Efficient radiative transfer in cloudy atmospheres

Abstract. Radiance measurements of solar radiation that is backscattered by the Earth’s atmosphere or surface contain information about the atmospheric composition and the state of the Earth’s surface. Retrieving such information from satellite-borne observations in nadir geometry employs a radiative transfer forward model. The forward model simulates the observed quantity, aiming to reproduce the observation. LINTRAN v2.0 is a linearised vector radiative transfer forward model, employing forward-adjoint theory, that is capable of modelling cloud contaminated satellite observations and their derivatives with respect to the state of the atmosphere and the Earth’s surface in a numerically efficient manner. A significant gain in efficiency with respect to its predecessor (LINTRAN v1.0) is achieved through a mathematical framework that combines an approximate iterative solving method using the forward-adjoint perturbation theory with separation of the first $N$ orders of scattering from the diffuse intensity vector field. Contributions to the observable up to order of scattering $N$ are recursively solved in an analytical manner. Contributions from higher orders of scattering are subsequently solved in a numerical manner, assuming that the intensity field varies linearly with the vertical coordinate within an optically homogeneous model layer. This method is implemented in LINTRAN v2.0, choosing $N=2$, within the general framework of forward-adjoint perturbation theory. This new approach allows us to decrease the number of model layers and the degree of angular quadrature within the numerical solver by a factor of 10 and 1.4 respectively, compared to LINTRAN v1.0, in a homogeneous atmosphere loaded with scattering Mie particles ($\chi \approx 35$). In this atmosphere, the reduced discretisation reduces the numerical effort associated with the numerical matrix solver by a factor of 42 relative to the previous model version, without a loss in accuracy.

This chapter has been published as Schepers, D. et al., LINTRAN v2.0: A linearised vector radiative transfer model for efficient simulation of satellite-born nadir-viewing reflection measurements of cloudy atmospheres Journal of Quantitative Spectroscopy and Radiative Transfer (2014)
3.1 Introduction

Observations of solar radiation that is backscattered by the Earth’s atmosphere and reflected by the Earth’s surface can be exploited to gain information about the atmospheric composition and the surface state. Such observations are provided by a range of nadir-observing satellite instruments covering several parts of the electromagnetic spectrum where scattering of light is significant. Among the currently operating nadir-viewing instruments are the GOME-2 (Callies et al., 2000) instruments on-board the MetOp series of satellites, measuring reflectance in the ultraviolet and visible part of the spectrum, and the Fourier Transform Spectrometer (FTS) on-board the Japan Aerospace Exploration Agency’s (JAXA) Greenhouse gas Observing Satellite (GOSAT) (Yokota et al., 2004; Kuze et al., 2009) that observes Earth radiances in the short-wavelength and thermal infrared (SWIR and TIR) spectral range. In the near future, the observational record will be extended using, among others, the TROPOMI instrument (Veefkind et al., 2012) on-board the European Space Agency’s (ESA) Sentinel-5 Precursor mission (S5-p), to be launched in 2015.

To retrieve the information about atmospheric trace gas concentrations in the Earth’s atmosphere from the observations of backscattered radiation, a forward model plays a crucial role. The forward model simulates the observed quantity $F$ for an atmospheric state $x$, aiming to reproduce the observation $F_{\text{meas}}$ with an accuracy $\epsilon$:

$$F_{\text{meas}} = F(x) + \epsilon$$  \hspace{1cm} (3.1)

Generally, the forward model describes a non-linear relationship between atmospheric and surface state and the observation. For that reason it should provide linearisations of the modelled observation with respect to state vector elements to facilitate an iterative retrieval.

Among existing methods to solve and linearise the radiative transfer equation, those based on splitting the model atmosphere in optically thin layers are numerically very efficient, especially in moderately scattering atmospheres. Applying a Fourier expansion for the azimuthal dependence and a Gaussian quadrature for the zenith dependence of the intensity fields, the radiative transfer equation can be rewritten as a linear system of equations in the intensity at the layer boundaries. Subsequently, this linear system can be solved using for instance Gauss-Seidel iterations or LU decomposition.

This represents the mathematical basis of the LINTRAN v1.0 radiative transfer model, developed by Landgraf et al. (2001) and Hasekamp and Landgraf (2002). It constitutes a plane-parallel vector radiative transfer code that is capable of simulating satellite-borne Earth-radiance measurements, including polarisation, with high accuracy. Linearisations with respect to atmospheric and
surface state parameters are provided through application of forward-adjoint perturbation theory. LINTRAN v1.0 has been widely used as a forward model in retrieval algorithms targeting a range of different trace gases as well as aerosol properties utilising satellite measurements in the near infra-red as well as ultraviolet part of the electromagnetic spectrum (e.g. Hasekamp and Landgraf, 2001; Van Diedenhoven et al., 2007; Hasekamp et al., 2011; Butz et al., 2011; Schepers et al., 2012; Guerlet et al., 2013). However, in an atmosphere containing a cloud layer, LINTRAN v1.0 quickly becomes very time consuming due to the increased scattering by cloud droplets. This implies that practical applications of trace gas retrievals that rely on modelling effective light scattering are limited to cloud-free observations only.

The numerical inefficiency in cloudy atmospheres stems from the fact that the LINTRAN v1.0 radiative transfer solver assumes the intra-layer intensity field to be constant, in order to iteratively solve the radiative transfer problem using forward-adjoint perturbation theory. Because of this and unlike radiative transfer solvers based on o.a. Discrete Ordinates Method (DOM) (e.g. Rozanov et al., 2014; McGarragh, 2012; Spurr, 2006) or Matrix Operator Method (MOM) (e.g. Hollstein and Fischer, 2012; Sanghavi et al., 2014), it relies on splitting the model atmosphere into optically thin layers to guarantee sufficient accuracy.

This work contains a series of updates to the LINTRAN v1.0 model that aims to remedy this. The advancement of the new model, designated LINTRAN v2.0, is based on the observation that the majority of structure in the diffuse intensity field originates from radiation that has only been scattered a few times i.e radiation of low order of scattering. Consequently, the diffuse field tends to get smoother with increasing scattering order. Following that line of reasoning, we developed a mathematical framework that allows the combination of the radiative transfer perturbation theory (e.g. Box et al., 1989) with the separation of the first $N$ orders of scattering from the diffuse intensity vector field. Measurement simulations and their derivatives are calculated by combining analytical expressions for low-order of scattering with the quasi-analytical approach of the forward-adjoint perturbation theory.

In the LINTRAN v2.0 model we implemented this method, separating the first 2 orders of scattering, within the general framework of forward-adjoint perturbation theory. Because the intensity field comprised of orders of scattering higher than 2 is relatively smooth, the discretisation density of the model atmosphere in both angular and vertical coordinates can be significantly relaxed compared to LINTRAN v1.0 without loss in accuracy. Furthermore, the numerical solver used by LINTRAN v2.0 assumes that the high-order diffuse field within a model layer behaves as a linear function of the vertical coordinate, instead of being constant throughout the layer, allowing further relaxation of
the vertical discretisation in the numerical solver.

In addition, the new model is capable of modelling chlorophyll fluorescence from photosynthesising vegetation as a source of the diffuse intensity field. Modelling and retrieving the fluorescence signal is of importance for trace gas retrievals because it interferes with absorption features and solar lines (e.g. Joiner et al., 2012; Frankenberg et al., 2012), potentially affecting retrieved trace gas concentrations. Furthermore, the retrieved fluorescence itself may provide useful information on the functional status of vegetation and gross primary productivity (e.g. Joiner et al., 2011; Frankenberg et al., 2011).

In the next section of this work (Sect. 3.2) we briefly introduce the theory of radiative transfer in the context of forward-adjoint perturbation theory, before presenting a mathematical framework for separating the first \( N \) orders of scattering from the diffuse field, in Sect. 3.3. Subsequently, we present a way to recursively solve the intensity fields associated with the first \( N \) orders of scattering as well as a numerical scheme to solve the high-order field associated with orders of scattering greater than \( N \) in Sections 3.4 and 3.5 respectively. Section 3.6 contains a detailed description of the implementation of these solvers in LINTRAN v2.0, while in Sects. 3.7 and 3.8 respectively, we verify the accuracy of the new model and estimate the gain in numerical efficiency it achieves. Conclusions are presented in Sect. 3.9.

### 3.2 The forward-adjoint radiative transfer theory

The transport equation for vector radiative transfer in an atmosphere that is illuminated by a radiation source \( S \) can, in its forward formulation, be written as

\[
\hat{L} \circ I = S, \quad (3.2)
\]

where \( I \) denotes the monochromatic intensity vector containing the four Stokes parameters,

\[
I = [I, Q, U, V]^T. \quad (3.3)
\]

The forward transport operator \( \hat{L} \), including surface reflection at the bottom boundary of the atmosphere, comprises an operator to describe extinction \( \hat{L}_e \) and a scattering operator \( \hat{L}_s \) to account for all scattering events (Ustinov, 2001; Landgraf et al., 2002):

\[
\hat{L} = \hat{L}_e - \hat{L}_s \quad (3.4)
\]

with

\[
\hat{L}_e = \left[ \mu \frac{\delta}{\delta z} + \beta_e (z) \right] E \quad (3.5)
\]
and

\[ \hat{L}_s = \int_{4\pi} d\tilde{\Omega} \left\{ \frac{\beta_e(z)}{4\pi} Z(z, \tilde{\Omega}, \Omega) + G_s(\tilde{\Omega}, \Omega) \delta(z) \Theta(\mu) \delta(-\tilde{\mu}) \Theta(\tilde{\mu}) \right\}. \] (3.6)

Here \( z \) denotes the vertical coordinate running from the surface to the top of the atmosphere, \( \Omega \) is the solid angle determined by the azimuth angle \( \phi \) and the cosine of the zenith angle \( \mu \) (\( \mu < 0 \) for downward directions, \( \mu > 0 \) for upward directions) and \( \beta_e \) and \( \beta_s \) represent the extinction and scattering coefficients, respectively. \( Z \) denotes the phase matrix defined relative to the local meridian plane and \( G_s \) represents the bidirectional reflection distribution function (BRDF) that characterises the surface reflection. Furthermore, \( E \) is the 4-by-4 identity matrix, \( \delta \) and \( \Theta \) represent the Dirac delta function and the Heaviside step function, respectively.

The source term on the right-hand side of Eq. (3.2) is composed of a unidirectional solar source \( S_\odot \) incident at the top of the atmosphere and an isotropic source \( S_f \) at the bottom of the atmosphere representing fluorescent emissions by photosynthesising vegetation:

\[ S = S_\odot + S_f, \] (3.7)

with

\[ S_\odot = \mu_\odot \delta(z-z_{\text{toa}}) \delta(\Omega - \Omega_\odot) F_\odot, \] (3.8)

\[ S_f = \mu \delta(z) \Theta(\mu) F_f. \] (3.9)

Here \( F_\odot = [F_\odot, 0, 0, 0]^T \) denotes a monochromatic solar flux of a certain wavelength incident on the top of the atmosphere (TOA) at \( z_{\text{toa}} \), along solid angle \( \Omega_\odot = (-\mu_\odot, \phi_\odot) \) (with \( \mu_\odot > 0 \) by definition ). Similarly, \( F_f = [F_f, 0, 0, 0]^T \) represents an isotropic monochromatic flux emitted at the bottom of the atmosphere, for instance due to fluorescence by vegetation.

Solving the transport equation produces the complete intensity vector field, although in the context of satellite remote sensing one is generally interested in simulating a certain observation. Any observable or radiative effect that is a linear function of the intensity field \( I \) can be described by a suitable response function \( R \) (Marchuk, 1964; Box et al., 1988) through an inner product:

\[ F = \langle R, I \rangle. \] (3.10)

Here, the inner product of two arbitrary vector functions \( a \) and \( b \) is defined as

\[ \langle a, b \rangle = \int dz \int d\Omega \ a^T(z, \Omega) b(z, \Omega). \] (3.11)
Considering a downward viewing instrument measuring reflectance in one of the Stokes parameters \( I, Q, U \) and \( V \) at the top of the atmosphere in viewing direction \( \Omega_v \), the response function is given by

\[
R_i(z, \Omega) = \frac{1}{F_{\odot}} \delta(\Omega - \Omega_v) \delta(z - z_{toa}) e_i,
\]

where \( e_i (i = 1, \ldots, 4) \) denotes the unity vector in the direction of the \( i \)th Stokes parameter.

To provide linearisation with respect to atmospheric and surface parameters we employ the forward-adjoint perturbation theory (e.g. Marchuk, 1964; Box et al., 1988). Thus, we introduce the adjoint intensity field \( I^\dagger \) defined by the adjoint transport equation taking the response function as the adjoint source, viz.

\[
\hat{L}^\dagger \circ I^\dagger = R_i
\]

Here \( \hat{L}^\dagger \) represents the adjoint radiative transfer operator (Box et al., 1988; Ustinov, 2001; Landgraf et al., 2002). Within the forward-adjoint perturbation theory, the adjoint intensity field can be interpreted as the importance of photons within the atmosphere for a given observation (Bell and Glasstone, 1970; Lewins, 1965). Given the forward and adjoint intensity fields and the associated source and response functions, the derivative of the observable with respect to an atmospheric parameter \( x \) is given by (Walter et al., 2004; Ustinov, 1991)

\[
\frac{dF_i}{dx} = -\langle I^\dagger, \hat{L}' \rangle + \langle I^\dagger, S' \rangle + \langle R'_i, I \rangle,
\]

where \( \hat{L}' \) denotes the derivative of the transport operator with respect to \( x \), i.e.

\[
\hat{L}' = \lim_{\Delta x \to 0} \frac{\Delta \hat{L}}{\Delta x}
\]

and \( S' \) and \( R'_i \) denote derivatives of the source and response functions, respectively.

Analytical expressions for \( \hat{L}' \) concerning the derivative with respect to absorption and scattering coefficients, phase function and BRDF parameters have previously been derived (e.g. Box et al., 1989; Hasekamp and Landgraf, 2002; Landgraf et al., 2002).

Because the fluorescence flux \( F_f \) acts as a source in the transport equation (Eq. (3.2)), the only contribution to its derivative stems from the second term on the right hand side of Eq. (3.14). The derivative follows directly from differentiation of Eq. (3.9), resulting in the following expression for the derivative of
the observable with respect to fluorescence flux
\[
\frac{dF}{dF_f} = \int_{4\pi} d\Omega \quad I^\dagger (0, \Omega) \mu \Theta (\mu).
\] (3.16)
The right hand side of Eq. (3.16) constitutes the definition of the upward adjoint flux at the bottom of the atmosphere.

### 3.3 Separating $N$ orders of scattering

When solving the transport equation for the intensity field $I$, it is a common practice to separate the unidirectional direct beam contribution from the diffuse part of the intensity field. The total intensity field is thus written as
\[
I = I_0 + I_{>0}
\] (3.17)
where a subscript has been introduced to distinguish between parts of the total intensity field according to orders of scattering. Thus, $I_0$ denotes that part of the intensity field that is scattered 0 times i.e. the direct beam contribution. Analogously, $I_{>0}$ denotes the part that is scattered more than 0 times: the diffuse field.

Using the notation introduced in Eq. (3.4), the direct beam solution $I_0$ can be readily solved from the unscattered source $S_0 \equiv S$ by applying the extinction operator:
\[
\mathbf{L}_e \circ I_0 = S_0
\] (3.18)
Solving Eq. (3.18), we can subsequently substitute the split intensity field (Eq. (3.17)) in the transport equation given in Eq. (3.2) which, after rearranging terms, gives
\[
\mathbf{L} \circ I_{>0} = \mathbf{L}_s \circ I_0 = S_1
\] (3.19)
Here $S_1$ is introduced to denote the first order scattering source. Thus $S_1 (z, \Omega)$ denotes the radiation that is scattered from the direct beam into the direction $\Omega$, at vertical location $z$. Equations (3.18) and (3.19) form a set of equations from which the total intensity field $I = I_0 + I_{>0}$ can be solved (see e.g. Hasekamp and Landgraf, 2002).

This technique of splitting the total intensity field is not limited to the direct beam and may in fact be generalised to any higher order of scattering thus separating orders of scattering up to a certain truncation order $N$, namely
\[
I = I_0 + I_1 + \ldots + I_N + I_{\geq N+1},
\] (3.20)
which, after substitution in the transport equation produces a recursive relationship for $I_n \ (n = 1, \ldots, N)$, in analogy with Eq. (3.18),

$$\hat{L}_\epsilon \circ I_n = S_n, \quad (3.21)$$

where $S_n$ denotes the source of light scattered $n$ times. Furthermore, in analogy with Eq. (3.19), the following holds for the cumulative radiation field resulting from orders of scattering greater than $N$:

$$\hat{L} \circ I_{\geq N+1} = S_{N+1}. \quad (3.22)$$

Equations (3.21) and (3.22) again form a set that allows solving the total intensity field. Here different solving techniques can be used for $I_0, \ldots, I_N$ on the one hand and $I_{\geq N+1}$ on the other.

The approach of splitting the intensity field according to order of scattering is extended to the calculation of linearisations by considering the following:

$$\frac{dF_i}{dx} = \frac{d}{dx} \langle R_i, I_0 \rangle + \ldots + \frac{d}{dx} \langle R_i, I_N \rangle + \frac{d}{dx} \langle R_i, I_{\geq N+1} \rangle. \quad (3.23)$$

Here, we made use of Eqs. (3.10) and (3.20) to separate contributions to the observable stemming from $I_0, \ldots, I_N$ and $I_{\geq N+1}$, respectively. We choose to do so because Eq. (3.21) provides an analytical expression for the intensity field up to order of scattering $N$, and all derivatives with respect to atmospheric or surface state parameters may be found by straightforward differentiation.

To provide derivatives of the higher order intensity field $I_{\geq N+1}$ we employ forward-adjoint perturbation theory. Thus the derivative with respect to model parameter $x$ can be found through (Walter et al., 2004; Ustinov, 1991)

$$\frac{d}{dx} \langle R, I_{\geq N+1} \rangle = - \langle I^\dagger, \hat{L}' I_{\geq N+1} \rangle + \langle I^\dagger, S'_{N+1} \rangle + \langle R', I_{\geq N+1} \rangle \quad (3.24)$$

Note that derivatives $R'$ and $S'_{N+1}$ are available in analytically closed form by differentiation of the expressions given in Eqs. (3.12) and (3.21), respectively. The order of scattering $N$ at which the recursive solver is truncated is chosen based on the relative advantages and disadvantages of the recursive and numerical solver and is discussed in Sect. 3.6.1.
3.4 Recursive solver for low-order intensity field

Using Eq. (3.21), one can recursively solve the intensity field up to order of scattering \( N \). The recursive series is initialised with the unscattered solar beam and fluorescence,

\[
I_0(z, \Omega) = \mathbf{F}_\odot e^{-\Delta \tau(z, z_{\mathrm{toa}}) / \mu_\odot} \delta(\mu - \mu_\odot) \delta(\varphi - \varphi_\odot) + \mathbf{F}_f e^{-\Delta \tau(0, z) / \mu} \Theta(\mu),
\]  

(3.25)

where we introduced

\[
\Delta \tau(z', z) = (\tau(z') - \tau(z)).
\]  

(3.26)

for ease of notation. The optical thickness coordinate \( \tau \) is measured from the top of the atmosphere downwards.

Let \( z_n \) denote the altitude at which the \( n \)th order scattering event takes place that scatters solar radiation from direction \( \Omega_{n-1} \) into direction \( \Omega_n \). Similarly, \( \tilde{z}_n, \tilde{\Omega}_{n-1} \) and \( \tilde{\Omega}_n \) describe the \( n \)th scattering event of radiation originating from the fluorescence source. By re-substitution of Eq. (3.21), the expression for \( I_n \) can be written as a sum of two integrals over altitude and solid angle that take into account all possible light paths comprising \( n \) scattering events (Maurellis et al., 2004):

\[
I_n(z, \Omega) = \mathbf{F}_0 \int_0^{z_{\mathrm{toa}}} dz_n \ldots dz_1 e^{-\Delta \tau(z_1, z_{\mathrm{toa}}) / \mu_\odot} \prod_{r=1}^n \frac{1}{|\mu_r|} \hat{L}_s e^{-\Delta \tau(z_r, z_{r+1}) / \mu_r} + \mathbf{F}_f \int_0^{z_{\mathrm{toa}}} d\tilde{z}_n \ldots d\tilde{z}_1 e^{-\Delta \tau(0, \tilde{z}_1) / \tilde{\mu}_0} \prod_{r=1}^n \frac{1}{|\tilde{\mu}_r|} \hat{L}_s e^{-\Delta \tau(\tilde{z}_r, \tilde{z}_{r+1}) / \tilde{\mu}_r}
\]  

(3.27)

where index \( n = 1 \ldots N \) denotes the scattering order while \( r = 1 \ldots n \) is introduced to distinguish between the different scattering events. In this notation we require \( z \equiv z_{n+1} \equiv \tilde{z}_{n+1} \) and \( \Omega \equiv \Omega_n \equiv \tilde{\Omega}_n \). Also, we use the scattering operator \( \hat{L}_s \) as defined in Eq. (3.6).

The first integral of Eq. (3.27) comprises all possible light paths originating from the solar source at the TOA that, after being scattered \( n \) times, arrive at altitude \( z \) in the direction defined by \( \Omega \). This is illustrated in Fig. 3.1 where one
such light path is drawn and annotated with the relevant variables and terms used in Eq. (3.27). Similarly, the second integral of Eq. (3.27) comprises all such light paths originating from the fluorescence source.

By means of Eq. (3.27), the diffuse intensity field after \( n \) orders of scattering is available in an analytically closed form. The integration over the unit sphere that is contained within the scattering operator \( \hat{L}_s \) can be evaluated by any suitable method. For instance by a finite element integration or by employing a Gaussian quadrature combined with a Fourier expansion in relative azimuth angle (see Sect. 3.5).

3.5 Solving the high-order intensity field

In order to solve the high-order intensity field \( I_{\geq N+1} \) from Eq. (3.22), we aim to use a numerical scheme. To facilitate the integration over azimuth we expand...
the phase matrix, intensity field and source field as a truncated Fourier series
in relative azimuth angle \( \Delta \varphi = \varphi_0 - \varphi_v \) as proposed by Hovenier and Van der
Mee (1983) and De Haan et al. (1987). Thus, \( I_{\geq N+1} \) is expanded as

\[
I_{\geq N+1} (z, \Omega) = \sum_{m=0}^{M} (2 - \delta_{m0}) \left[ B^+m (\varphi_0 - \varphi) I^+_{\geq N+1} (z, \mu) \right.
\]

\[
+ B^-m (\varphi_0 - \varphi) I^-_{\geq N+1} (z, \mu) \right] \tag{3.28}
\]

Here, the superscript \( m \) denotes the \( m \)-th component of the Fourier expansion,
which is truncated in \( M \)-th order. Subsequently the \( m \)-th Fourier term of the
phase matrix is expanded using generalised spherical functions (De Rooij and
Van der Stap, 1984; Domke, 1975; Siewert, 1982; Sanghavi, 2014)

\[
Z^m (z, \mu', \mu) = (-1)^m \sum_{l=m}^{M} P^l_m (\mu) S^l (z) P^l_m (\mu'), \tag{3.29}
\]

for \( m = 0, \ldots, M \). The matrices \( P^l_m \) contain the generalised spherical functions
for the expansion while \( S^l \) contains the expansion coefficients which follow
directly from the scattering phase matrix:

\[
S^l = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & s_3^l & s_6^l \\
0 & s_5^l & s_2^l & 0 \\
s_1^l & s_5^l & s_2^l & 0 \\
0 & 0 & -s_6^l & s_4^l \\
0 & 0 & s_3^l & s_6^l
\end{pmatrix} \tag{3.30}
\]

Analogously, Eq. (3.22) decomposes into a set of similar equations per Fourier
component of the intensity and source fields

\[
\tilde{L}^m \circ I^m_{\geq N+1} = S^m_{N+1}. \tag{3.31}
\]

To handle integration over zenith angle cosine \( \mu \), we introduce a double Gaussian quadrature of total order \( 2I \), letting \( \mu_i \) denote the Gaussian points and \( a_i \)
their corresponding weights. For convenience, we introduce the single scattering
albedo \( \omega = \beta_s / \beta_e \) and convert the vertical coordinate \( z \) to optical depth \( \tau \),
considering that \( d\tau = -\beta_e dz \). Also, we consider an atmosphere which consists
of \( K \) layers assuming constant absorption and scattering properties within each
layer. Thus, for layer \( k \) out of \( K \) homogeneous layers, we assume

\[
Z^m (\tau, \mu_i', \mu_i) = Z^m_k (\mu_i', \mu_i) \quad \text{for} \quad \tau_{k-1} < \tau < \tau_k \tag{3.32}
\]

\[
\omega (\tau) = \omega_k \quad \text{for} \quad \tau_{k-1} < \tau < \tau_k \tag{3.33}
\]
where $\tau_{k-1}$ and $\tau_k$ represent the optical depth at the top and bottom of model layer $k$, respectively.

Equation (3.22) can now be transformed into a set of two integral equations for each model layer, Fourier component and quadrature point. In particular, integrating from the bottom of a layer at $\tau_k$ up to an optical depth $\tau > \tau_{k-1}$ results in an equation describing upward streams:

$$I_{m \geq N+1}^{m+1}(\tau, \mu_i) = I_{m \geq N+1}^{m+1}(\tau_k, \mu_i) e^{-(\tau_k - \tau)/\mu_i} +$$

$$\int_{\tau_k}^{\tau} e^{-(\tau'-\tau)/\mu_i} J_{m \geq N+1}^{m+1}(\tau', \mu_i) \frac{d\tau'}{\mu_i},$$

(3.34)

while performing an integration over optical depth from the top of layer $k$ at $\tau_{k-1}$ downward until an optical depth $\tau < \tau_k$ yields for downward streams:

$$I_{m \geq N+1}^{m+1}(\tau, -\mu_i) = I_{m \geq N+1}^{m+1}(\tau_{k-1}, -\mu_i) e^{-(\tau - \tau_{k-1})/\mu_i} +$$

$$\int_{\tau_{k-1}}^{\tau} e^{-(\tau'-\tau)/\mu_i} J_{m \geq N+1}^{m+1}(\tau', -\mu_i) \frac{d\tau'}{\mu_i}.$$

(3.35)

The source function $J_{m \geq N+1}^{m+1}(\tau, \mu_i)$ contains the discretised scattering operator applied to $I_{m \geq N+1}^{m+1}$ and the initialising radiation source of order $N + 1$ (see Eq. (3.31)):

$$J_{m \geq N+1}^{m+1}(\tau, \mu_{i'}) = \frac{\omega_k}{2} \sum_{i'=-I}^{I} a_i z_k^{m+1}(\mu_i, \mu_{i'}) I_{m \geq N+1}^{m+1}(\tau, \mu_i)$$

$$+ S_{m \geq N+1}^{m+1}(\tau, \mu_{i'}).$$

(3.36)

Here, subscripts $i$ and $i'$ are used as an index for the streams of the double Gaussian quadrature of order $2I$.

Given a truncation scattering order $N$, we assume a linear dependence of $I_{m \geq N+1}^m$ on optical depth $\tau$. Any higher order dependence of $I_{m \geq N+1}^m$ on $\tau$ can be mitigated by splitting model layers into several, sufficiently thin sub-layers. Thus, for upward and downward streams we write, respectively

$$I_{m \geq N+1}^{m+1}(\tau, \mu_i) = c_0^{k,i} + c_1^{k,i}(\tau_k - \tau),$$

$$I_{m \geq N+1}^{m+1}(\tau, -\mu_i) = c_0^{k,i} + c_1^{k,i}(\tau - \tau_{k-1})$$

(3.37)

(3.38)

for $\tau_{k-1} \leq \tau \leq \tau_k$. The choice of truncation order $N$ and the aforementioned assumption will be more thoroughly discussed in Sects. 3.6.1 and 3.6.3 respectively.
After substituting the linear approximations for $I_{m \geq N+1}$ in Eq. (3.36), the integration of the layer-internal intensity field in Eqs. (3.34) and (3.35) can be performed analytically, to yield:

$$I_{m \geq N+1}(\tau, \mu_i) = I_{m \geq N+1}(\tau_k, \mu_i) e^{-(\tau_k - \tau)/\mu_i}$$

$$+ \frac{\omega_k}{2} \sum_{i'=-I}^{I} a_{i'} Z^m_k (\mu_{i'}, \mu_i)$$

$$c^{k,i'}_0 \left[ 1 - e^{-(\tau_k - \tau)/\mu_i} \right]$$

$$+ \frac{\omega_k}{2} \sum_{i'=-I}^{I} a_{i'} Z^m_k (\mu_{i'}, \mu_i)$$

$$c^{k,i'}_1 \left[ (\tau_k - \tau) - \mu_i \left( 1 - e^{-(\tau_k - \tau)/\mu_i} \right) \right]$$

$$\delta I_{m \geq N+1}(\tau, \mu_i)$$

(3.39)

for upward streams and the corresponding expression for downward streams. We introduced $\delta I_{m \geq N+1}$ to denote the integral in Eq. (3.34) applied to $S^m_{m \geq N+1}$.

By expressing the linear coefficients $c^{k,i}_0$ and $c^{k,i}_1$ in terms of $I_{m \geq N+1}$ at the layer boundaries and subsequently matching the incoming and outgoing intensities at those boundaries given by Eq. (3.39) and its downward counterpart, a system of equations can be constructed for the intensities at all layer interfaces $k$ as was shown by Hasekamp and Landgraf (2002) for a layer-average approximation of the total diffuse intensity field.

$$\Phi^k = A_{+-} \Phi^{-k} + A_{-+} \Phi^k + B_{+-} \Phi_{-+}$$

$$\Gamma^k = \Phi^k + \Phi^k$$

(3.40)

In the remaining part of this section, we will present updated definitions of the vectors and (sub-)matrices defined by Hasekamp and Landgraf (2002) such that they incorporate the splitting of low and high-order intensity fields as well as the linear approximation of $I_{m \geq N+1}$.

For $k = 1, \ldots, K$, the $4I$-dimensional vectors $\Phi^k_\pm$ and $\Gamma^k_\pm$ are defined as

$$\Phi^k_\pm = \begin{pmatrix} I^m_{m \geq N+1}(\tau_k, \mu_{\pm1}) \\ \vdots \\ I^m_{m \geq N+1}(\tau_k, \mu_{\pm1}) \end{pmatrix}, \quad \Gamma^k_\pm = \begin{pmatrix} \delta I^m_{m \geq N+1}(\tau_k, \mu_{\pm1}) \\ \vdots \\ \delta I^m_{m \geq N+1}(\tau_k, \mu_{\pm1}) \end{pmatrix}$$

(3.41)
and the matrices $A^k_{\pm \pm}$ and $B^k_{\pm \pm}$ are defined as

$$
A^k_{\pm \pm} = \left( \alpha^k_{\pm i', \pm i} \right),
$$

$$
B^k_{\pm \pm} = \left( \beta^k_{\pm i', \pm i} \right),
$$

with sub-matrices containing a linear representation of the intensity field:

$$
\alpha^k_{\pm i, \pm i'} = \frac{\omega_k}{2} a_{i'} Z^m_k (\mu_{\pm i'}, \mu_{\pm i}),
$$

$$
\beta^k_{\pm i, \pm i'} = \frac{\omega_k}{2} a_i Z^m_k (\mu_{\pm i'}, \mu_{\pm i})
$$

\begin{align*}
&\left[ 1 - \frac{\mu_{i}}{\Delta \tau_k} \left( 1 - e^{-\Delta \tau_k / \mu_{i}} \right) \right],
\end{align*}

$$
+ \delta_{ii'} e^{-\Delta \tau_k / \mu_{i}} E.
$$

Furthermore, at the top boundary of the atmosphere, we define

$$
\Phi_0^- = \begin{pmatrix}
0 \\
0 \\
\vdots \\
0
\end{pmatrix}
$$

The surface reflection as well as the fluorescent emission at the lower atmospheric boundary is accounted for by requiring

$$
\Phi^K_+ = A_s \Phi^K_- + \Gamma_s F_0 e^{-\tau_K / \mu_\odot}
$$

$$
+ \delta_{om} \begin{pmatrix}
F_f \\
\vdots \\
F_f
\end{pmatrix}
$$

with the $4I$ square matrix $A_s$ and the $4I$ vector $\Gamma_s$ defined as

$$
A_s = 2 \begin{pmatrix}
\mu_1 G^m_s (\mu_1, \mu_1) & \cdots & \mu_I G^m_s (\mu_I, \mu_1) \\
\vdots & \ddots & \vdots \\
\mu_1 G^m_s (\mu_1, \mu_I) & \cdots & \mu_I G^m_s (\mu_I, \mu_I)
\end{pmatrix},
$$

$$
\Gamma_s = \begin{pmatrix}
\mu_1 G^m_s (\mu_1, \mu_1) \\
\vdots \\
\mu_1 G^m_s (\mu_1, \mu_I) \\
\mu_I G^m_s (\mu_1, \mu_1) \\
\mu_I G^m_s (\mu_I, \mu_1) \\
\vdots \\
\mu_I G^m_s (\mu_I, \mu_I)
\end{pmatrix}.
$$
\[ \Gamma_s = \frac{\mu_\odot}{\pi} \begin{pmatrix} \Gamma_{s}^m (\mu_\odot, \mu_1) \\ \vdots \\ \Gamma_{s}^m (\mu_\odot, \mu_I) \end{pmatrix}. \] (3.48)

and \( \Gamma_{s}^m \) denotes the \( m \)-th coefficient of the Fourier-expanded surface reflection matrix.

Combining Eqs. (3.40), (3.45) and (3.46) for the entire atmosphere, a linear system can now be constructed (Hasekamp and Landgraf, 2002)

\[ \mathbf{M} \mathbf{I} = \mathbf{C} \] (3.49)

such that \( \mathbf{M} \) is a \((2K+1)4I \times (2K+1)4I\) matrix containing the submatrices \( \mathbf{A}_{\pm}^k \) and \( \mathbf{B}_{\pm}^k \) \((k = 0, \ldots, K)\) in a band structure around the diagonal. Analogously, \( \mathbf{I} \) and \( \mathbf{C} \) are \((2K+1)4I\)-dimensional vectors containing of the vectors \( \mathbf{\Phi}_{\pm}^k \) and \( \mathbf{\Gamma}_{\pm}^k \), respectively.

### 3.6 Model implementation

In the previous sections we have presented the mathematical framework to separate the first \( N \) orders of scattering from the diffuse intensity field and to solve \( \mathbf{I}_1, \ldots, \mathbf{I}_N \) recursively in an analytical manner. The residual high-order field \( \mathbf{I}_{\geq N+1} \), containing radiation that is scattered more than \( N \) times, is subsequently solved employing a numerical scheme. This numerical scheme relies on the assumption that \( \mathbf{I}_{\geq N+1} \) can be approximated as a linear function of optical depth \( \tau \) within an atmospheric model layer. In this section we will elaborate further on how this mathematical framework is implemented in the LINTRAN v2.0 model.

#### 3.6.1 Truncation scattering order \( N \)

For numerical implementation one has to realise that the numerical cost of the recursive solver described in Sect. 3.4 increases dramatically for third and higher orders of scattering. Hence, in this work we consider the implementation for \( N = 2 \), thus separating the first and the second order of scattering from the diffuse field to be solved analytically. Figure 3.2 shows the dependence of \( \mathbf{I}_1, \mathbf{I}_2 \) and \( \mathbf{I}_{\geq 3} \) along the line of sight (LOS) defined by \( \mu = \pm \cos(80^\circ) \), assuming a homogeneous scattering atmosphere of unity optical thickness. A Lambertian BRDF is assumed, equivalent to an albedo of 0.2. A LOS with a large zenith angle was chosen because it provides an exemplary case for this discussion while such slant light paths contribute significantly to the diffuse intensity field.
Figure 3.2 – Transects of the intensity field contributions $I_1$, $I_2$ and $I_{\geq 3}$ (Stokes parameter $I$) within a homogeneous atmospheric layer of optical thickness 1, solar zenith angle $0^\circ$ and $\omega = 1.0$. The two upper panels show the downwelling and upwelling radiation associated with the three intensity field contributions along a line of sight for which $\mu = \cos(80^\circ)$. The lower panel shows the contributions of the three different intensity fields at the top of atmosphere as function of zenith angle $\mu$. The relative zenith angle $\Delta \varphi$ is zero and $\mu_\odot = \cos(0^\circ)$. Calculations are performed for a pure Mie scattering matrix assuming a size parameter $\chi \approx 35$, which corresponds to a 4.3 $\mu$m diameter scattering particle at 773 nm.
Figure 3.3 – Simplified illustration of the single scattering geometry in a homogeneous atmosphere, with the unidirectional solar source $S_\odot$ illuminating the top of the atmosphere. Downward and upward lines of sight are drawn from A to C and A’ to C’, respectively.

The downwelling $I_1$ field shows a distinct peak around a quarter of the total optical path length before decaying seemingly exponentially with increasing optical depth. This characteristic feature is a direct consequence of the singly scattered nature of $I_1$.

Figure 3.3 illustrates that the diffuse downward intensity at location B along a downward line of sight results from the accumulation of light scattered into the LOS and its extinction along the LOS between point A at the TOA and point B. In case of singly scattered light $I_1$, for which the direct beam acts as radiation source, the accumulating effect is especially strong at low optical depth because both the solar beam and the radiation along the line of sight are not significantly attenuated. Going to higher optical depth, the attenuation along the line of sight and the direct beam becomes dominant, causing a decay in intensity.

In the same manner, $I_2$ is shaped by the competing effects of accumulation and attenuation. However, in this case $I_1$ serves as the source for radiation scattered into the line of sight instead of the solar beam. Thus, in this case the source is zero at the top of the atmosphere and increases to a maximum before
decaying. Hence, the accumulation of double scattered radiation at low optical depth is less strong than it is for $I_1$, resulting in a less pronounced peak in the double scattering field $I_2$ as well as in $I_{\geq 3}$.

For an upward line of sight, $I_1$ is already far less structured than its downwelling counterpart. Here, the attenuation of the direct sunlight by the atmosphere above point B’ is balanced by the contribution of the surface reflection. Moreover, attenuation along the upward LOS is countered by the increased strength of the direct beam, preventing a decay in intensity.

An analogous reasoning holds for the angular smoothness of the diffuse intensity as illustrated in the bottom panel of figure 3.2. It shows variation of $I_1$, $I_2$ and $I_{\geq 3}$ with zenith angle $\mu$. It is clear that the shape of the single-scattering field is dominated by the characteristics of the scattering phase function, which in this case follows from Mie theory assuming a size parameter of $\chi \approx 35$. In the double scattering field the backscatter peaks are already significantly smoothed, while the high-order field shows even less of those structures. The importance of this smoothing effect becomes apparent when considering the numerical solver that is used to solve $I_{\geq N+1}$ because it relies on discretising the high-order field in $\tau$ and $\Omega$. To capture all structures in low-order fields like $I_1$ and $I_2$ requires a dense angular discretisation. The smoother high-order field on the other hand can be sampled less densely, directly reducing numerical cost involved with the numerical solver for $I_{\geq 3}$. Overall, this motivates the choice for $N = 2$ as it is implemented in LINTRAN v2.0.

### 3.6.2 Angular integration within recursive solver

Describing the solid angle integration by employing a double Gaussian quadrature in combination with a Legendre expansion of the phase function and the intensity field that is expanded in a Fourier series in relative azimuth angle (see Eq. (3.28)) is very efficient. It is therefore preferable to use this technique in the recursive solver based on Eq. (3.27) as well. However, it should be noted that in such a case, we can define two independent quadratures and expansion orders for the recursive and the numerical solver, respectively. This is especially important when considering a phase function containing many angular features, such that a high-order quadrature, and associated phase function expansion, is needed to capture all structures in $I_2$. Such a high order quadrature is inexpensive in the recursive solver. The numerical solver can subsequently use a significantly lower order quadrature. For all results presented in this paper we follow this approach.
3.6.3 Layer splitting and quadrature order

Although \( I_{\geq 3} \) is relatively smooth, it clearly deviates from depending linearly on the optical depth coordinate \( \tau \). Because the assumption of linearity is valid for sufficiently optically thin model layers we split atmospheric layers with a scattering or absorbing optical thickness that do not exceed given thresholds \( \Delta_s \) and \( \Delta_a \) respectively. Effectively, the layer splitting thresholds govern the density of discretisation in \( \tau \). Because this method increases the dimension of matrix equation (3.49), an increase in accuracy through denser discretisation comes at a numerical cost. Eventually, the values of \( \Delta_s \) and \( \Delta_a \) should be chosen as a compromise between accuracy required and numerical effort involved in solving \( I_{\geq 3} \). Therefore, the threshold will differ per application.

Moreover, the accuracy of the diffuse intensity fields is governed by both the order of the Gaussian quadrature \( I \) and the order of the Fourier expansion \( M \). Requiring conservation of energy, the normalisation of the phase matrix can only be guaranteed for \( M \leq 2I - 1 \) orders of Fourier expansion. Thus, the accuracy of our solver is determined by both the maximum allowable layer thickness and the order of the Gaussian quadrature. The choice of \( \Delta_a, \Delta_s \) and \( I \) is discussed further in Sect. 3.8.

3.6.4 Techniques for solving the linear system \( MI = C \)

The linear system given in Eq. (3.49) can be solved using several techniques available of which we selected two: the Gauss-Seidel (GS) iterative method and LU decomposition.

Generally, the Gauss-Seidel method (or any iterative method) is effective when it is initialised close to the final solution. Within the framework presented here, the GS solver is initialised with \( I_2 \). For weakly scattering conditions the iterative approach converges relatively fast, whereas in heavily scattering conditions like a cloud or thick aerosol layer, the GS solver is initialised far away from the final solution causing slow convergence in such cases. The LU decomposition on the other hand suffers from computational overhead from floating point operations involved in restructuring and decomposing matrix \( M \). This overhead is independent from the state of the atmosphere, and thus LU decomposition will perform similarly for any atmospheric state considering a given layer splitting.

3.6.5 The adjoint transport operator and its pseudo-forward formulation

The forward and adjoint transport operators \( \hat{L} \) and \( \hat{L}^\dagger \) generally are different in nature and therefore two dedicated algorithms are required to simulate the
forward and adjoint intensity fields. However, due to the reciprocal nature of light it is possible to transform the adjoint problem in Eq. (3.13) into a quasi-forward form (Bell and Glasstone, 1970; Box et al., 1988)

\[ \hat{L} \circ \Psi = S_{\Psi}, \]  
(3.50)

by reversing the direction \( \Omega \) and applying the appropriate transformations to the source term and adjoint (i.e. transposed) phase matrix (Hovenier, 1969):

\[ \Psi(z, \Omega) = I^\dagger(z, -\Omega), \]
\[ S_{\Psi}(z, \Omega) = R_i(z, -\Omega), \]
\[ Z^T_{\Psi}(z, -\Omega, -\tilde{\Omega}) = T Z \left( z, \tilde{\Omega}, \Omega \right) T, \]  
(3.51)

with \( T = \text{diag}(1, 1, 1, -1) \). Because the quasi-forward formulation makes use of the forward transport operator and because the source function \( S \) and the response function \( R_i \) both constitute the same type of source, the pseudo-forward problem may be solved using the exact same algorithm as the forward problem in Eq. (3.2). This is desirable because it reduces the overall complexity of the algorithm.

### 3.7 Model verification

In this section, we verify the new model version (LINTRAN v2.0) which uses the analytical solution of the first and second order of scattering and the numerical solution of the high-order intensity field assuming a linear dependence on the optical depth coordinate \( \tau \). We compare the new model version against the previous implementation (LINTRAN v1.0). The model version v1.0 combines the analytical solution of the first order of scattering field with the numerical solution of the diffuse intensity field of higher scattering order. For the numerical solution of the diffuse field, LINTRAN v1.0 assumes that the intensity field within a model layer does not vary with the optical depth coordinate within that layer. In practice this means that the intra-layer intensity is set to the average of the intensities at both layer boundaries. For the comparison we focus on the treatment of the diffuse field in both model versions, hence the accuracy of the simulated reflected radiances in viewing direction at the TOA is a good indicator for model performances.

First, we investigate the numerical advantages of the new solver for a homogeneous model layer illuminated at the top by the solar beam. The surface source \( F_f \) and the surface reflection are set to zero, to create a worst case scenario for modelling the diffuse intensity field. For the performance analysis, we disabled the layer splitting for both model versions.
As a reference, we employ simulations \( F_{\text{ref}} \) that are modelled with extremely fine layer splitting \((\Delta_a = \Delta_s = 0.01)\). For a quantitative analysis, we define the relative model accuracy as the difference

\[
\Delta F = \frac{F - F_{\text{ref}}}{F_{\text{ref}}}.
\]  

(3.52)

Figure 3.4 summarises the model accuracies as a function of scattering optical thickness \( \tau_s \) for varying absorption optical thickness, \( 0 < \tau_a < 1 - \tau_s \), assuming either isotropic scattering or a Henyey-Greenstein phase function with asymmetry parameter \( g = 0.8 \). First of all, it clearly shows that the accuracy of both versions deteriorates with increasing scattering optical thickness. This confirms the need for layer splitting in both versions. More important however, it shows that v2.0 tolerates significantly thicker layers than v1.0 when requiring a given model accuracy, for both the isotropic or the Henyey-Greenstein scattering phase function. Thus considering the implementation of v2.0, the layer splitting criterion can be significantly less strict compared to v1.0, while achieving the same accuracy in \( F \). The clouds of data points in Fig. 3.4 are bounded at the lower edge (highest absolute error) by cases of conservative scattering, while the most accurate results on the upper edge are those with maximum absorption optical thickness \( (\tau_a = 1 - \tau_s) \).

Subsequently, we investigate the sensitivity of \( F \) to the discretisation in its angular coordinates \( \mu \) and \( \Delta \phi \) i.e. the degree of the Gaussian quadrature in zenith angle and the truncation order of the Fourier expansion in relative azimuth angle, respectively. To this end, we assume a simple homogeneous atmosphere of total optical thickness \( \tau_e = 1.0 \) albeit this time with a fixed single scattering albedo of \( \omega = 0.9 \). The angular structure in \( I \) is predominantly governed by the characteristic of the scattering phase function. Thus, for this assessment to be significant we assume the Mie phase function that was used for Fig. 3.2. To isolate the effect of angular discretisation, \( \Delta_s \) is set to 0.01 for both LINTRAN v1.0 and v2.0.

Discretisation in zenith angle \( \mu \) is directly governed by the order of the Gaussian quadratures \( I \) (see Sect. 3.5). Thus in a similar way as before, we model a reflectance measurement using both model versions while varying the quadrature order \( I \). The results (Fig. 3.5) show that model v1.0 is significantly more sensitive to reduced discretisation in \( \mu \) than version v2.0. Thus given a certain accuracy requirement, the latter allows for using lower order Gaussian quadratures than version v1.0. Through a similar exercise we find that a significant reduction can also be achieved in the minimum Fourier expansion truncation order \( M \), as shown in Fig. 3.6.

Overall, these three experiments show that the discretisation in \( \tau \), as well as the number of quadrature points and Fourier expansion terms can be sig-
Figure 3.4 – Relative error on the first Stokes parameter of the reflectance vector in viewing direction ($\mu_v = \cos(15^\circ)$, $\mu_\odot = \cos(30^\circ)$, $\Delta \varphi = 60^\circ$) calculated using LINTRAN v1.0 and v2.0. Varying combinations of single scattering albedo $\omega$ and total optical thickness $\tau_a$ have been collapsed onto the x-axis as $\tau_s$. The error ranges are limited at the high-error side by non-absorbing atmospheres. The low-error limit is described by cases with maximum absorption. The upper panel shows the results assuming isotropic scattering, the lower panel assumes a Henyey-Greenstein phase function ($g = 0.8$).
Figure 3.5 – Relative absolute error on the first Stokes parameter of the reflectance vector averaged over a range of viewing angles ($\cos^{-1}(\mu_v) = 0^\circ, \ldots, 85^\circ$) while $\Delta \varphi = 0^\circ$ and $\mu_0 = \cos(50^\circ)$. Results for LINTRAN v1.0 and v2.0 are shown as function of Gaussian quadrature order $I$ ($M = 2I - 1$ Fourier terms are considered). A homogeneous atmosphere with an optical thickness of 1.0 and single scattering albedo of 0.9 is assumed. The phase function stems from Mie theory with size parameter $\chi \approx 35$.

Significantly reduced in LINTRAN v2.0 compared to v1.0, for a given accuracy requirement on $\mathcal{F}$. These reductions directly reduce the dimension of the linear system in Eq. (3.49), in turn reducing the numerical effort needed to solve it.

In the remainder of this work we assess the performance of LINTRAN v2.0 in more realistic atmospheric scenarios for satellite based reflectance measurements involving the $\text{O}_2$ absorption lines in the near infrared (NIR) region of the electromagnetic spectrum. Generally, in the NIR region, $\Delta \mathcal{F}$ is significantly more sensitive to $\Delta \sigma$ than it is to $\Delta \alpha$. Thus, in the following discussions we specify $\Delta \sigma = 0.1$ and $\Delta \alpha \rightarrow \infty$. The latter effectively means that no layer splitting is applied based on absorption optical thickness.

The base for the following scenarios constitutes an atmosphere including Rayleigh scattering and absorption by oxygen, to which an aerosol layer characterised by a Gaussian vertical distribution with a full width at half maximum (FWHM) of 2 km, centred at the ground surface, is added. The total optical
thickness of the boundary layer aerosol $\tau_{aer}$ is set to 0.3 and the aerosol single scattering albedo is fixed at 0.85 with an associated Henyey-Greenstein scattering phase function ($g = 0.60$). Absorption and scattering characteristics of oxygen follow from a spectroscopic parameter database (Rothman et al., 2009) and Rayleigh scattering calculations (Bucholtz, 1995), and are shown in Fig. 3.7. At the surface, a (spectrally constant) Lambertian BRDF is assumed, equivalent to an albedo of 0.15. Added to this is a fluorescence flux. The spectral shape of the latter, plotted in Fig. 3.7, is approximated by two co-added Gaussian functions (Frankenberg et al., 2012). The emitted flux is normalised with its value at 755 nm, which is set to $1 \text{ mW nm}^{-1} \text{ sr}^{-1} \text{ m}^{-2}$.

Given this scenario we calculate two reflectance observations ($\mu_v = \cos(15^\circ)$, $\varphi_v = 60^\circ$) of the oxygen-A absorption features between 757 and 773 nm, one assuming cloud-free conditions, and the other assuming a stratified cloud layer at an altitude of 3 km. This cloud layer is modelled using a Gaussian non-absorbing scattering layer of optical thickness 3.0, centred at 3 km, with a FWHM of 2 km. For the cloud droplets a Henyey-Greenstein ($g = 0.80$) phase function is assumed. In addition to reflectance spectra, linearisations with respect to surface and atmospheric parameters are also calculated. At 773 nm, with $\Delta_s = 0.1$,
the cloudy and cloudless atmosphere are split into $K = 76$ and $K = 51$ model layers, respectively. The reference model splits both atmospheres into 399 and 98 layers.

Both modelled reflectance observations are plotted in the top panel of Fig. 3.8 while the bottom panel shows the corresponding residuals relative to the reference simulation which are well within 0.2% for the entire spectral range covered. Derivatives with respect to surface albedo and fluorescence at 755 nm, with their respective residuals, are plotted in Fig. 3.9. One effect of fluorescence on the modelled measurement constitutes the filling up of Fraunhofer lines, resulting in the above-continuum level peaks in the derivative with respect to fluorescence in Fig. 3.9. Height-resolved derivatives of $F$ with respect to the absorption coefficient, the scattering coefficient, and the first moment of the scattering phase function expansion $s_1$ (see Eq. (3.30)) are shown in Fig. 3.10 for two selected wavelengths. The two top panels show the derivatives and their residuals at a continuum wavelength (773 nm), while the plots in the two bottom panels correspond to a wavelength characterised by moderate molecular absorption (760 nm). Comparing the residuals at these two wavelengths, it is clear that the accuracy of LINTRAN v2.0 improves with increasing absorption. The residuals on the derivatives plotted in Figs. 3.9 and 3.10 are of similar magnitude as those on the spectra in Fig. 3.8 and are solely introduced by the numerical solver through the discretisation of the high-order intensity field in the optical depth coordinate.

3.8 Model efficiency

Based on the test cases that were presented in the previous section, we can make an estimate of the relative numerical efficiency of the numerical solvers in LINTRAN v1.0 and v2.0. Thus, this analysis does not include the effort involved in separately solving the double scattering contribution $I_2$ which, because of the analytical approach used to solve it, involves relatively little numerical effort when compared to the numerical solver used to solve the high-order field $I_{\geq 3}$.

To compare both model versions, we point out that the numerical complexity, or the number of floating point operations $\mathcal{E}$ involved in executing the LU-decomposition of matrix $M$ is proportional to the number of atmospheric model layers $K$, the number of terms in the Fourier expansion $M$ and the quadrature order $I$

$$\mathcal{E}^{LU} \propto K M I^3,$$

(3.53)

for a sufficiently large matrix $M$.

Subsequently, we use Figs. 3.4 and 3.5 to select the parameters $\Delta_s$ and
Figure 3.7 – Vertically integrated absorption and scattering optical thickness of the cloudless test atmosphere ($\tau_a$ and $\tau_s$, left axis) and fluorescence flux ($F_f$, right axis) between 757 nm and 773 nm. The inset axis shows the spectral shape of the fluorescence flux on a broader scale, illustrating the co-added Gaussian functions.

$I$ for both LINTRAN v1.0 and v2.0 such that both produce the observable $F$ with a given accuracy. The Fourier truncation order $M$ is set to its maximum allowable value $M = 2I - 1$ (see Sect. 3.6.3), ignoring any earlier convergence of the Fourier series. Table 3.1 shows the selected parameter values for v1.0 and v2.0, requiring $\Delta F \approx 0.5\%$ and assuming that errors on $F$ introduced through the reduction in the number of model layers and the quadrature order can be considered independently.

Given Eq. 3.53 and the values in Table 3.1, it is possible to make a rough estimate of the difference in numerical effort involved with LU-decomposition, when using LINTRAN v1.0 or v2.0

$$\frac{\mathcal{E}_{LU}^{v1.0}}{\mathcal{E}_{LU}^{v2.0}} \propto \left(\frac{MKI^3}{v1.0}\right) \approx 42$$

Thus, assuming a non-absorbing cloud of spherical particles with size parameter $\chi \approx 35$ and requiring an accuracy of 0.5% or better on the observable, the reduced number of model layers and quadrature order that are allowed by LIN-
Figure 3.8 – Top panel: Calculated reflectance between 757 nm and 773 nm for the cloudless as well as the cloudy atmospheric scenario ($\mu_n = \cos(15^\circ)$, $\mu_r = \cos(30^\circ)$, $\Delta \varphi = 60^\circ$). In both cases $I$ and $M$ are set to 8 and 15 respectively. Bottom panel: Residuals of the calculated reflectance with respect to the reference simulation. The residuals are normalised with the reference reflectance at 757 nm to avoid artificially large residuals for vanishing reflectances.

TRAN v2.0, results in a speed-up of the LU-decomposition of roughly a factor of 42.

3.9 Conclusions

We presented a new vector radiative transfer model, LINTRAN v2.0, to be used for retrieving atmospheric trace gas concentrations from satellite-based observations of the Earth’s reflectance. The new model is designed to be numerically more efficient than its predecessor when modelling atmospheres with high scattering optical thickness to enable modelling of cloud-contaminated satellite measurements. In addition, we implemented a fluorescence source at the bottom of the atmosphere, enabling the modelling and retrieval of fluorescence using LINTRAN v2.0.

We developed a mathematical framework that combines the forward-adjoint
perturbation theory with separation of the first $N$ orders of scattering from the diffuse intensity vector field. Contributions of these low-order fields to the observable are recursively solved in an analytical manner. The residual high-order field, containing radiation that is scattered more than $N$ times, is subsequently solved in a numerical manner assuming linearity of the intensity field in the vertical coordinate. The reasoning behind this separation approach is that structures in the intensity field are predominantly caused by low order of scattering contributions, leaving the high-order field relatively smooth. Because of its analytical nature, the recursive solver is very well suited for solving the highly structured intensity fields that results from low order scattering, although numerical effort increases significantly with increasing scattering order. On the other hand, the numerical solver is generally most efficient for solving relatively smooth intensity fields like the one associated with high-order scattering while it tends to become numerically inefficient for highly structured fields. Thus, by
Figure 3.10 – Height-resolved derivatives of the modelled reflectance (Stokes parameter $I$) with respect to normalised absorption and scattering coefficients per layer as well as with respect to the first moment of the phase function expansion $s_1$. Residual errors on derivatives for the cloudy scenario calculated using LINTRAN v2.0 ($\Delta s = 0.1$) with respect to the reference model are shown in the two upper panels for a (continuum) wavelength of 773 nm. The observation geometry is assumed to be $\mu_v = \cos(15^\circ)$, $\mu_\odot = \cos(30^\circ)$ and $\Delta \varphi = 60^\circ$. Each tick on the y-axis denotes a model layer boundary. The derivative with respect to $s_1$ has been scaled by a factor 10, $I$ and $M$ are set to 8 and 15 respectively. Two lower panels: Idem for a wavelength of 760 nm characterised by moderate molecular absorption by oxygen.
choosing truncation order $N$ such that most structures are represented in the low order field, while keeping numeral effort limited for the recursive solver, we optimally combine the two solving methods.

This concept is implemented in LINTRAN v2.0 for $N = 2$, thus producing the single and double scattering fields analytically, within the general framework of forward-adjoint perturbation theory. Separately solving the low-order intensity field allows us to decrease the density of the discretisation within the numerical solver by a factor of 10 in the vertical coordinate and a factor of 1.4 in the angular coordinates compared to the previous model version, assuming a homogeneous atmosphere loaded with scattering Mie particles ($\chi \approx 35$). In this homogeneous atmosphere, the reduced discretisation sampling in turn reduces the numerical effort associated with the numerical solver by a factor 42 relative to the previous model version, without a loss in model accuracy.

### Table 3.1 – The number of model layers $K$, order of the Gaussian quadratures $I$ and the number of Fourier expansion terms $M$ needed to achieve a 0.5% accuracy on the observable with LINTRAN v1.0 and v2.0, in a homogeneous atmosphere of unity optical thickness, assuming a Mie phase function ($\chi \approx 35$).

| $|\Delta F| \simeq 0.5\%$ | $K$ | $I$ | $M$ |
|---------------------|-----|-----|-----|
| LINTRAN v1.0        | 100 | 100 | 199 |
| LINTRAN v2.0        | 10  | 70  | 139 |