by Ustinov [1992] and Sendra and Box [2000] for the linearization with respect to atmospheric scattering properties. Another approach for the linearization of scalar radiative transfer has been followed by Spurr et al. [2001], who developed an analytical linearization with respect to absorption and scattering properties for the discrete ordinate method for scalar radiative transfer [Chandrasekhar, 1960; Stamnes et al., 1988]. For plane parallel vector radiative transfer an analytical linearization with respect to atmospheric absorption properties has been developed by Hasekamp and Landgraf [2002], who extended the forward-adjoint perturbation theory to include polarization. This approach has been used by Walter et al. [2004] for the linearization of radiative transfer with respect to atmospheric absorption properties in a pseudospherical atmosphere. Recently, Postylyakov [2004] achieved a linearization of vector radiative transfer with respect to atmospheric absorption properties for a full spherical geometry.

An analytical linearization of vector radiative transfer with respect to atmospheric scattering properties has not been achieved yet, which means that currently no linearized vector radiative transfer model exists that is suitable for aerosol retrieval from satellite measurements of intensity and polarization. For all vector radiative transfer models developed so far the Jacobian matrix needed in (2) must be estimated by finite differencing. Here two independent radiative transfer calculations are needed to approximate the derivative of the forward model with respect to an element \( x_k \) of the state vector \( x \): one for an unperturbed atmosphere and the other for an atmosphere for which \( x_k \) has been perturbed by a small amount. Depending on the number of fit parameters, such a method may require a large computational effort, because for each element of the state vector a separate radiative transfer calculation has to be performed. In addition to the time consuming nature of the finite difference approach the accuracy depends in a rather ad hoc manner on the magnitude of the numerical perturbation. Thus, aerosol retrievals from intensity and polarization measurements will greatly benefit from an analytical linearization of vector radiative transfer with respect to aerosol properties.
The aim of this paper is to develop an analytical linearization of vector radiative transfer with respect to physical aerosol properties. The linearization will be performed in two steps. In the first step we calculate the derivatives of the Stokes parameters with respect to the optical input parameters of the radiative transfer equation employing the forward adjoint perturbation theory. In the second step we calculate the derivatives of the optical input parameters of the radiative transfer equation with respect to physical aerosol parameters (refractive index, parameters describing the size distribution). Here we assume spherical aerosols which allows the use of Mie theory to relate the optical properties of aerosols to their physical properties. The linearization of Mie theory can be obtained in an analytical way. In section 2 the radiative transfer model is described whereas section 3 summarizes the Mie calculations. The linearization of the radiative transfer model and the Mie calculations will be described in section 4. In section 5 we discuss the numerical implementation of the linearization approach and show results for derivatives of the intensity and polarization at the top of the atmosphere with respect to several aerosol parameters, relevant for aerosol retrieval. Finally, in section 6 we demonstrate the use of the linearized radiative transfer model for the retrieval of column integrated aerosol properties using synthetic measurements of intensity and polarization of GOME-2. Here we consider the retrieval of total aerosol loading, real refractive index, and parameters describing the aerosol size distribution. For this particular retrieval problem we study the use of an iterative inversion approach based on linearized radiative transfer, and additionally we study the validity of an error analysis performed using the linear approximation.

2. Radiative Transfer Model

The radiance and state of polarization of light at a given wavelength can be described by an intensity vector $\mathbf{I}$ which has the Stokes parameters as its components [see, e.g., Chandrasekhar, 1960]:

$$\mathbf{I} = [I, Q, U, V]^T,$$

(4)

where $T$ indicates the transposed vector, and the Stokes parameters are defined with respect to a certain reference plane. The angular dependence of single scattering of polarized light can be described by means of the scattering phase matrix $\mathbf{P}$. We will restrict ourselves to scattering phase matrices of the form

$$\mathbf{P}(\theta) = \begin{pmatrix} p_1(0) & p_2(0) & 0 & 0 \\ p_3(0) & p_2(0) & 0 & 0 \\ 0 & 0 & p_3(0) & p_6(0) \\ 0 & 0 & -p_6(0) & p_4(0) \end{pmatrix},$$

(5)

where $p_1, p_2, \ldots, p_6$ are arbitrary functions of scattering angle $\theta$ and the scattering plane is the plane of reference. This type of scattering matrix is valid for [see, e.g., van de Hulst, 1957] (1) scattering by an assembly of randomly oriented particles each having a plane of symmetry, (2) scattering by an assembly containing particles and their mirror particles in equal numbers and with random orientations, (3) Rayleigh scattering with or without depolarization effects.

To discuss the single scattering properties of aerosol particles we will use the scattering plane as the plane of reference. However, for the atmospheric radiative transfer calculations in this paper we will use the local meridian plane, defined as the plane going through the direction of propagation and the vertical direction, as reference plane.

We consider a plane-parallel, macroscopically isotropic atmosphere bounded below by a reflecting surface. Furthermore, we ignore inelastic scattering and thermal emission. The equation of transfer for polarized light is now given in its forward formulation by

$$\mathbf{L}_1 \mathbf{I} = \mathbf{S},$$

(6)

where the transport operator

$$\mathbf{L}_1 = \int_{4\pi} d\Omega \left\{ \left[ \mu \frac{\partial}{\partial \mu} + \beta' \right] b(\Omega - \Omega) \mathbf{F} - \frac{\beta'}{4\pi} \mathbf{Z}(z, \Omega, \Omega) \right\} \sigma,$$

(7)

is adopted from scalar radiative transfer [Marchuk, 1964; Box et al., 1988; Ustinov, 2001; Landgraf et al., 2002]. Here $z$ describes altitude, the direction $\Omega$ is given by ($\mu, \varphi$) where $\varphi$ is the azimuthal angle measured clockwise when looking downward and $\mu$ is the cosine of the zenith angle ($\mu < 0$ for downward directions and $\mu > 0$ for upward directions). Furthermore, $d\Omega = d\mu \, d\varphi$, $\mathbf{F}$ is the $4 \times 4$ unity matrix, $\beta'$ and $\beta''$ represent the extinction and scattering coefficients, respectively, $\Theta$ represents the Heaviside step function, and $\delta$ is the Dirac-delta function with $\delta(\Omega - \Omega) = \delta(\mu - \mu') \delta(\varphi - \varphi')$. The first term of the radiative transfer operator describes the extinction of light, whereas the second term represents scattering of light from direction $\Omega$ to $\Omega$ with the phase matrix $\mathbf{Z}(z, \Omega, \Omega)$, defined with respect to the local meridian plane. The last term on the right-hand side of (7) describes the surface reflection at the lower boundary of the atmosphere with reflection matrix $\mathbf{R}_o$. The right-hand side of (6) provides the source of light and can either be a volume source inside the atmosphere or a surface source chosen to reproduce the incident flux conditions at the boundaries of the atmosphere, or some combination of the two. In the UV and visible part of the spectrum the radiation source $\mathbf{S}$ is determined by the unpolarized sunlight that illuminates the top of the Earth atmosphere:

$$\mathbf{S}(z, \Omega) = \mu_o \delta(z - z_{top}) b(\Omega - \Omega_o) \mathbf{F}_o.$$  

(8)

Here $z_{top}$ is the height of the model atmosphere, $\Omega_o = (-\mu_o, \varphi_o)$ describes the geometry of the incoming solar beam (we define $\mu_o > 0$), and $\mathbf{F}_o$ is given by

$$\mathbf{F}_o = [F_o, 0, 0, 0]^T,$$

(9)

where $F_o$ is the solar flux per unit area perpendicular to the direction of the solar beam. Because the reflection of light at
the ground surface is already included in the radiative transfer operator (7) and the incoming solar beam is represented by the radiation source of (8), the intensity vector \( I \) is subject to homogeneous boundary conditions:

\[
I_{\text{top}}(\Omega) = [0, 0, 0, 0]^T \quad \text{for } \mu < 0
\]

\[
I(0, \Omega) = [0, 0, 0, 0]^T \quad \text{for } \mu > 0.
\]

In conjunction with these boundary conditions, the radiation source \( S \) can be interpreted as located at a vanishingly small distance below the upper boundary. Similarly, the surface reflection takes place at a vanishingly small distance above the lower boundary [see, e.g., Morse and Feshbach, 1953].

[14] In order to handle the integration over azimuth angle in (6) we use a decomposition of the radiative transfer equation into corresponding equations per Fourier component [Hovenier and van der Mee, 1983; de Haan et al., 1987]:

\[
L^m \mathbf{I}^m = \mathbf{S}^m,
\]

with

\[
\mathbf{L}^m = \int_0^1 d\mu \left\{ \left[ \mu \frac{\partial}{\partial \mu} + \beta^m(z) \right] \delta(\mu - \tilde{\mu}) \mathbf{E} - \frac{\beta^m(z)}{2} \mathbf{Z}^m(z, \tilde{\mu}, \mu) \\
- \delta(z) \Theta(\mu) |\mu| \mathbf{R}^m(\tilde{\mu}, \mu) \Theta(-\tilde{\mu}) |\tilde{\mu}| \right\} \cdot .
\]

[15] The corresponding Fourier expansion of the intensity vector is given by

\[
I(z, \Omega) = \sum_{m=0}^{\infty} (2 - \delta_{m0}) \left[ B^m(\psi_0 - \varphi) I^m(z, \mu) + B^{-m}(\psi_0 - \varphi) I^{-m}(z, \mu) \right] + B^{m}(\psi_0 - \varphi) I^{m}(z, \mu) \right),
\]

where \( \delta_{m0} \) is the Kronecker delta, and

\[
\begin{align*}
B^m(\varphi) &= \text{diag}[\cos m\varphi, \cos m\varphi, \sin m\varphi, \sin m\varphi] \\
B^{-m}(\varphi) &= \text{diag}[-\sin m\varphi, -\sin m\varphi, \cos m\varphi, \cos m\varphi].
\end{align*}
\]

[16] The Fourier coefficients of the intensity vector are given by

\[
I^m(z, \mu) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \ B^m(\psi_0 - \varphi) I(z, \Omega)
\]

\[
I^{-m}(z, \mu) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \ B^{-m}(\psi_0 - \varphi) I(z, \Omega).
\]

Similarly, a Fourier expansion of the radiation source \( S(z, \Omega) \) is obtained, with Fourier coefficients

\[
S^m(z, \mu) = \frac{1}{2\pi} \mu_o \delta(z - z_{\text{top}}) \delta(\mu_o + \mu) F_0
\]

\[
S^{-m}(z, \mu) = [0, 0, 0, 0]^T.
\]

From (10) and (17) it follows that \( I^{-m} = 0 \), so the Fourier expansion of the intensity vector contains terms of \( I^m \) only. [17] The Fourier expansion of the phase matrix is given by

\[
Z(z, \mu, \Omega) = \frac{1}{2} \sum_{m=0}^{\infty} (2 - \delta_{m0}) \left[ B^m(\tilde{\varphi} - \varphi) Z^m(z, \mu, \mu) (\mathbf{E} + \mathbf{A}) + \mathbf{B}^{-m}(\tilde{\varphi} - \varphi) Z^{-m}(z, \mu, \mu) (\mathbf{E} - \mathbf{A}) \right],
\]

where

\[
\mathbf{A} = \text{diag}[1, 1, -1, -1].
\]

[18] The \( m \)-th Fourier coefficient of the phase matrix can be calculated by

\[
Z^m(z, \mu, \mu) = (-1)^m \sum_{l=-m}^{m} P^l_m(-\mu) S^l(z) P^l_m(\tilde{\mu}),
\]

where \( L \) is a suitable truncation index [Ustinov, 1988] and \( P^l_m \) is the generalized spherical function matrix given by

\[
P^l_m(\mu) = \begin{pmatrix}
P^0_m(\mu) & 0 & 0 & 0 \\
0 & P^l_{m+1}(\mu) & P^l_{m-1}(\mu) & 0 \\
0 & P^l_{m+1}(\mu) & P^l_{m-1}(\mu) & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

where

\[
P^l_{m\pm} = \frac{1}{2} \left( P^l_{m+2} \pm P^l_{m-2} \right)
\]

and \( P^l_{m\pm}(\mu) \) are the generalized spherical functions [Gel’fand et al., 1963], which were introduced in atmospheric radiative transfer by Kašic’er and Ribarić [1959]. \( S^l \) is the expansion coefficient matrix having the form

\[
S^l = \begin{pmatrix}
\alpha^l_1 & \alpha^l_2 & 0 & 0 \\
\alpha^l_2 & \alpha^l_2 & 0 & 0 \\
0 & 0 & \alpha^l_3 & \alpha^l_3 \\
0 & 0 & -\alpha^l_3 & \alpha^l_3
\end{pmatrix},
\]

where the expansion coefficients follow from the scattering phase matrix \( \mathbf{P} \) in (5) [see, e.g., de Rooij and van der Stap, 1984]:

\[
\alpha^l_1 = \frac{2l + 1}{2} \int_{-1}^{1} P^l_{00}(\cos \theta) p_1(\theta) \ d(\cos \theta),
\]

\[
\alpha^l_2 = \frac{2l + 1}{2} \sqrt{\frac{(l - 2)!}{(l + 2)!}} \int_{-1}^{1} P^l_{22}(\cos \theta) \left[ p_2(\theta) + p_3(\theta) \right] \ d(\cos \theta).
\]
\[ \alpha_2^l - \alpha_3^l = -\frac{2l+1}{2} \left( \frac{(l-2)!}{(l+2)!} \right) \int_{-1}^{1} P_{l-2}^0(\cos\theta)(p_2(\theta) + p_3(\theta)) \cdot d(\cos\theta), \] \hspace{1cm} (26)

\[ \alpha_4^l = \frac{2l+1}{2} \int_{-1}^{1} P_{l,0}^0(\cos\theta)p_4(\theta) \cdot d(\cos\theta), \] \hspace{1cm} (27)

\[ \alpha_5^l = \frac{2l+1}{2} \int_{-1}^{1} P_{l,2}^0(\cos\theta)p_5(\theta) \cdot d(\cos\theta), \] \hspace{1cm} (28)

\[ \alpha_6^l = \frac{2l+1}{2} \int_{-1}^{1} P_{l,2}^0(\cos\theta)p_6(\theta) \cdot d(\cos\theta). \] \hspace{1cm} (29)

[19] In this paper we assume that the surface reflection matrix obeys the same symmetry relations as the scattering phase matrix [Hovenier, 1969] and thus can also be expanded in a Fourier series. The Fourier coefficients \( R^m_\mu \) of the surface reflection matrix \( R \) are given by

\[ R^m_\mu(\mu, -\mu) = \frac{1}{2\pi} \int_0^{2\pi} d(\varphi - \varphi') \left[ B^m(\varphi - \varphi) + B^{*m}(\varphi + \varphi') \right] \cdot R_\mu(\Omega, \Omega). \] \hspace{1cm} (30)

[20] In order to solve the radiative transfer equation per Fourier coefficient (11) for a vertically inhomogeneous atmosphere, the model atmosphere has to be divided in a number of homogeneous layers, where each layer is characterized by a height independent scattering coefficient, extinction coefficient, and scattering matrix. Several numerical models exist to solve the corresponding radiative transfer problem. We will use the Gauss-Seidel model described by Landgraf et al. [2002] and Hasekamp and Landgraf [2002].

3. Mie Scattering Calculations

[21] The optical input parameters of the radiative transfer equation (6) are for each homogeneous layer the extinction and scattering coefficients \( \beta^e \) and \( \beta^s \), respectively, and the phase matrix \( Z \) in the form of expansion coefficient matrices \( S^l \). These parameters are determined by scattering and absorption by aerosols, scattering by air molecules, and absorption by atmospheric gases, and are obtained from these different components by

\[ \beta^e = \beta^e_a + \beta^e_r + \beta^e_g \] \hspace{1cm} (31)

\[ \beta^s = \beta^s_a + \beta^s_r \] \hspace{1cm} (32)

\[ \alpha = \frac{\beta^e_m}{\beta^e} + \frac{\beta^e_m}{\beta^s} \] \hspace{1cm} (33)

where the subscript \( a \) denotes aerosol, the subscript \( r \) denotes Rayleigh scattering, the subscript \( g \) denotes gas absorption, and we omitted the sub- and superscripts of the expansion coefficients \( \alpha^l \).

[22] The optical properties of aerosols depend on the size, shape, and type of aerosols. In this paper we restrict ourselves to spherical aerosols which means that the optical properties of aerosols can be calculated using Mie theory. Here we will summarize the most important formulas needed for Mie calculations [see, e.g., de Rooij and van der Stap, 1984]. A complete overview of Mie scattering theory is given by van de Hulst [1957].

[23] In order to calculate the elements of the Mie scattering phase matrix \( P \) in (5), we first consider the transformation matrix \( F \) [van de Hulst, 1957] which is defined as

\[ F = \frac{k^2 \sigma_{\text{sc}}}{4\pi} \cdot P. \] \hspace{1cm} (34)

with elements \( f_1, f_2, \ldots, f_6 \) analogous to the elements \( p_1, p_2, \ldots, p_6 \) in (5). In (34) \( \sigma_{\text{sc}} \) is the scattering cross-section, and \( k = \frac{2\pi}{\lambda} \) where \( \lambda \) denotes wavelength. For a single sphere of radius \( r \) the elements of the transformation matrix \( F \) are given by

\[ f_1 = \frac{1}{2} (S_1 S_1^e + S_2 S_2^e) \] \hspace{1cm} (35)

\[ f_2 = f_1 \] \hspace{1cm} (36)

\[ f_2 = \frac{1}{2} (S_1 S_1^s + S_2 S_2^s) \] \hspace{1cm} (37)

\[ f_4 = f_3 \] \hspace{1cm} (38)

\[ f_5 = \frac{1}{2} (S_1 S_1^s - S_2 S_2^s) \] \hspace{1cm} (39)

\[ f_6 = \frac{i}{2} (S_1 S_2^s - S_2 S_1^s) \] \hspace{1cm} (40)

where we omitted the dependence on scattering angle \( \theta \), and particle radius \( r \) of \( S_1 \) and \( S_2 \). In (35)–(40) \( S_1 \) and \( S_2 \) are the elements of the two-by-two scattering amplitude matrix relating the electric field vector (containing the component parallel and the component perpendicular to the scattering plane) of the scattered beam to that of the incoming beam, and the asterisk denotes the complex conjugate. The functions \( S_1 \) and \( S_2 \) are given by

\[ S_1(\theta) = \sum_{n=0}^{\infty} \frac{2n+1}{n(n+1)} (a_n \tau_n(\theta) + b_n \tau_n(\theta)) \] \hspace{1cm} (41)

\[ S_2(\theta) = \sum_{n=0}^{\infty} \frac{2n+1}{n(n+1)} (b_n \tau_n(\theta) + a_n \tau_n(\theta)), \] \hspace{1cm} (42)
where $\tau_a$ and $\tau_n$ are functions of only scattering angle and are expressed in associated Legendre functions as

$$\tau_a(0) = \frac{1}{\sin \theta} p^1_n(\cos \theta)$$

(43)

$$\tau_n(0) = \frac{d}{d\theta} p^1_n(\cos \theta).$$

(44)

The most substantial part of the Mie calculations is the computation of the Mie coefficients $a_n$ and $b_n$ in (41) and (42) which are functions of the particle’s complex refractive index $m = m_r + im_i$ and the size parameter $k$. A numerical procedure for calculating $a_n$ and $b_n$ is given by de Rooij and van der Stap [1984], and is summarized in Appendix A. The scattering and extinction cross-sections, $\sigma_{sca}$ and $\sigma_{ext}$, of a single sphere with radius $r$ can also be calculated using the coefficients $a_n$ and $b_n$:

$$\sigma_{sca}(r) = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \left[ |a_n|^2 + |b_n|^2 \right]$$

(45)

$$\sigma_{ext}(r) = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}(a_n + b_n).$$

(46)

[24] Equations (35)–(42), (45), and (46) provide expressions for the scattering matrix and absorption and extinction cross sections for a single sphere. In nature a distribution of particles with different sizes is normally encountered. Under the assumption of independent scattering [see, e.g., Hansen and Travis, 1974] the scattering and extinction cross section for a size distribution are given by

$$\bar{\sigma}_{sca} = \int_0^\infty \sigma_{sca}(r) n(r) \, dr$$

(47)

$$\bar{\sigma}_{ext} = \int_0^\infty \sigma_{ext}(r) n(r) \, dr,$$

(48)

where $n(r)$ is the aerosol size distribution normalized to unity.

[25] Similarly, element $f_j$ of the transformation matrix $\mathbf{F}$ (34) for a size distribution is given by

$$f_j = \int_0^\infty f_j(r) n(r) \, dr.$$  

(49)

[26] In this paper the integrations over size distribution are approximated by a sum over different size bins. Here, for a function $g(r)$, the integral over size distribution is approximated by

$$\bar{g} \approx \sum_{i=1}^N g(r_i) n_i \Delta r_i,$$

(50)

where $r_i$ is the middle of size interval $i$, $n_i = n(r_i)$ and $\Delta r_i$ is the width of size interval $i$.

[27] The elements $p_j$ of the scattering phase matrix $\mathbf{P}$ of an ensemble with given size distribution can be obtained from $f_j$ and $\bar{\sigma}_{sca}$ via

$$p_j = \frac{4\pi}{k^2} \frac{f_j}{\bar{\sigma}_{sca}}.$$  

(51)

[28] The expansion coefficients $\alpha_j$ can now be calculated from the elements of the scattering phase matrix $\mathbf{P}$ using (24)–(29). Here the integrals over cos $\theta$ can be calculated analytically [Domke, 1975] or numerically [de Rooij and van der Stap, 1984]. The latter approach will be adopted for the calculations in this paper. Furthermore, the aerosol extinction and scattering coefficients $\beta_a$ and $\beta_s$ for each homogeneous layer are obtained by multiplying the corresponding cross-section by the aerosol density in that layer.

4. Linearization of the Forward Model

[29] As follows from the previous section, the relevant optical properties of spherical aerosols can be obtained from the aerosol size distribution, the aerosol number density, and the aerosol refractive index. Often, the size distribution consists of different modes, where each mode contains particles of the same refractive index. Thus, in the most general case, the elements of the state vector $\mathbf{x}$ for aerosol retrieval in (1) are for each homogeneous layer and mode of the size distribution the real part of the refractive index $m_r$, the imaginary part of the refractive index $m_i$, the elements $n_i$ of the discretized aerosol size distribution, and the aerosol number density.

[30] The elements of the forward model vector $\mathbf{F}$ are in the most general case modeled values of intensity and polarization quantities at the top of the model atmosphere, at different wavelengths, in different viewing directions of the satellite. We will use the symbol $E_i$ to refer to the modeled value of the $i$-th Stokes parameter at the top of the atmosphere, at a given wavelength and viewing direction of the satellite measurement. $E_i$ is called a radiative effect. The radiative effect $E_i$ can be extracted from the intensity vector field $\mathbf{I}$ (i.e. the solution of the radiative transfer equation (6)) with a suitable response vector function $\mathbf{R}_i$ via the inner product [see, e.g., Marchuk, 1964]:

$$E_i = \langle \mathbf{R}_i, \mathbf{I} \rangle.$$  

(52)

Here the inner product of two arbitrary vector functions $\mathbf{a}$ and $\mathbf{b}$ is defined by

$$\langle \mathbf{a}, \mathbf{b} \rangle = \int d\Omega \int d\Omega' a^*(\zeta, \Omega') b(\zeta, \Omega') \sin \theta,$$

(53)

with integration over full solid angle and altitude range of the model atmosphere. The response functions $\mathbf{R}_i$ are given by

$$\mathbf{R}_i(z, \Omega) = \delta(z - z_{top}) \delta(\Omega - \Omega_i) \mathbf{e}_i,$$

(54)

where $\mathbf{e}_i$ is the unity vector in the direction of the $i$-th component of the intensity vector, and $\Omega_i = (\theta_i, \phi_i)$ denotes the viewing direction of the instrument. In this context the
response function formalism may seem somewhat awkward, but it is essential for a proper presentation of the adjoint formulation of radiative transfer, which will be described in section 4.1.

[31] The requested derivatives of the elements of the forward model vector $\mathbf{F}$ in (2) can be expressed by the corresponding derivatives of the radiative effects $E_i$. Thus, the derivatives that we need to calculate are the derivatives $\partial E_i / \partial x_k$. These derivatives can be written as

$$\frac{\partial E_i}{\partial x_k} = \sum_{j=1}^{N} \sum_{l=0}^{L} \frac{\partial E_{ij}}{\partial \lambda_l} \frac{\partial \lambda_l}{\partial x_k} + \frac{\partial E_{ij}}{\partial \alpha_k} \frac{\partial \alpha_k}{\partial x_k} + \frac{\partial E_{ij}}{\partial \beta_k} \frac{\partial \beta_k}{\partial x_k}.$$  

(55)

Thus, the linearization corresponds to the calculation of two types of derivatives: (1) the derivatives $\partial E_{ij} / \partial \lambda_l$, $\partial E_{ij} / \partial \alpha_k$, $\partial E_{ij} / \partial \beta_k$ and (2) the derivatives $\partial \lambda_l / \partial x_k$, $\partial \alpha_k / \partial x_k$, and $\partial \beta_k / \partial x_k$. In the following we present an analytical approach to calculate these derivatives.

4.1. Linearization of Radiative Transfer

4.1.1. Forward-Adjoint Perturbation Theory

[32] For the linearization of radiative transfer with respect to the optical input parameters of the radiative transfer equation we will employ the forward-adjoint perturbation theory. Here the adjoint formulation of radiative transfer is of essential importance. The transport operator adjoint to $L$, which is called $L^\dagger$, is defined by requiring that [see, e.g., Marchuk, 1964; Box et al., 1988]

$$(I_2, L I_1) = (L^\dagger I_1, I_2)$$  

(56)

for arbitrary vector functions $I_1$ and $I_2$. The adjoint vector field $I^\dagger$ is the solution of the adjoint transport equation

$$I^\dagger = S^\dagger$$  

(57)

with any suitable adjoint source $S^\dagger$. The adjoint operator $L^\dagger$ is given by [Marchuk, 1964; Carter et al., 1978]

$$L^\dagger = \int_4 d\Omega \left\{ -\frac{1}{4} \frac{\partial}{\partial \Omega} + \beta^2(z) \right\} \delta(\Omega - \Omega') e^{i \delta(z)} Z^T(z, \Omega, \Omega')$$

$$- \delta(z) \Theta(-\mu) \mu |R^T(\Omega, \Omega') \Theta(\mu)| \mu | \right\} .$$  

(58)

The inclusion of the surface reflection term (last term on the right-hand side) is discussed by Ustinov [2001] and Landgraf et al. [2002]. We see that compared to the forward operator $L$ the adjoint operator $L^\dagger$ has a different sign in the first term, and the phase matrix $Z(z, \Omega, \Omega')$ and the surface reflection matrix $R(z, \Omega, \Omega')$ are replaced by $Z^T(z, \Omega, \Omega')$ and $R^T(\Omega, \Omega')$, respectively. The adjoint vector field $I^\dagger$ has to fulfill the boundary conditions [Box et al., 1988]

$$I^\dagger(x_{top}, \Omega) = [0, 0, 0, 0]^T \quad \text{for } \mu > 0$$  

$$I^\dagger(0, \Omega) = [0, 0, 0, 0]^T \quad \text{for } \mu < 0.$$  

(59)

[33] The forward radiative transfer equation (6) and the adjoint transport equation (57) do not describe two independent problems. The solutions $I$ and $I^\dagger$ are linked by the relation

$$\langle S^\dagger, I \rangle = \langle I^\dagger, S \rangle$$  

(60)

which can be derived in a straightforward fashion using (6), (56), and (57). We now take the response vector function $R_i$ of (54) as the adjoint source $S^\dagger_i$. In this particular case, the left-hand side of (60) represents the definition of the radiative effect $E_i$. Thus we see from (60) that there are two ways of computing the radiative effect $E_i$. The first is the forward approach: solve the radiative transfer equation (6) and take the inner product of the response function $R_i$ with the solution $I$. The second is the adjoint approach: solve the adjoint transport equation (57) for the adjoint source $S^\dagger_i = R_i$ and take the inner product of its solution $I^\dagger$ with the radiation source $S$. Now also the physical meaning of the adjoint vector field $I^\dagger$ becomes clear: it can be interpreted as the importance of a radiation source anywhere in the atmosphere regarding the radiative effect $E_i$ [Lewins, 1965]. Thus, if the adjoint vector field is known, the radiative effect $E_i$ can be calculated for any radiation source via (60).

[34] Let us consider an atmosphere with a set of optical parameters (the $\alpha_i$, $\beta_i$, and $\beta_i$) contained in the vector $g$. We call this atmosphere the unperturbed atmosphere. We denote the corresponding vector intensity field by $I_0$, and the adjoint field corresponding to the adjoint source $R_i$ by $I_0^\dagger(R_i)$. We also consider a perturbed atmosphere with a vector of optical parameters $g = g_0 + \Delta g$, where the optical parameters are perturbed in one layer of the model atmosphere. The radiative effect $E_i$ for the perturbed atmosphere is given by [Marchuk, 1964]

$$E_i(g) = E_i(g_0) - \langle I_0^\dagger(R_i), \Delta L, I_0 \rangle + O(\Delta g^2).$$  

(61)

where $O(\Delta g^2)$ denotes second and higher order terms. The change $\Delta L$ in the radiative transfer operator $L$ caused by the perturbation $\Delta g$ can be written as:

$$\Delta L = \sum_{k=1}^{K} \Delta g_k \Delta L_k.$$  

(62)

where $\Delta L_k$ is the the change in $\Delta L$ per unit in parameter $g_k$, and $K$ is the total number of optical parameters. The explicit form of $\Delta L_k$ follows from the definition of the transport operator $L$ (7). Substitution of (62) in (61) and comparison with a Taylor expansion yields the requested derivatives of the radiative effect $E_i$ with respect to the optical parameters $g_k$:

$$\frac{\partial E_i}{\partial g_k} = -\langle I_0^\dagger(R_i), \Delta L_k, I_0 \rangle.$$  

(63)

[35] So, in order to calculate the requested derivative the intensity vector field $I_0$ is required as well as the adjoint fields $I_0^\dagger$ for the adjoint sources $R_i$ with $i = 1, \ldots, 4$.

4.1.2. Transformation to Pseudoforward Problem

[36] The adjoint field can be calculated with the same radiative transfer model as the forward intensity field, because the adjoint transport equation (57) may be trans-
formed to a pseudofoward problem. For this purpose we consider the vector function

$$
\Psi(z, \Omega) = I^l(z, -\Omega).
$$

(64)

With substitution of equation (64) in equation (57), and with the symmetry relation of the scattering phase matrix [Hovenier, 1969]

$$
Z^T(z, -\Omega, -\Omega) = QZ(z, -\Omega, -\Omega)Q.
$$

(65)

with

$$
Q = \text{diag}[1, 1, 1, -1],
$$

(66)

and a similar relation for the surface reflection matrix $R_s$, the adjoint transport equation transforms to a pseudofoward equation

$$
L_\Psi \Psi = S_\Psi
$$

(67)

with

$$
S_\Psi(z, \Omega) = R_s(z, -\Omega).
$$

(68)

Here the transport operator $L_\Psi$ is the same as $L$ defined in equation (7), except that $Z(z, \Omega, \Omega)$ is replaced by $QZ(z, -\Omega, -\Omega)Q$ and $R_s(z, \Omega, \Omega)$ is replaced by $QR_s(z, -\Omega, -\Omega)Q$. According to equations (64) and (59), $\Psi$ has to fulfill the same boundary conditions as $I$ in equation (10).

[37] For the pseudofoward problem a Fourier expansion can be made as described in section 2. However, here the Fourier coefficients $S_\Psi^m(z, \Omega)$ of the pseudofoward source $S_\Psi(z, \Omega) = R_s(z, -\Omega)$ depend on the index $i$, indicating the radiative effect $E_i$ under consideration. For $i = 1, 2$, i.e. for the calculation of the derivatives of $I$ and $Q$, we obtain

$$
S_\Psi^m(z, \mu) = \frac{1}{2\pi} \delta(z-z_{\lambda\mu}) \delta(\mu+\mu_\mu) \textbf{e}_i,
$$

(69)

$$
S_\Psi^m(z, \mu) = [0, 0, 0, 0]^T.
$$

Hence, for the corresponding pseudofoward problems, we obtain a Fourier expansion of $\Psi$ containing terms of $\Psi^m$ only. For $i = 3, 4$, i.e. for the calculation of the derivatives of $U$ and $V$, we obtain

$$
S_\Psi^m(z, \mu) = [0, 0, 0, 0]^T,
$$

$$
S_\Psi^m(z, \mu) = \frac{1}{2\pi} \delta(z-z_{\lambda\mu}) \delta(\mu+\mu_\mu) \textbf{e}_i.
$$

(70)

Hence, for the corresponding pseudofoward problems, we obtain a Fourier expansion of $\Psi$ containing terms of $\Psi^m$ only.

### 4.1.3. Calculation of the Derivatives

[38] In the following we will work out the expressions for the derivatives with respect to the expansion coefficients $\alpha_j$, the scattering coefficient $\beta$, and the extinction coefficient $\beta^e$. Hereto, we write instead of (62)

$$
\Delta L = \sum_{j=1}^6 \sum_{i=0}^7 \Delta \alpha_j \Delta L_j^i + \Delta \beta \Delta L_s + \Delta \beta^e \Delta L_s.
$$

(71)

where

$$
\Delta L_j^i = \frac{\beta^e}{4\pi} \int_4 d\Omega \frac{\partial Z(z, \Omega, \Omega)}{\partial \alpha_j^i}
$$

(72)

$$
\Delta L_s^j = \frac{1}{4\pi} \int_4 d\Omega Z(z, \Omega, \Omega)
$$

(73)

$$
\Delta L_s^j = \frac{1}{4\pi} \int_4 d\Omega \delta(\Omega - \Omega) E
$$

(74)

In order to obtain expressions for the derivatives with respect to $\alpha_j$, $\beta$, and $\beta^e$, we substitute $\Delta L_j^i$, $\Delta L_s$, and $\Delta L_s^j$ in (63), respectively. Additionally, we use the Fourier expansion of $I$, $\Psi$, and $Z$, and evaluate the integrals over azimuth angle. We then obtain expressions in the form of cosine- and sine expansions which have a similar form for the three types of derivatives. For the radiative effects $E_i$ with $i = 1, 2$ (i.e. corresponding to Stokes parameters $I$ and $Q$, respectively) the derivatives are given by a cosine expansion:

$$
\frac{\partial E_i}{\partial g_k} = -\sum_{m=0}^\infty (2 - \delta_{00}) \cos m(\phi_\mu - \phi_0) K_{i,m}^m(g_k).
$$

(75)

[39] For the radiative effects $E_i$ with $i = 3, 4$ (i.e. corresponding to Stokes parameters $U$ and $V$, respectively) the derivatives are given by a sines expansion:

$$
\frac{\partial E_i}{\partial g_k} = -\sum_{m=0}^\infty (2 - \delta_{00}) \sin m(\phi_\mu - \phi_0) K_{i,m}^m(g_k).
$$

(76)

[40] The specific integral kernels for $\alpha_j$, $\beta$, and $\beta^e$ are determined by $\Delta L_j^i$, $\Delta L_s$, and $\Delta L_s^j$, respectively. For the derivative of the radiative effect $E_i$ with respect to the expansion coefficient $\alpha_j$ we obtain for the integral kernel

$$
K_{i,m}^{\alpha_j} = \frac{\pi}{4} \int_{\theta_{00}}^{\theta_{00}} d\theta \beta \beta^e \int_{-1}^{1} d\mu d\eta \Psi_{\theta, \mu}^{\alpha_j}(R_s, z, -\mu) A
$$

(77)

$$
\frac{\partial Z_m(z, \mu)}{\partial Q_j} = (-1)^m P_{m}(\mu) P_{m}(\mu).
$$

(78)

Here the matrix $E_j$ has the same structure as the expansion coefficient matrix (23) and is given by

$$
E_j = \begin{pmatrix}
\delta_{j1} & \delta_{j5} & 0 & 0 \\
\delta_{j5} & \delta_{j2} & 0 & 0 \\
0 & 0 & \delta_{j3} & \delta_{j6} \\
0 & 0 & -\delta_{j6} & \delta_{j4}
\end{pmatrix},
$$

(79)

where $\delta$ is the Kronecker delta.
[41] The integral kernel corresponding to the derivative of the radiative effect \( E_i \) with respect to \( \beta^j \) is given by

\[
K_j^{\pm m}(\beta^j) = \frac{\pi}{4} \int_{z_{\text{to}}}^{z_{\text{bot}}} dz \int_{-1}^{1} d\mu \frac{\Psi_{\omega}^{\pm m}(\mathbf{R}_i, z, -\mu) \Delta Z_{\omega}(z, \bar{\mu}, \mu)}{\Delta \omega^m(z, \mu)}, \tag{80}
\]

and the integral kernel corresponding to the derivative of the radiative effect \( E_i \) with respect to \( \beta^j \) is given by

\[
K_j^{\pm m}(\beta^j) = 2\pi \int_{z_{\text{to}}}^{z_{\text{bot}}} dz \int_{-1}^{1} d\mu \frac{\Psi_{\omega}^{\pm m}(\mathbf{R}_i, z, -\mu) \Delta \mathbf{I}_{\omega}^{m}(z, \mu)}{\Delta \omega^m(z, \mu)}. \tag{81}
\]

[42] Equations (75) and (76), together with (77)–(81), provide analytical expressions for the derivatives of the radiative effects \( E_i \) with respect to the expansion coefficients \( \alpha_j \), the scattering coefficient \( \beta^j \), and the extinction coefficients \( \beta^j \), respectively. Thus, to calculate these derivatives one needs the forward intensity field and the pseudoforward fields for the sources \( \mathbf{S}_\omega(z, \Omega) = \mathbf{R}_i(z, -\Omega) \), with \( i = 1, 4 \). These fields can be determined by any vector radiative transfer model that calculates the internal radiation of the atmosphere, such as the doubling and adding model of Stammes et al. [1989], the Discrete Ordinate model VDISORT of Schulz et al. [1999], and the Gauss-Seidel model of Hasekamp and Landgraf [2002]. The latter model is used for all numerical simulations in this paper. The corresponding integral kernels of equations (77)–(81) are worked out by Landgraf et al. [2004] for this model.

### 4.2. Linearization of the Mie Calculations

[43] The derivatives of the optical input parameters of the radiative transfer equation with respect to the different elements \( x_i \) of the state vector can be found from the corresponding derivatives of the optical aerosol parameters (see equations (31)–(33)):

\[
\frac{\partial \beta^j}{\partial x_k} = \frac{\partial \beta^j}{\partial \alpha_a} \frac{\partial \alpha_a}{\partial x_k}
\]

\[
\frac{\partial \beta^j}{\partial x_k} = \frac{\partial \beta^j}{\partial \alpha_a} \frac{\partial \alpha_a}{\partial x_k}
\]

\[
\frac{\partial \alpha_a}{\partial x_k} = \frac{\beta^j}{\beta^j} \frac{\partial \alpha_a}{\partial x_k} + \alpha_a \frac{\partial \beta^j}{\partial x_k} \frac{\partial \beta^j}{\beta^j} \frac{\partial \beta^j}{\partial x_k} = \frac{\beta^j}{\beta^j} \frac{\partial \alpha_a}{\partial x_k} \frac{\partial \beta^j}{\partial x_k}, \tag{84}
\]

where we omitted the indices for the expansion coefficients \( \alpha_j \). In this subsection we will derive expressions for the derivatives \( \partial \alpha_a/\partial x_k \), \( \partial \beta^j/\partial x_k \), and \( \partial \beta^j/\partial x_k \). For notational convenience we will omit the subscript \( a \) for the expansion coefficients in the remainder of this subsection.

[44] In order to calculate the derivatives of the expansion coefficients \( \alpha_j \) with respect to the real and imaginary part of the refractive index, \( m_r \) and \( m_i \), respectively, we first need to calculate the corresponding derivatives of the elements \( f_j \) of the transformation matrix \( \mathbf{F} \) in (34). These derivatives are expressed by the derivatives of \( S_1 \) and \( S_2 \) (see (35)–(40)):

\[
[f_j]' = \frac{1}{2} \left( S_1[S_2]' + |S_1|^2 S_2' + S_2[S_1]' + |S_2|^2 S_1' \right)
\]

\[
[f_j]' = [f_j]
\]

\[
[f_j]' = \frac{1}{2} \left( S_1[S_2]' + |S_1|^2 S_2' + S_2[S_1]' + |S_2|^2 S_1' \right)
\]

\[
[f_j]' = [f_j]' + [f_j]
\]

\[
[f_j]' = \frac{1}{2} \left( S_1[S_2]' + |S_1|^2 S_2' - S_2[S_1]' + |S_2|^2 S_1' \right)
\]

\[
[f_j]' = \frac{1}{2} \left( S_1[S_2]' + |S_1|^2 S_2' - S_2[S_1]' + |S_2|^2 S_1' \right)
\]

Here the prime denotes the derivative with respect to either \( m_r \) or \( m_i \). The derivatives of \( S_1 \) and \( S_2 \) are given by

\[
[S_1]' = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} (a_n \tau_n + |b_n|^2 \tau_n)
\]

\[
[S_2]' = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} (|b_n|^2 \tau_n + a_n \tau_n).
\]

[45] The derivatives of the scattering and extinction coefficients with respect to \( m_r \) and \( m_i \) follow from the corresponding derivatives of the scattering and extinction cross-sections. These derivatives also depend on the derivatives of \( a_n \) and \( b_n \):

\[
[\sigma_{\text{sc}}]' = \frac{4\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \left( a_n a_n^* + a_n b_n^* + b_n a_n^* + b_n b_n^* \right)
\]

\[
[\sigma_{\text{sc}}]' = \frac{4\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \text{Re} \left( a_n a_n^* + b_n b_n^* \right)
\]

Thus, all derivatives with respect to \( m_r \) and \( m_i \) depend on the corresponding derivatives of the Mie coefficients \( a_n \) and \( b_n \), for which analytical expressions are given in Appendix A.

[46] The derivatives of \( f_j \), \( \sigma_{\text{sc}} \), and \( \sigma_{\text{ext}} \) with respect to \( m_r \) and \( m_i \) given above all correspond to a single sphere with a given radius. The derivatives for an ensemble of particles with a given size distribution can be easily obtained via integration over the size distribution as in (50). The derivatives of the elements \( f_j \) of the scattering phase matrix \( M \) for the size distribution can then be calculated using the derivatives of \( f_j \) and \( \sigma_{\text{sc}} \), namely,

\[
[p_j]' = \frac{4\pi}{k^2} \left( \frac{f_j'}{\sigma_{\text{sc}}'} \frac{f_j}{\sigma_{\text{sc}}^2} \right)
\]

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The derivatives of the expansion coefficients \( \alpha'_j \) can be calculated from the derivatives of \( p_j \) equivalent to (24)–(29).

The other type of derivatives that are needed are the derivatives with respect to the elements \( n_i \) of the discretized size distribution (see (50)). These derivatives can be calculated in a straightforward manner. The derivative of an averaged element \( f' \) of the transformation matrix \( F \) with respect to \( n_i \) is given by

\[
\frac{\partial f'}{\partial n_i} = f'(n) \Delta n_i, \tag{96}
\]

and similar expressions hold for the derivatives of \( \bar{\sigma}_{sca} \) and \( \bar{\sigma}_{ext} \) with respect to \( n_i \). Using the derivatives of \( f_j \) and \( \bar{\sigma}_{sca} \) with respect to \( n_i \), the derivatives of the elements \( p_j \) of the scattering phase matrix (5) with respect to \( n_i \) can now be calculated similar to (95). The corresponding derivatives of the aerosol expansion coefficients \( \alpha'_j \) can be calculated equivalent to (24)–(29).

For aerosol retrieval it is often useful to describe the size distribution by a limited number of parameters, for example, the effective radius \( R_{eff} \) and the effective variance \( V_{eff} \) \cite{Hansen:1974} of a prescribed size distribution (e.g., a lognormal distribution). For such retrievals one needs to calculate the derivatives with respect to these parameters. For an averaged optical parameter \( g \) this derivative is given by

\[
\frac{\partial g}{\partial R_{eff}} = \sum_{i=1}^{N} \frac{\partial n_i}{\partial R_{eff}} \frac{\partial g}{\partial n_i}, \tag{97}
\]

and a similar expression holds for the derivative with respect to \( V_{eff} \).

5. Numerical Implementation and Results

The linearization approach described in section 4 has been implemented in the Gauss-Seidel vector radiative transfer model described by Landgraf et al. \cite{Landgraf:2002} and Hasekamp and Landgraf \cite{Hasekamp:2002}, combined with the Mie scattering algorithm of de Rooij and van der Stap \cite{DeRooij:1987}. Expressions for the integral kernels of section 4.1 can be found in the paper of Landgraf et al. \cite{Landgraf:2004} for our Gauss-Seidel radiative transfer model.

The Gauss-Seidel radiative transfer approach is based on the integral form of the radiative transfer equation \cite[see, e.g., Lenoble, 1985]{Lenoble:1985}. When we approximate the integral over zenith angle in the Fourier components of the radiative transfer equation (11) by a Gaussian quadrature, and we assume a height independent multiply scattered radiation field within the homogeneous layers of the inhomogeneous atmosphere, the integral form of the radiative transfer equation per Fourier component can be written as a matrix equation \cite{Landgraf:2002, Hasekamp:2002}. This matrix equation is solved using the Gauss-Seidel iterative method \cite[see, e.g., Herman and Browning, 1965; Strang, 1986]{Herman:1965, Strang:1986}, yielding the Fourier component under consideration of the intensity vector field at the layer boundaries and Gaussian streams (angles). Of course, the accuracy of the radiative transfer calculations depends on the optical thickness of the layers in which the model atmosphere is divided. For all calculations in this paper we used model layers for which the scattering optical thickness <0.005 and the absorption optical thickness <0.01. For this choice of layer thickness we compared radiative transfer calculations of our model with reference Doubling-Adding calculations at an accuracy of \( 10^{-9} \) \cite{deHaan:1987}. We found that the relative error caused by the assumption of a height independent multiply scattered radiation field within the model layers is smaller than \( 10^{-6} \) for all Stokes parameters, which is negligible compared to the errors in any satellite measurement. In order to enhance the numerical efficiency of our radiative transfer calculations we employ the analytical separation of single scattering as described by de Haan et al. \cite{deHaan:1987}, which significantly reduces the number of terms needed in the Fourier series.

All radiative transfer calculations in this paper were performed for a model atmosphere that includes Rayleigh scattering and scattering and absorption by spherical aerosols. All aerosols were homogeneously distributed over the lowest 2 km of the atmosphere. We used a bimodal lognormal aerosol size distribution, with a mode containing small particles referred to as the small mode and a mode containing large particles referred to as the large mode. For this model atmosphere the aerosols are characterized by 10 parameters, i.e. 5 per mode of the size distribution. These parameters are: per mode the effective radius \( R_{eff} \), the effective variance \( V_{eff} \) the aerosol column \( N \), and the real and imaginary part of the refractive index \( m \).

In order to verify the analytical derivatives of the radiative effects \( E_i \) with respect to the 10 aerosol parameters in our model atmosphere, calculated by the approach of sections 4.1 and 4.2, we compared them with corresponding derivatives calculated by finite differencing:

\[
\frac{\partial E_i}{\partial x_k} (x_k) \approx \frac{E_i(x_k + \Delta x_k) - E_i(x_k)}{\Delta x_k}, \tag{98}
\]

where \( \Delta x_k \) is the perturbation in \( x_k \). The value of \( \Delta x_k \) determines the accuracy of the derivative calculated by finite differencing. \( \Delta x_k \) should be chosen as small as possible, but if the difference \( E_i(x_k + \Delta x_k) - E_i(x_k) \) becomes too small numerical rounding errors become important. Starting with a value for \( \Delta x_k = 0.01x_k \), we gradually decreased the value for \( \Delta x_k \) and evaluated the differences between the analytical derivatives and derivatives calculated by (98). The relative difference decreased to about \( 10^{-6} \) for \( \Delta x_k \approx 10^{-7}x_k \) and then increased again because the numerical derivatives calculated by (98) became unstable. The small differences between the analytical derivatives and derivatives calculated by (98) indicate that the linearization approach of sections 4.1 and 4.2 has been implemented correctly in our model.

Figures 1 and 2 show the derivatives of Stokes parameters \( I \) and \( Q \) at the top of the atmosphere with respect to the logarithm of the 10 aerosol parameters in our model atmosphere, as a function of viewing zenith angle for a solar zenith angle of 40°, for a wavelength of 350 nm and 800 nm, respectively. The relative azimuth angle \( \phi_\alpha = \phi_\alpha = 180^\circ \) for negative viewing zenith angles and \( \phi_\phi = \phi_\phi = 0^\circ \) for positive viewing zenith angles. For these geometries the Stokes parameters \( U \) and \( V \) are equal to zero, so Stokes
Figure 1. Derivatives of the Stokes parameters $I$ (left panels) and $Q$ (right panels) at the top of the atmosphere (TOA), with respect to the logarithm of (A) $R_{\text{eff}}$, (B) $V_{\text{eff}}$, (C) $m_r$, (D) $m_i$, and (E) the aerosol column $N$. The solid lines correspond to parameters of the small mode, and the dashed lines correspond to parameters of the large mode. The derivatives are shown as a function of viewing zenith angle (VZA), where $VZA < 0$ refer to the relative azimuth angle $\phi_o - \phi_v = 180^\circ$, and $VZA > 0$ refer to $\phi_o - \phi_v = 0^\circ$. The solar zenith angle is $40^\circ$, and the calculation is performed for a wavelength of 350 nm. The solar and viewing zenith angles are defined as the smallest angle between the zenith direction and the solar and viewing direction, respectively. The range $-60^\circ$ to $60^\circ$ of viewing zenith angles used in this figure corresponds to a horizon-to-horizon scan for a satellite at approximately 800 km. The internal radiation field was discretized in 16 Gaussian streams. A bimodal aerosol size distribution was used with $R_{\text{eff}} = 0.05$ for the small mode, $R_{\text{eff}} = 0.75$ for the large mode, $V_{\text{eff}} = 0.2$ for both modes, $m_r = 1.45$, $m_i = -0.0045$, the optical thickness at 550 nm is 0.15 with equal contribution from the small and the large mode.
parameter $Q$ fully describes the polarization of the back-scattered light at the top of the atmosphere. The derivative with respect to the logarithm of a given aerosol parameter is a measure for the sensitivity of $I$ and $Q$ to a relative change in this aerosol parameter, which is a convenient quantity in order to compare the sensitivities to the different parameters.

The angular dependence of the derivatives is caused by the angular dependence of the following effects: (1) the derivatives of the relevant elements of the aerosol scattering phase matrix with respect to the different aerosol parameters. (2) The light path inside the aerosol layer, which increases with viewing zenith angle. This causes an increase in sensitivity up to a certain viewing angle because an increasing fraction of the light is scattered by aerosols. However, if the viewing angle becomes too large this effect causes a decrease in sensitivity because of increasing extinction within the aerosol layer along the line of sight. (3) Multiple scattering effects, which in general smear out the angular effects of the aerosol scattering phase matrix.

Figure 2. Same as Figure 1, but for a wavelength of 800 nm.
From Figure 1 it follows that at 350 nm the sensitivities of both \( I \) and \( Q \) with respect to the parameters of the small mode are much larger than the corresponding sensitivities with respect to the parameters of the large mode, which are in general negligibly small at 350 nm. The angular dependence of the derivatives of the intensity in Figure 1 is relatively weak which is caused by the weak angular dependence of the corresponding derivatives of element (1, 1) of the scattering phase matrix (except for the forward scattering direction, which is not shown in Figure 1). The derivatives with respect to the different aerosol parameters of element (2, 1) of the scattering phase matrix has a larger angular dependence, which is the most dominant effect in the right panels of Figure 1. Also multiple scattering effects can be seen here, because both the Rayleigh and aerosol scattering optical thickness are relatively large at 350 nm. For example, in the backward scattering direction element (2, 1) of the scattering phase matrix is zero independent of the aerosol properties, i.e. it is insensitive with respect to aerosol properties. However, the sensitivity of Stokes parameter \( Q \) is not zero in the backward single scattering direction (viewing angle = \(-40^\circ\)), because the sensitivity is influenced by aerosol scattering in all directions via multiple scattering.

At 800 nm (Figure 2) the derivatives of both \( I \) and \( Q \) with respect to the parameters of the large mode, are significantly larger than at 350 nm, while the derivatives with respect to the parameters of the small mode are much smaller. The angular dependence of the derivatives of the phase matrix plays the most important role at 800 nm, especially for the derivatives of Stokes parameter \( Q \). Here the strong angular variation in the derivatives of \( Q \) around the single scattering backward direction (\(-40^\circ\)) is also present in the sensitivity of the (2, 1)-element of the aerosol scattering phase matrix. A similar, but weaker effect can be seen in the derivatives of the intensity with respect to parameters of the large mode. Another effect that can be seen in Figure 2 is the slight increase in sensitivity towards larger (absolute values of) viewing zenith angle. This increase in sensitivity is caused by an enhanced light path inside the aerosol layer.

The different sensitivities at 350 nm and 800 nm to the different aerosol parameters demonstrates the need to use multispectral measurements of intensity and polarization for aerosol remote sensing. As shown by Chowdhary et al. [2001, 2002], the sensitivity with respect to parameters of the large mode can be significantly increased by including longer wavelengths up to about 2 \( \mu m \). The dependence of sensitivity on viewing angle demonstrates the need of using multi-viewing angle measurements [Mishchenko and Travis, 1997a]. Furthermore, a clear feature in the derivatives at both 350 nm and 800 nm is the higher sensitivity of both \( I \) and \( Q \) to the effective radii, the real part of the refractive indices, and the aerosol column, than to the effective variances and the imaginary part of the refractive indices. This may be an indication that it is more difficult to retrieve the effective variances and imaginary parts of the refractive indices from satellite measurements in the range 350–800 nm.

6. Application to Aerosol Retrieval

In this section we demonstrate the use of the linearized radiative transfer model presented in this paper for aerosol retrieval from measurements of the Global Ozone Monitoring Experiment-2 (GOME-2), which is due for launch on EUMETSAT’s METOP satellite in 2005. The Polarization Measuring Device (PMD) of GOME-2 measures the 312–800 nm spectral range using 200 detector pixels with a spectral resolution of 2.8 nm at 312 nm and about 40 nm at 800 nm, with an integration time of 23 ms. The components of the intensity polarized parallel and perpendicular to the optical plane are measured simultaneously. These components are denoted by \( I_p \) and \( I_s \), respectively, for detector pixel \( i \). The measurement \( I_i \) is given by

\[
I_i = \int_0^\infty d\lambda S(\lambda) I'(\lambda),
\]

where the integration over wavelength \( \lambda \) describes the effect a Gaussian spectral response function \( S(\lambda) \), where \( I'(\lambda) \) denotes the \( I \) component of the intensity at the entrance of the instrument. The measurement \( I_i \) is defined in the same manner as in (99). From the measured intensities \( I_p \) and \( I_s \) the Stokes parameters \( I \) and \( Q \) can be obtained, namely,

\[
I_i = I_p^i + I_s^i
\]

\[
Q_i = I_p^i - I_s^i.
\]

The accuracy of the PMD measurements of the relative Stokes parameter \( q_i = Q_i/I_i \) is expected to be better than 0.005 [Hartmann et al., 2003]. For the study in this paper we assume that this value represents the standard deviation \( \sigma_q \) of a random Gaussian error on \( q_i \) for all scenarios, and thus do not include the dependence on signal strength which is present in for example shot noise. So, this is a rather conservative noise estimate, but this is suitable for the purpose of this study. Given the fact that \( I \) and \( Q \) are obtained from the same measurements \( I_p \) and \( I_s \), the standard deviation on \( I_p \) and \( Q_p \) is expected to have the same value \( \sigma_q \), which is given by

\[
\sigma_q = \frac{\sigma_q I_p}{\sqrt{1 + q_i^2}}.
\]

Due to limitations in the GOME-2 data rate the information of the 200 detector pixels has to be co-added onboard to form 15 programmable bands. The expected spectral situation for these bands is denoted in Table 1. For aerosol retrieval it is anticipated to use band 7–15. The intensity \( I_{pmd} \) for a given PMD band is given by

\[
I_{pmd} = \sum_{i=1}^N I_i,
\]

where the summation in (103) describes the co-adding over a number of \( N \) detector pixels. The Stokes parameter \( Q_{pmd} \)
In principle, the number of unknown aerosol parameters in a retrieval is 10 for the given setup, since we use the same aerosol model as described in the previous section. However, the corresponding inverse problem is ill posed if one tries to fit all 10 aerosol parameters. This means that different combinations of aerosol parameters produce the same measurement, within the noise. Therefore, the number of fit parameters needs to be reduced by choosing fixed a priori values for some aerosol parameters. We found that a stable inversion is obtained if we choose fixed a priori values for the refractive index.

The model atmosphere was bounded below by a rough ocean surface (wind speed of 7 m/s). Here we used the wind speed dependent distribution of surface slopes of Cox and Munk [1954] from which we calculated the Fresnel reflection on the waves using the method described by Mishchenko and Travis [1997a]. For each retrieval the iteration was started with values of the aerosol parameters in the middle of the specified range, i.e., 0.06 for the refractive index of the small mode, 0.9 for the refractive index of the large mode, 1.3–1.7 for the optical thickness of both modes, and 1.5 for the real part of the refractive index.

To illustrate the retrieval results from the synthetic measurements, Figure 3 shows for the effective radius of the small mode and the refractive index the retrieved values against the true values. The 1σ error bars calculated using (105) are also indicated in this figure. In general the retrieved values match the true values well, taking into account the error bars. It can be seen that the size of the error bars varies considerably for different retrievals. The reason for this is that the different retrievals in Figure 3 correspond to different values of the aerosol optical thickness, and the errors on the retrieved parameters generally increase with decreasing aerosol optical thickness.

If (105) would correctly describe the ‘true’ uncertainties in the retrieved aerosol parameters, then the distribution of \((x'_r - x_r)/\sigma_r\) is given by a Gaussian with a mean value of 0 and a full width at half maximum of 2. Here \(x'_r\) is the i-th element of the retrieved state vector, \(x_r\) is the corresponding true value, and \(\sigma_r\) the standard deviation that follows from (105). For the retrievals on the 1000 synthetic measurements described above the corresponding distribution is depicted in Figure 4. The shown distribution contains the values \((x'_r - x_r)/\sigma_r\) for all 5 state vector elements.

From Figure 4 it follows that the distribution of the retrieved aerosol parameters reproduces the general features of a Gaussian distribution well, except for the fact that the wings of the distribution are too wide and the maximum is somewhat flatter. In order to investigate whether the outliers
in Figure 4 are caused by local minima or by nonlinearity within the error range, we repeated the 1000 retrievals but now the iteration was started using the true aerosol parameters. For these first guess parameters it is very unlikely that the inversion will end up in a local minimum. The corresponding distribution is shown in Figure 5. It can be seen that virtually all outliers are not present anymore, which demonstrates that the outliers in Figure 4 were mainly caused by local minima. An inspection of the data corresponding to Figure 4 shows that by far most of the outliers (and thus the local minima) correspond to retrievals where the effective radius of the small mode was smaller than about 0.03 \( \mu \text{m} \) and the effective radius of the large mode was larger than about 1.3 \( \mu \text{m} \). So, still for a broad range of true aerosol parameters the global minimum of the inversion problem was found, which demonstrates a relatively weak dependence on the first guess aerosol parameters.

In order to investigate the effect of nonlinearity within the range of the error we compare the distribution of Figure 5 with a distribution based on the same retrieved parameters but now with \( \sigma_i \) calculated using the linearization around the true state vector instead of the retrieved state vector. Here we choose the true state vector as linearization point because \( \left( x_i^t / C_0 \right) / \sigma_i \) is a good measure for the error range. The corresponding distribution is shown in Figure 6. It can be seen that the distributions of Figures 5 and 6 only show some small differences. This means that the effect of nonlinearity within the error range is present but small.

To summarize, the results presented in this section demonstrate that an iterative retrieval approach based on a linearized radiative transfer model is well suited for aerosol retrieval from GOME-2 measurements. Furthermore, the retrieval error covariance matrix calculated by the linear approximation (105) yields a good description of the precision of the retrieved aerosol parameters.

## 7. Conclusion

An analytical linearization of vector radiative transfer with respect to physical properties of spherical aerosols has been presented. The linearization consists of two steps: The first step is the calculation of the derivatives of the four Stokes parameters at the top of the atmosphere with respect to scattering coefficient, absorption coefficient, and the expansion coefficients of the scattering phase matrix. These derivatives are calculated analytically employing the forward-adjoint perturbation theory. Here general expressions are presented that can be applied for the linearization of any vector radiative transfer model that calculates the internal radiation field in the model atmosphere. The second step is the calculation of the derivatives of the scattering coefficient, absorption coefficient, and the expansion coefficients of the scattering phase matrix, with respect to the real and imaginary part of the refractive index, and parameters describing the size distribution (e.g., effective radius, effec-

![Figure 3.](image3.png) **Figure 3.** (left) Retrieved refractive index with 1σ error bar versus true refractive index for the 1000 synthetic retrievals. (right) Retrieved effective radius of the small mode with 1σ error bar versus true effective radius of the small mode for the 1000 synthetic retrievals.

![Figure 4.](image4.png) **Figure 4.** Solid line: distribution of \( \left( x_i^r - x_i^t \right) / \sigma_i \) for the 1000 retrievals on synthetic GOME-2 measurements. \( N / N_{\text{tot}} \) indicates the number of points in a certain size bin normalized to the total number of points. Dashed line: Gaussian with a full width at half maximum of 2. The distribution contains 101 bins between −8 and 8.
Figure 5. Same as Figure 4, but for the iteration started with the true aerosol parameters.

Appendix A: Mie Coefficients and Their Derivatives

The Mie coefficients $a_n$ and $b_n$ are calculated using the method of de Rooij and van der Stap [1984]. Here we will summarize the relevant formulas and for further details we refer to the corresponding paper. Furthermore, we give expressions for the derivatives of $a_n$ and $b_n$ with respect to the real and imaginary part of the refractive index, needed in section 4.2. The Mie coefficients are given by [see, e.g., Deirmendjian, 1969]:

$$a_n = \frac{(D_n(z)/m + n/x) \Psi_n(x) - \Psi_{n-1}(x)}{(D_n(z)/m + n/x) \zeta_n(x) - \zeta_{n-1}(x))}$$  \hspace{1cm} (A1)

$$b_n = \frac{(mD_n(z) + n/x) \Psi_n(x) - \Psi_{n-1}(x)}{(mD_n(z) + n/x) \zeta_n(x) - \zeta_{n-1}(x))}$$ \hspace{1cm} (A2)

where $m$ is the complex refractive index $m_r + im_i$, $x$ is the size parameter $2\pi r/\lambda$, and $z = mx$. Furthermore,

$$\Psi_n(x) = x j_n(x)$$  \hspace{1cm} (A3)

$$\zeta_n(x) = \Psi_n(x) + ix \chi_n(x),$$  \hspace{1cm} (A4)

with

$$\chi_n(x) = -x j_n(x)$$  \hspace{1cm} (A5)

where $j_n(x)$ and $y_n(x)$ are the spherical Bessel functions of the first and second kind respectively. $D_n(z)$ is the only function that depends on refractive index and is given by

$$D_n(z) = \frac{d}{dz} \ln \Psi_n(z) = -\frac{n}{z} \frac{\Psi_{n+1}(z)}{\Psi_n(z)}.$$  \hspace{1cm} (A6)

[70] The functions $\Psi_n(x)$ and $\chi_n(x)$ and $D_n(z)$ are all calculated using recurrence relations. Here $\chi_n(x)$ is calculated upward recursion using the recurrence relation

$$\chi_{n+1}(x) = \frac{2n+1}{x} \chi_n(x) - \chi_{n-1}(x)$$  \hspace{1cm} (A7)

with initial functions

$$\chi_{-1}(x) = \sin x, \hspace{1cm} \chi_0(x) = \cos x.$$  \hspace{1cm} (A8)

[71] $\Psi_n(x)$ is calculated using downward recursion:

$$\Psi_n(x) = r_n(x) \Psi_{n-1}(x)$$  \hspace{1cm} (A9)

where

$$r_n(x) = \left[\frac{2n+1}{x} - r_{n+1}(x)\right]^{-1}.$$  \hspace{1cm} (A10)

Figure 6. Same as Figure 5, but the standard deviation is calculated using the linearization around the true aerosol parameters.
The recursion is started at \( n = N_1(x) \) where

\[
N_1(x) = x + 4.05x^{4/3} + 60
\]  
(A11)

and \( r_{z0}(x) = 0 \) \cite{deRooijandvanderStap,1984}.\footnote{De Rooij and van der Stap, 1984.}

\[ D_n(z) \] is calculated using the following downward recursion relation:

\[
D_n(z) = \frac{n+1}{z} - \left( D_{n+1}(z) + \frac{n+1}{z} \right)^{-1},
\]

(A12)

where the recursion is started at \( n = N_2(z) \) with

\[
N_2(z) = z + 4.05z^{4/3} + 10
\]  
(A13)

and \( D_N(z) = 0 \) \cite{deRooijandvanderStap,1984}.\footnote{De Rooij and van der Stap, 1984.}

The derivatives of \( a_n \) and \( b_n \) with respect to the real and imaginary part of the refractive index are given by

\[
[a_n]' = \frac{(D_n(z)/m - D_n(z)/m^2)(\Psi_{n-1} - \Psi_{n+1})}{[(D_n(z)/m + n/x) \zeta_n(x) - \zeta_n(x)]}
\]

where \( \pi \) is the prime indicates the derivative with respect to either \( m, \) or \( \imath \).

Here it is important to note that in section 4.2 we use the derivatives with respect to \( m \) which follow directly from the here given derivatives with respect to \( \imath \). The derivative \( [D_n(z)]' \) is found by backward recursion via

\[
[D_n(z)]' = -\frac{x(n+1)}{z^2} + \left( D_{n+1}(z) + \frac{x(n+1)}{z^2} \right)
\]

(A16)

starting the recursion at \( N_2 \) with \([D_N(z)]' = 0\).

\[ \begin{align*}
[D_n(z)]' &= -\frac{x(n+1)}{z^2} + \left( D_{n+1}(z) + \frac{x(n+1)}{z^2} \right) \\
&= \frac{n+1}{z}.
\end{align*} \]

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O. P. Hasekamp and J. Landgraf, Space Research Organization Netherlands, Sorbonnelaan 2, 3584 CA Utrecht, Netherlands. (o.hasekamp@sron.nl; j.landgraf@sron.nl)