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Fast and simple model for atmospheric radiative transfer

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Abstract

Radiative transfer models (RTMs) are of utmost importance for quantitative remote sensing, especially for compensating atmospheric perturbation. A persistent trade-off exists between approaches that prefer accuracy at the cost of computational complexity, versus those favouring simplicity at the cost of reduced accuracy. We propose an approach in the latter category, using analytical equations, parameterizations and a correction factor to efficiently estimate the effect of molecular multiple scattering. We discuss the approximations together with an analysis of the resulting performance and accuracy. The proposed Simple Model for Atmospheric Radiative Transfer (SMART) decreases the calculation time by a factor of more than 25 in comparison to the benchmark RTM 6S on the same infrastructure. The approximative computation of the atmospheric reflectance factor by SMART has an uncertainty ranging from about 5% to 10% for nadir spaceborne and airborne observational conditions. The combination of a large solar zenith angle (SZA) with high aerosol optical depth (AOD) at low wavelengths lead to uncertainties of up to 15%. SMART can be used to simulate the hemispherical conical reflectance factor (HCRF) for spaceborne and airborne sensors, as well as for the retrieval of columnar AOD.

1 Introduction

The terrestrial atmosphere attenuates the propagation of the solar radiation down to the Earth's surface and back up to a sensor. The scattering and absorption processes involved disturb the retrieval of quantitative information on surface properties. Radiative transfer models (RTMs) and their inversions are commonly used to correct for such effects on the propagation of light. Well-known RTMs are 6S (Second Simulation of a Satellite Signal in the Solar Spectrum) (Vermote et al., 1997), SCIATRAN (Roazanov et al., 2005), SHARM (Muldashev et al., 1999; Lyapustin, 2005), RT3 (Evans and Stephens, 1991), RTMOM (Govaerts, 2006), RAY (Zege and Chaikovskaya, 1996), STAR (Ruggaber et al., 1994) and Pstar2 (Nakajima and Tanaka, 1986; Ota et al., 2010), as well as DISORT (Stamnes et al., 1988), which is used in MODTRAN (Berk

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et al., 1989), STREAMER (Key and Schweiger, 1998) and SBDART (Ricchiazzi et al., 1998). These accurate but complex RTMs are frequently run in a forward mode, generating look-up tables (LUTs), which are later used during the inversion process for atmospheric compensation (Gao et al., 2009) or aerosol retrieval (Kokhanovsky, 2008; Kokhanovsky and Leeuw, 2009; Kokhanovsky et al., 2009), for instance. There are also a series of highly accurate, but computationally intensive Monte Carlo photon transport codes available. However, the best accuracy may not be always desirable for an RTM. Approximative equations have been developed before computers were widely available (Hammad and Chapman, 1939; Sobolev, 1972). With regard to the growing size and frequency of remote sensing datasets, approximative and computationally fast RTMs are becoming relevant again (Kokhanovsky, 2006; Katsev et al., 2010). In particular, RTMs of the vegetation canopy and further algorithms that exploit data from imaging spectroscopy instruments (Itten et al., 2008) often relay on fast atmospheric RTM calculations.

In this context, we propose the fast Simple Model for Atmospheric Radiative Transfer (SMART). It is based on approximative analytical equations and parameterizations, which represent an favourable balance between speed and accuracy. We consider minimised complexity and computational speed as important assets for downstream applications. Nevertheless, we define an acceptable uncertainty range of between 5% and 10% for the modelled reflectance factor at the sensor level, under typical mid-latitude remote sensing conditions. SMART can therefore be used as a physical model, maintaining a cause-and-effect relationship in atmospheric radiative transfer. Instead of depending on the classic LUT approach, it permits parameter retrieval in near-real-time. This enables the rapid assessment of regional data requiring exhaustive correction, such as imaging spectrometer data. Furthermore, it supports the straightforward inversion of aerosol optical depth (AOD; $\tau_{\lambda}^{\text{aer}}$) by implementing the radiative transfer equations as a function of $\tau_{\lambda}^{\text{aer}}$. The theoretical feasibility for the retrieval of aerosols in terms of the sensor performance of the APEX instrument (Itten et al., 2008) was shown in Seidel et al. (2008).

In this paper, we describe the two-layer atmospheric model with the implementation of approximative radiative transfer equations in both layers and at the Earth's surface. We then assess the accuracy and performance of SMART in comparison with 6S.

2 SMART – a Simple Model for Atmospheric Radiative Transfer

A remote sensing instrument measures the spectral radiance $L_\lambda(\tau_\lambda, P_\lambda(\Theta), \omega_\lambda; \mu_0, \mu, \phi)$ as function of the spectral atmospheric properties and the illumination/observation geometry. However, from a modelling perspective, it is more convenient to use a dimensionless reflectance function. The relationship between radiance and the reflectance is given by:

$$R_\lambda(\tau_\lambda, P_\lambda(\Theta), \omega_\lambda; \mu_0, \mu, \phi - \phi_0) = \frac{\pi L_\lambda(\tau_\lambda, P_\lambda(\Theta), \omega_\lambda; \mu_0, \mu, \phi)}{\mu_0 F_{0,\lambda}}, \quad (1)$$

where τ_λ is the optical depth, $P_\lambda(\Theta)$ is the phase function at the scattering angle Θ , ω_λ is the single scattering albedo, $\mu_0 = \cos\theta_0$, $\mu = \cos\theta$, θ_0 and θ represent the solar and viewing zenith angles (SZA, VZA), $\phi - \phi_0$ is the relative azimuth between viewing and solar directions, and $F_{\lambda,0}$ is the spectral solar flux or irradiance on the unit area perpendicular to the beam. For readability, we will omit the arguments and use R_λ instead of $R_\lambda(\tau_\lambda, P_\lambda(\Theta), \omega_\lambda; \mu_0, \mu, \phi - \phi_0)$. The subscripted wavelength denotes spectral dependence.

SMART assumes a plane-parallel, two-layer atmosphere. We will use the superscript I to denote the upper layer, superscript II for the lower layer. While the lower layer contains aerosol particles and molecules, the upper layer contains only molecules. The surface elevation, the transition altitude of the two layers, as well as the top-of-atmosphere (TOA) altitude can be chosen freely. The planetary boundary layer (PBL) height is a good estimate for the vertical extent of the lower layer. The sensor altitude can be equal to the TOA or any altitude within the atmosphere. Altitudes are related to air pressure p according to the hydrostatic equation. This 1-D coordinate system is

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used in Eqs. (3) and (18) to determine τ_λ and to scale the atmospheric reflectance and transmittance function corresponding to a specific altitude within atmosphere.

The code can be run at any combination of τ_λ , θ_0 , θ and λ . The current implementation executes on the 2-D array $[\lambda, \tau_{550\text{ nm}}^{\text{aer}}]$, where $\lambda \in [400\text{nm}, 800\text{nm}]$ and $\tau_{550\text{ nm}}^{\text{aer}} \in [0.0, 0.5]$. The spectral dependence of the AOD is approximated by:

$$\tau_\lambda^{\text{aer}} = \tau_{550\text{ nm}}^{\text{aer}} \left(\frac{\lambda}{550\text{ nm}} \right)^{-\alpha}, \quad (2)$$

according to the Ångström's law (Ångström, 1929). Aerosol optical properties, such as g_λ^{aer} , $\omega_\lambda^{\text{aer}}$ and the Ångström parameter α are taken from d'Almeida et al. (1991) for the following aerosol models: clean-continental, average-continental, urban, clean-maritime, maritime-polluted and maritime-mineral.

2.1 Radiative transfer in layer I

By definition, the layer I contains no aerosols and the total optical depth is therefore given by $\tau_\lambda^{\text{I}} = \tau_\lambda^{\text{mic}} (1 - h^{\text{PBL}})$, where

$$h^{\text{PBL}} = \frac{\rho^{\text{SFC}} - \rho^{\text{PBL}}}{\rho^{\text{SFC}} - \rho^{\text{TOA}}} \quad (3)$$

is the relative height of the PBL within the atmosphere. It ranges from 0 at the surface to 1 at TOA. Values for $\tau_\lambda^{\text{mic}}$ are computed using semi-empirical equations from Bodhaine et al. (1999).

The downward total transmittance $T_\lambda^{\text{I}\downarrow}$ is the sum of the downward direct transmittance $T_\lambda^{\text{I}\downarrow\text{dir}}$ and the downward diffuse transmittance $T_\lambda^{\text{I}\downarrow\text{dfs}}$:

$$T_\lambda^{\text{I}\downarrow} = T_\lambda^{\text{I}\downarrow\text{dir}} + T_\lambda^{\text{I}\downarrow\text{dfs}} = e^{-\frac{\tau_\lambda^{\text{I}}}{\mu_0}} + \tau_\lambda^{\text{I}} e^{\left(-u_0 - v_0 \tau^{\text{I}} - w_0 (\tau_\lambda^{\text{I}})^2\right)}. \quad (4)$$

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$T_{\lambda}^{\downarrow\text{dfs}}$ is approximated by using a fast and accurate parameterization suggested by Kokhanovsky et al. (2005) where the parameters u_0 , v_0 , w_0 and associated constants are provided with respect to g_{λ} . The upward transmittance T_{λ}^{\uparrow} is defined according to Eq. (4) by substituting μ_0 , u_0 , v_0 , w_0 for μ , u , v , w , respectively.

The transmitted light is scattered in all directions. The ratio of scattering to total light extinction ω_{λ} and the angular distribution of the scattered light $P_{\lambda}(\Theta)$ are used to describe the scattering process. To simplify the approach, the total intrinsic atmospheric scattering function can be decomposed into the single scattering approximation (SSA) and multiple scattering. The first order atmospheric reflectance function $R_{\lambda}^{\text{I,SSA}}$ can be expressed using the analytical equation as given in van de Hulst (1948); Sobolev (1972); Hansen and Travis (1974); Kokhanovsky (2006):

$$R_{\lambda}^{\text{I,SSA}} = \frac{\omega_{\lambda}^{\text{mlc}} P_{\lambda}^{\text{mlc}}(\Theta)}{4(\mu_0 + \mu)} \left(1 - e^{-m\tau_{\lambda}^{\text{I}}}\right), \quad (5)$$

where the molecular single scattering albedo $\omega_{\lambda}^{\text{mlc}} := 1$ and the molecular (Rayleigh) scattering phase function for unpolarised solar radiation is

$$P_{\lambda}^{\text{mlc}}(\Theta) = \frac{3}{4} \left(1 + \cos^2 \Theta\right) \quad (6)$$

with the scattering angle $\Theta = \arccos \left[-\mu_0 \mu + \cos(\phi - \phi_0) \sqrt{(1 - \mu_0)(1 - \mu)} \right]$ and the geometrical air mass factor $m = \left(\mu_0^{-1} + \mu^{-1} \right)$. $P_{\lambda}^{\text{mlc}}(\Theta)$ is plotted in Fig. 1.

Standard RTMs spend most of their computational time calculating multiple scattering with iterative integration procedures. In the case of layer I, we therefore suggest a generic correction factor f^{corr} to approximate Rayleigh multiple scattering. We derive one f^{corr} per SZA as a function of λ and τ from accurate MODTRAN/DISORT calculations, however without polarisation. The correction factor is defined as the ratio

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between the total reflectance and the SSA at sensor level:

$$f_{\mu_0}^{\text{corr}}(\lambda, \tau) = \frac{R_{\lambda}^{\text{sensor,MODTRAN}}}{R_{\lambda}^{\text{sensor,SSA,MODTRAN}}} \quad (7)$$

The total reflectance function of layer I is then given by Eqs. (5) and (7):

$$R_{\lambda}^{\text{I}} = R_{\lambda}^{\text{I,mlc}} = \frac{\omega_{\lambda}^{\text{mlc}} P_{\lambda}^{\text{mlc}}(\Theta)}{4(\mu_0 + \mu)} \left(1 - e^{-m\tau_{\lambda}^{\text{I}}}\right) f_{\mu_0}^{\text{corr}} \quad (8)$$

2.2 Radiative transfer in layer II

The down- and upward total transmittances $T_{\lambda}^{\text{II}\downarrow}, T_{\lambda}^{\text{II}\uparrow}$ in layer II are calculated according to Eq. (4) by using g_{λ}^{aer} and substituting $\tau_{\lambda}^{\text{I}}$ to the total spectral optical depth of layer II $\tau_{\lambda}^{\text{II}} = \tau_{\lambda}^{\text{aer}} + \tau_{\lambda}^{\text{mlc}} h^{\text{PBL}}$.

The atmospheric reflectance function of layer II is simplified by the decomposition into molecular and aerosol parts. As a consequence, the aerosol-molecule scattering interactions are neglected. The related error is examined in Sect. 3.1.4. The molecular reflectance function $R_{\lambda}^{\text{II,mlc}}$ is derived directly from Eq. (8), where $\tau_{\lambda}^{\text{I}}$ is changed to $\tau_{\lambda}^{\text{mlc}} h^{\text{PBL}}$. Thus, the total reflectance function of layer II is given by:

$$R_{\lambda}^{\text{II}} = R_{\lambda}^{\text{II,mlc}} + \underbrace{\frac{\omega_{\lambda}^{\text{aer}} P_{\lambda}^{\text{aer}}(\Theta)}{4(\mu_0 + \mu)} \left(1 - e^{-m\tau_{\lambda}^{\text{aer}}}\right)}_{R_{\lambda}^{\text{aer}}} + \underbrace{R_{\lambda}^{\text{aer,MS}}}_{\text{second order}} \quad (9)$$

The aerosol phase function $P_{\lambda}^{\text{aer}}(\Theta)$ is defined by the approximate Henyey-Greenstein (HG) phase function (Henyey and Greenstein, 1941), which depends on the aerosol

asymmetry factor g_{λ}^{aer} and the scattering angle Θ :

$$P_{\lambda}^{\text{aer}}(\Theta) = \frac{1 - (g_{\lambda}^{\text{aer}})^2}{\left[1 + (g_{\lambda}^{\text{aer}})^2 - 2g_{\lambda}^{\text{aer}} \cos\Theta\right]^{2/3}}. \quad (10)$$

This HG phase function is plotted in Fig. 1 with $g_{550 \text{ nm}}^{\text{aer}} = 0.63$ for a dry water soluble aerosol according to d'Almeida et al. (1991). The exact phase function derived from the Lorenz-Mie theory is superimposed to illustrate the imperfection of the HG approximation in the forward scattering domain for $\Theta > 150^\circ$. This influence on the accuracy of SMART is discussed in the Sect. 3.1.2.

The second order (or secondary) scattering is calculated according to the Successive Orders of Scattering (SOS) method described by Hansen and Travis (1974):

$$R^{\text{aer,MS}}(\mu, \mu_0, \phi - \phi_0) = \frac{\omega^{\text{aer}} \tau^{\text{aer}}}{4\pi} \left(\frac{1}{\mu_0} + \frac{1}{\mu} \right)^{-1} \cdot \int_0^{2\pi} \int_0^1 \left[\frac{1}{\mu} P_{\text{t}}^{\text{aer}}(\mu, \mu', \phi - \phi') R^{\text{SSA}}(\mu', \mu_0, \phi' - \phi_0) + \frac{1}{\mu_0} R^{\text{SSA}}(\mu, \mu', \phi - \phi') P_{\text{t}}^{\text{aer}}(\mu', \mu_0, \phi' - \phi_0) - \frac{e^{-\frac{\tau^{\text{aer}}}{\mu_0}}}{\mu_0} T^{\text{SSA}}(\mu, \mu', \phi - \phi') P_{\text{r}}^{\text{aer}}(\mu', \mu_0, \phi' - \phi_0) - \frac{e^{-\frac{\tau^{\text{aer}}}{\mu}}}{\mu} P_{\text{r}}^{\text{aer}}(\mu, \mu', \phi - \phi') T^{\text{SSA}}(\mu', \mu_0, \phi' - \phi_0) \right] d\mu' d\phi'. \quad (11)$$

λ and other non-angular arguments are omitted for the sake of readability. $P_{\text{r}}^{\text{aer}}$ and $P_{\text{t}}^{\text{aer}}$ denote the aerosol HG phase function given by Eq. (10) using the reflectance scattering

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angle $\Theta_r = \arccos \left[-\mu_0\mu + \cos(\phi - \phi_0) \sqrt{(1 - \mu_0)(1 - \mu)} \right]$ or the transmittance scattering angle $\Theta_t = \arccos \left[\mu_0\mu + \cos(\phi - \phi_0) \sqrt{(1 - \mu_0)(1 - \mu)} \right]$ respectively. The single scattering transmittance T_{λ}^{SSA} is given in van de Hulst (1948); Sobolev (1972); Hansen and Travis (1974); Kokhanovsky (2006):

$$T_{\lambda}^{\text{SSA}} = \frac{\omega_{\lambda}^{\text{aer}} P_{\lambda}^{\text{aer}}(\Theta)}{4(\mu_0 - \mu)} \left(e^{-\frac{\tau_{\lambda}^{\text{aer}}}{\mu_0}} - e^{-\frac{\tau_{\lambda}^{\text{aer}}}{\mu}} \right). \quad (12)$$

To avoid indeterminacy at $\mu_0 = \mu$, we modify Eq. (12) by using l'Hôpital's (Bernoulli's) rule:

$$T_{\lambda}^{\text{SSA}} = \frac{\omega_{\lambda}^{\text{aer}} P_{\lambda}^{\text{aer}}(\Theta)}{4\mu^2} \tau_{\lambda}^{\text{aer}} e^{-\frac{\tau_{\lambda}^{\text{aer}}}{\mu}}. \quad (13)$$

We use a numerical approximation to calculate the integrals of Eq. (11). This is by far the most computationally intensive step in SMART. Therefore, we currently neglect scattering orders higher than two. A third order term could be added to Eq. (11) as given by Hansen and Travis (1974). However, for our accuracy requirements and under favourable remote sensing conditions, second order scattering is sufficient. More details are given in Sect. 3.

If low computation time is more important than accuracy, $R_{\lambda}^{\text{aer,MS}}$ can be substituted by $f_{\mu_0}^{\text{corr}}(\lambda, \tau_{550}^{\text{aer}})$ from Eq. (7), at the expense of an increased uncertainty of roughly 20%.

2.3 Radiative transfer at the surface

The modelling of optical processes at the surface can be elaborate due to directional effects. Here we assume the simple case with isotropically reflected light on a homogeneous surface according to Lambert's law (Ångström, 1925; Chandrasekhar, 1960;

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Sobolev, 1972):

$$R_{\lambda}^{\text{SFC}} = \frac{a_{\lambda}}{1 - s_{\lambda} a_{\lambda}}, \quad (14)$$

where a_{λ} is the surface albedo and s_{λ} is the spherical albedo to account for multiple interaction between surface and atmosphere. We use the parameterization given in Kokhanovsky et al. (2005) for s_{λ} . The resulting R_{λ}^{SFC} is also known as the hemispherical conical reflectance factor (HCRF) according to Schaepman-Strub et al. (2006).

2.4 At-sensor reflectance function

Finally, we put the above equations together along the optical path to resolve the reflectance function R_{λ}^{S} . Multiple retro-reflections between layers I and II are neglected. A sensor at TOA or within levels I or II is simulated as follows:

$$R_{\lambda}^{\text{S,TOA}} = R_{\lambda}^{\text{I}} + T_{\lambda}^{\text{I}\downarrow} \left[R_{\lambda}^{\text{II}} + R_{\lambda}^{\text{SFC}} T_{\lambda}^{\text{II}\downarrow} \right] T_{\lambda}^{\text{I}\uparrow}, \quad (15)$$

$$R_{\lambda}^{\text{S,I}} = R_{\lambda}^{\text{I}} sh^{\text{I}} + T_{\lambda}^{\text{I}\downarrow} \left[R_{\lambda}^{\text{II}} + R_{\lambda}^{\text{SFC}} T_{\lambda}^{\text{II}\downarrow} \right] \left(1 - sh^{\text{I}} + sh^{\text{I}} T_{\lambda}^{\text{I}\uparrow} \right), \quad (16)$$

$$R_{\lambda}^{\text{S,II}} = T_{\lambda}^{\text{I}\downarrow} \left[R_{\lambda}^{\text{II}} sh^{\text{II}} + T_{\lambda}^{\text{II}\downarrow} R_{\lambda}^{\text{SFC}} \left(1 - sh^{\text{II}} + sh^{\text{II}} T_{\lambda}^{\text{II}\uparrow} \right) \right]. \quad (17)$$

where $T_{\lambda}^{\text{II}\downarrow} := T_{\lambda}^{\text{II}\downarrow} T_{\lambda}^{\text{II}\uparrow}$,

$$sh^{\text{I}} = \frac{\rho^{\text{PBL}} - \rho^{\text{Sensor}}}{\rho^{\text{PBL}} - \rho^{\text{TOA}}} \quad \text{and} \quad sh^{\text{II}} = \frac{\rho^{\text{SFC}} - \rho^{\text{Sensor}}}{\rho^{\text{SFC}} - \rho^{\text{PBL}}}. \quad (18)$$

These scaling factors are used to account for the relative height of the sensor within the corresponding layer. sh^{I} ranges from 1 at TOA to 0 at the PBL, while sh^{II} varies from 1 at the PBL to 0 at the Earth's surface (SFC).

3 Accuracy assessment

For typical airborne remote sensing conditions in the mid-latitudes we choose the representative uncertainty of imaging spectroscopy data of approximately 5% (Itten et al., 2008) as the accuracy requirement for SMART. Less typical conditions are analysed as well; in these cases we will accept larger errors. The definition of the conditions is given in Table 2. The AOD range was chosen according to the findings of Ruckstuhl et al. (2008), the wavelength range selected with regard to the optimal sensor performance (Seidel et al., 2008), while also avoiding strong water vapour absorption. We assume a black surface at the sea level ($a_\lambda=0$) to focus on the atmospheric part of SMART. Furthermore, we solely use the nadir viewing direction ($\mu=1$), which is approximated by small field-of-view ($FOV < 30^\circ$) sensors.

This section evaluates if the prior accuracy requirements can be met by SMART. We compare SMART with an assumed virtual truth computed by the well known RTM 6SV1.1. It accounts for polarisation and uses the SOS method as well as aerosol phase matrices based on Lorenz-Mie scattering theory (Vermote et al., 1997). It was validated and found to be consistent to within 1% when compared to other RTMs by (Kotchenova et al., 2006). We use the default accuracy mode of 6S with 48 Gaussian scattering angles and 26 atmospheric layers. The use of more calculation angles and layers would be possible, but the accuracy increase would be 0.4% at best (Kotchenova et al., 2006) and therefore is negligible for our study. The two layers of SMART were chosen to interface at 2 km above the surface. The lower layer includes dry water soluble aerosols and molecules distributed along the exponential vertical air pressure gradient. The corresponding aerosol optical parameters g_λ^{aer} , ω_λ^{aer} and α_λ are taken from d'Almeida et al. (1991) for SMART and 6S. All results in this study are calculated with identical input parameters in SMART and in 6S, which are provided in Table 1.

In the following, the accuracy of SMART is investigated for specific approximation uncertainties, as well as for the overall accuracy. As an indicator of the accuracy, we

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calculate the relative or percent error of the reflectance function:

$$\delta R \cdot 100 = \frac{R_{\text{SMART}}^{\text{S}} - R_{6\text{S}}^{\text{S}}}{R_{6\text{S}}^{\text{S}}} \cdot 100. \quad (19)$$

3.1 Approximation uncertainties

All calculations in this subsection are performed for a sensor at TOA.

3.1.1 Rayleigh scattering and polarisation

The total Rayleigh scattering is $R_{\lambda}^{\text{mlc}} = R_{\lambda}^{\text{mlcl}} + R_{\lambda}^{\text{mlcII}}$ as given by Eqs. (8) and (9). The associated approximations include the Rayleigh scattering phase function (Eq. 6), the multiple scattering correction factor from MODTRAN (Eq. 7) and the neglected polarisation due to the scalar equations. The uncertainty is a distinct function of the wavelength and SZA, induced mainly by polarisation. Figure 2 shows that it grows towards shorter wavelengths and larger SZA. It is known that the scalar approximation can introduce uncertainties of up to 10% in the blue spectral region (van de Hulst, 1980; Mishchenko et al., 1994). The SZA dependency of this uncertainty is shown in Fig. 3, where it was seen that the backscattering calculations at SZA=0 suffer from a numerical artefact. At 550 nm, the Rayleigh scattering uncertainty in the typical SZA range from 20° to 50° is below 3%.

3.1.2 Aerosol scattering with Mie phase function

The aerosol scattering involves approximations mainly through double scattering (Eq. 11) and the HG phase function (Eq. 10). In this subsection, we extract the phase function from 6S and used it in SMART. In this way, both models use exactly the same phase function, derived from the Lorenz-Mie scattering theory. This bypass isolates the uncertainties of the aerosol scattering, which are not related to the HG approximation.

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The remaining uncertainty is plotted in Figs. 4, 5 and 6. It is obvious that the uncertainty is increasing for larger AOD due to the missing higher scattering orders (see Fig. 5), while the uncertainty is lower for shorter wavelengths. The latter contributes an approximately constant absolute error over the spectra, but the reflectance is higher at shorter wavelengths and the relative error is therefore smaller (see Fig. 4). The same is the case for the nearly-constant percent error in Fig. 5 for AOD larger than 0.3. Figure 6 shows that smaller SZA leads to overestimation, higher SZA to underestimation of the atmospheric reflectance.

3.1.3 Aerosol scattering with HG phase function

In order to study the accuracy of the total aerosol scattering R_{λ}^{aer} , as given in Eq. (9), we include the approximative HG phase function in SMART. 6S uses the same Mie phase function as before. The input parameter for the HG phase function g_{λ}^{aer} corresponds to the same dry water soluble aerosol, which is used in 6S. The exact Mie and the approximative HG phase function are shown in Fig. 1 for the same aerosol. The latter provides a reasonable approximation for scattering angles around 130° , which corresponds to a 50° SZA for nadir observations. The resulting relative error of Eq. (9) is examined in Figs. 4, 5 and 6. It shows the combination of the aerosol scattering error with the HG approximation error. It also suggests that the use of the HG approximation does not introduce large uncertainties within the range of typical SZA, as defined in Table 2. Given a 30° SZA, SMART is quite accurate at all investigated wavelengths and AOD values. By comparing Fig. 4 with Figs. 7 and 5 with 8, it can be seen that the HG approximation reverses some of the errors encountered in Sect. 3.1.3.

3.1.4 Coupling of Rayleigh and aerosol scattering

The current version of SMART does not yet account for the scattering interaction between molecules and aerosols. We analyse this effect by comparing 6S computations with the coupling switched on and off. The relative errors related to this specific

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approximation are shown in Figs. 10, 11 and 12. They are mainly within about 3%, reaching a maximum at a large SZA (see Fig. 12) and short wavelengths (see Fig. 10). With errors of less than 2%, small SZAs are virtually uninfluenced by the coupling. There is also no distinct dependency on the AOD noticeable.

3.2 Overall accuracy

The previous Sect. 3.1 clearly demonstrated that the approximations in SMART are adequate and well within the desired accuracy range of $\pm 5\%$ for investigated conditions as defined in Table 2. In the following, we examine the overall accuracy of SMART by comparing with independent computations of SMART and 6S according to Eq. (19). The computations of SMART are performed by Eq. (15) for a TOA sensor altitude at 80 km and by Eq. (16) for an airborne sensor altitude at 5500 m a.s.l. The uncertainty due to the excluded coupling between molecules and aerosols is inherent in the results of this subsection.

Figure 13 visualises the result with respect to λ and $\tau_{550\text{ nm}}^{\text{aer}}$ of two independent calculations using 6S (bright yellow surface plot) and SMART (black surface plot). The sensor is located at TOA and the SZA is 30° . The qualitative agreement between the two models is evident. A quantitative perspective by statistical means of the overall accuracy is provided in Table 3, where

$$R^2 = 1 - \frac{\sum \left(R_{\text{SMART}}^{\text{S}} - R_{6\text{S}}^{\text{S}} \right)^2}{\sum \left(R_{6\text{S}}^{\text{S}} - \bar{R}_{6\text{S}}^{\text{S}} \right)^2}, \quad (20)$$

is the squared correlation coefficient between the two models,

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum \left(R_{\text{SMART}}^{\text{S}} - R_{6\text{S}}^{\text{S}} \right)^2}, \quad (21)$$

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is the root mean square error and

$$\text{NRMSE} = \frac{\text{RMSE} \cdot 100}{\max(R_{\text{SMART}}^{\text{S}}) - \min(R_{\text{SMART}}^{\text{S}})}, \quad (22)$$

is the normalised RMSE. The statistics are derived from all combinations of input parameters defined in Tables 1 and 2 within the limited conditions. The resulting correlation between SMART and 6S is almost perfect. The RMSE is approximately 0.16 reflectance values and the NRMSE is between 1.8% and 3.5%. The differences are smaller at TOA in comparison to those at 5500 m.

In the following, we analyse the overall accuracy of Eq. (15) by Eq. (19) in more details with respect to wavelength, SZA and AOD. SMART computes very similar results compared to 6S at TOA with an SZA between 30° and 40°. This conclusion can be drawn from the combination of Figs. 3, 9 and 12, as well as from the total uncertainty in Fig. 14. The overall uncertainty does not exceed ±5% at any investigated wavelength or AOD. At the large SZA of 60°, SMART overestimates $R_{\lambda}^{\text{S,TOA}}$ by more than 10% at short wavelengths. Nevertheless, the overall accuracy is still well within the acceptable range of 10% at any wavelength larger than 450 nm (see Fig. 15). At 550 nm, only the combination of very small SZA with a strong AOD or a high SZA with low AOD leads to uncertainties just outside of the desired 5% margin (see Fig. 16). In the blue part of the spectrum, high or low SZA lead to significant uncertainties in a pure Rayleigh scattering atmosphere (see Fig. 17). The same is true in an atmosphere containing aerosols, where the aerosols introduce additional uncertainties in the red part of the spectrum for small SZAs (see Figs. 18 and 19).

Since SMART is also intended for the use with airborne remote sensing data, we additionally analyse the overall accuracy of Eq. (16) by Eq. (19). We place the sensor at 5500 m above the assumed black surface at sea level. The airborne scenario is more sensitive to the approximative two-layer setup in SMART. The 26 atmospheric layers in 6S can better account for the vertically inhomogeneous atmosphere. In fact, the uncertainty is slightly larger in the airborne case in comparison with the TOA case. The

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error distribution in the contour plots of Figs. 20–25 show that SMART underestimates the reflectance factors at 5500 m. Nevertheless, the hypothetical pure Rayleigh atmosphere still performs well, with a maximum uncertainty of 6% (see Figs. 20, 21 and 23). The aerosols worsen the underestimation in the lower half of the visible spectrum, especially at very small and very large SZAs. At 550 nm and a 30° SZA, the uncertainty is 6% or less for an AOD up to 0.5. With the same constellation but an extreme SZA, the uncertainties reach about 10% (see Figs. 22, 24 and 25). The largest offset between SMART and 6S is found at 60° SZA, 400 nm and an AOD of 0.5 with 18% relative difference.

However, it should be noted that the absolute uncertainty $R_{\text{SMART}}^{\text{S}} - R_{\text{6S}}^{\text{S}}$ is in fact smaller in the airborne case compared to the TOA case (not shown). Nonetheless, the relative error given by Eq. (19) is larger due to the smaller R_{6S}^{S} in the denominator.

4 Performance assessment

SMART is designed to optimally balance the opposing needs for accuracy and computational speed; the speed decreases with increasing model complexity and accuracy. We use the 6S vector version 1.1 (Vermote et al., 1997) as a benchmark RTM (same as in Sect. 3) to assesses the performance of SMART. 6S is compiled with GNU Fortran and SMART is implemented in IDL. Both run on the same CPU infrastructure.

SMART needs only approximately 0.05 s for the calculation of one reflectance factor value. The more complex 6S needs about 1.4 s under identical conditions. Consequently, SMART computes more than 25 times faster. If $R_{\lambda}^{\text{aer,MS}}$ (Eq. 11) is substituted by a simple $f_{\mu_0}^{\text{corr}}(\lambda, \tau)$ for aerosol multiple scattering (similar to Eq. 7), SMART runs more than 5500 times faster than 6S.

5 Summary and conclusions

We introduced SMART, as well as its approximative radiative transfer equations and parameterizations. Results of the atmospheric at-sensor reflectance function computed by SMART were compared with benchmark results from 6S for accuracy and performance. The overall uncertainty was examined and discussed, as were the individual errors resulting from Rayleigh scattering, aerosol scattering and molecule-aerosol interactions. The aerosol scattering was compared to 6S with and without the effect of the HG phase function approximation.

We found that SMART fulfils its design principle: it is fast and simple, yet accurate enough for a range of applications. One example may include the assessment of atmospheric effects when inspecting the quality of airborne or spaceborne data against ground truth measurements in near-real-time. The generation of atmospheric input parameters for vegetation canopy RTM inversion schemes, could be another application. SMART computes more than 20 reflectance results per second on a current customary desktop computer. This is more than 25 times faster than the benchmark RTM. The overall uncertainty under typical mid-latitude remote sensing conditions was found to be about 5% for the spaceborne and 5% to 10% for the airborne case. Large AOD or SZA values lead to larger uncertainties of up to 15%. In general, the included approximations are sensitive to the strong scattering in the blue spectral region, which leads to larger uncertainties. Together with the effect of polarisation, the total uncertainty of SMART exceeds the desired accuracy goal of 5% only in the blue region. It is therefore suggested that SMART be used preferably in the spectral range between roughly 500 nm and 680 nm, avoiding the blue and strong absorption bands.

SMART can be improved by implementing other phase functions instead of the HG approximation, including those derived from Lorenz-Mie theory, geometrical optics (ray-tracing), and T-matrix approaches (Liou and Hansen, 1971; Mishchenko et al., 2002). Further refinements may include the coupling between molecules and aerosols, as well as the implementation of freely mixable aerosol components and hygroscopic growth

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(Hess et al., 1998). To account for polarisation, the scalar equations can be extended to the vector notation. Furthermore, a similar approach as used for the Rayleigh multiple scattering in this study (Eq. 7) may perhaps be used to perform a rough polarisation correction. Other issues for further developments may include additional atmospheric layers, gaseous absorption and the treatment of a directional, non-Lambertian surface.

A recent inter-comparison study for classic RTMs such as 6S, RT3, MODTRAN and SHARM, found discrepancies of $\delta R \leq 5\%$ at TOA (Kotchenova et al., 2008). Even larger uncertainties were found when polarisation was neglected or the HG phase function was used. SMART does not yet account for polarisation and uses the HG approximation by default, however with the option to include pre-calculated Mie phase functions. Therefore, the overall accuracy achieved by SMART under given conditions can be regarded as satisfactory, especially when a computationally fast RTM is required.

Acknowledgements. The work of A. A. Kokhanovsky was performed in the framework of DFG Project Terra. Suggestions from D. Schlaepfer and A. Schubert were very much appreciated.

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Table 1. Summary of the input parameters used in SMART and 6S for the accuracy assessment, with the aerosol and molecular optical depth $\tau_{550\text{ nm}}^{\text{aer}}$ and $\tau_{550\text{ nm}}^{\text{mic}}$, the solar and viewing zenith angle SZA and VZA, the aerosol asymmetry factor and single scattering albedo $g_{550\text{ nm}}^{\text{aer}}$ and $\omega_{550\text{ nm}}^{\text{aer}}$, the Ångström parameter $\alpha_{550\text{ nm}}$, the surface albedo a_λ , as well as the air pressure at the surface and the planetary boundary layer p^{SFC} and p^{PBL} and the corresponding scaling factor h^{PBL} .

parameter	$\tau_{550\text{ nm}}^{\text{aer}}$	$\tau_{550\text{ nm}}^{\text{mic}}$	SZA	VZA	$g_{550\text{ nm}}^{\text{aer}}$	$\omega_{550\text{ nm}}^{\text{aer}}$	$\alpha_{550\text{ nm}}$	a_λ	p^{SFC}	p^{PBL}	h^{PBL}
value	0–0.5	0.097	nadir–70°	nadir	0.638	0.963	1.23	0	1013 mb	800 mb	0.211

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Table 2. Definition of the conditions and the related accuracy requirements for SMART. The limited conditions refer to typical airborne remote sensing needs in the mid-latitudes, which SMART was developed for. The analysed conditions refer to the accuracy assessment.

remote sensing conditions	limited	analysed
$\tau_{550\text{ nm}}^{\text{aer}}$	0–0.5	0–0.5
solar zenith angle, degrees	20–60	nadir–70
viewing zenith angle	nadir	nadir
wavelength, nm	500–700	400–800
surface albedo	0	0
accuracy requirement, %	5	15

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Table 3. Quantitative comparison between SMART and 6S by statistical means for the limited conditions as defined in Table 2. SMART uses the HG phase function; 6S used the phase function from Mie calculations. R^2 denotes the squared correlation coefficient, RMSE the root mean square error and NRMSE the normalised RMSE.

sensor altitude	R^2	RMSE	NRMSE
TOA	0.998	0.157	1.77%
5500 m	0.998	0.167	3.52%

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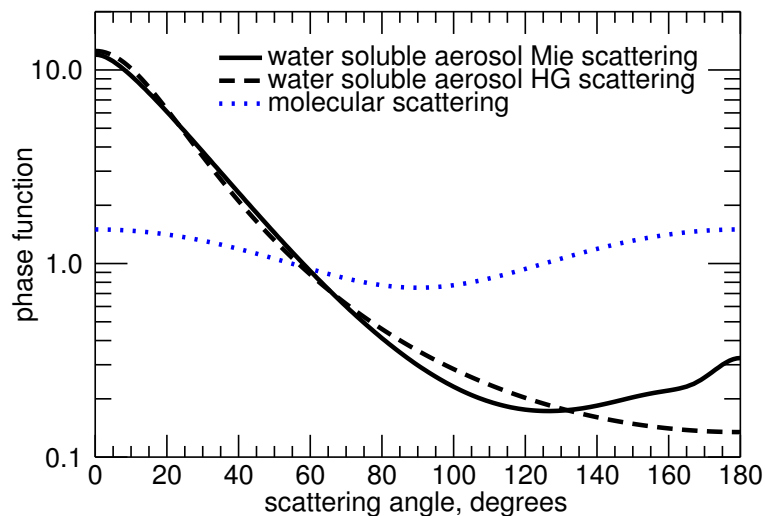


Fig. 1. Phase functions at 550 nm for molecules and dry water soluble aerosols derived from the Henyey-Greenstein (HG) approximation with $g_{550\text{ nm}}^{\text{aer}} = 0.63$ and the exact Lorenz-Mie theory.

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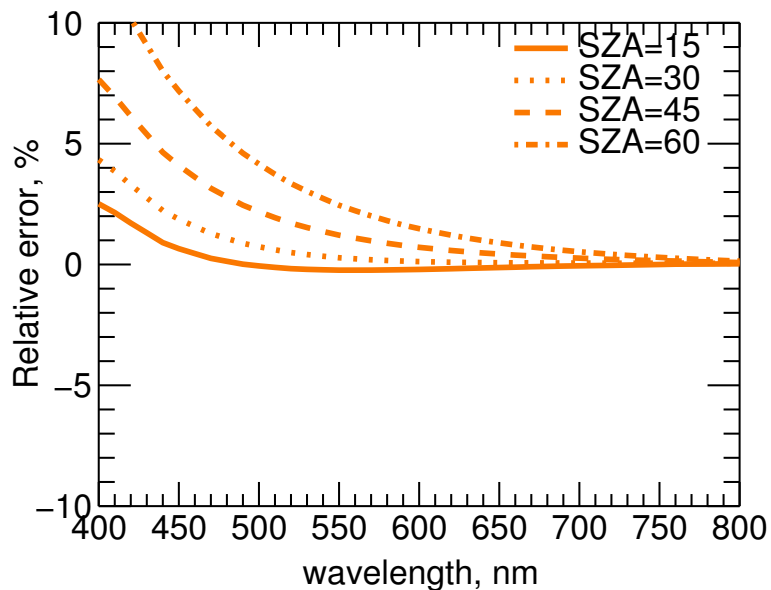


Fig. 2. $\delta R_{\lambda}^{\text{mic}}(\lambda) \cdot 100$. Percent error due to Rayleigh scattering and polarisation with respect to wavelength.

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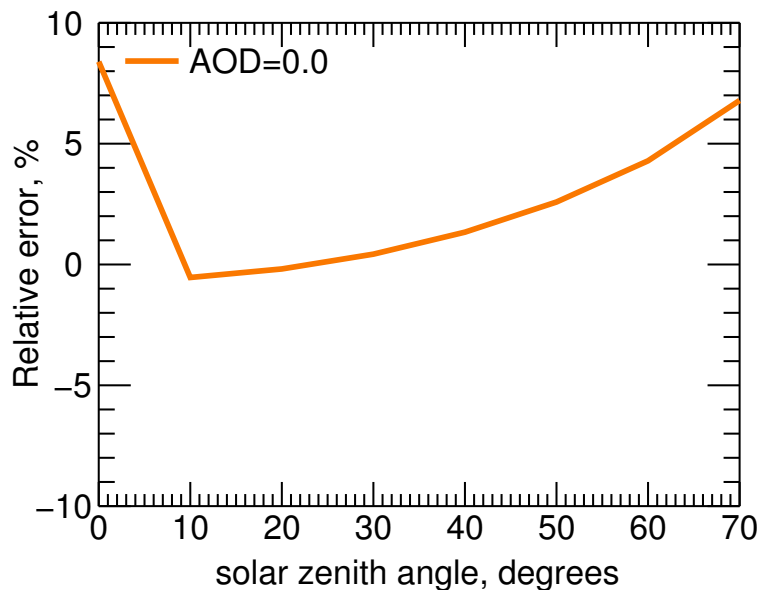


Fig. 3. $\delta R_{550\text{ nm}}^{\text{mlc}}(\text{SZA}) \cdot 100$. Percent error due to Rayleigh scattering and polarisation with respect to solar zenith angle (SZA).

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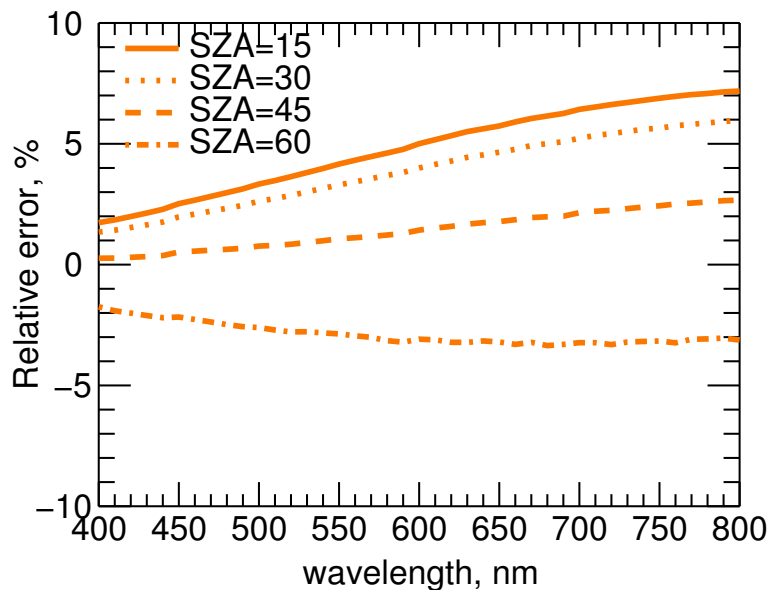


Fig. 4. $\delta R^{\text{aerMie}}(\lambda) \cdot 100$. Percent error of the SMART reflectance function due to aerosol scattering with respect to wavelength. SMART and 6S use the same phase function from Lorenz-Mie theory.

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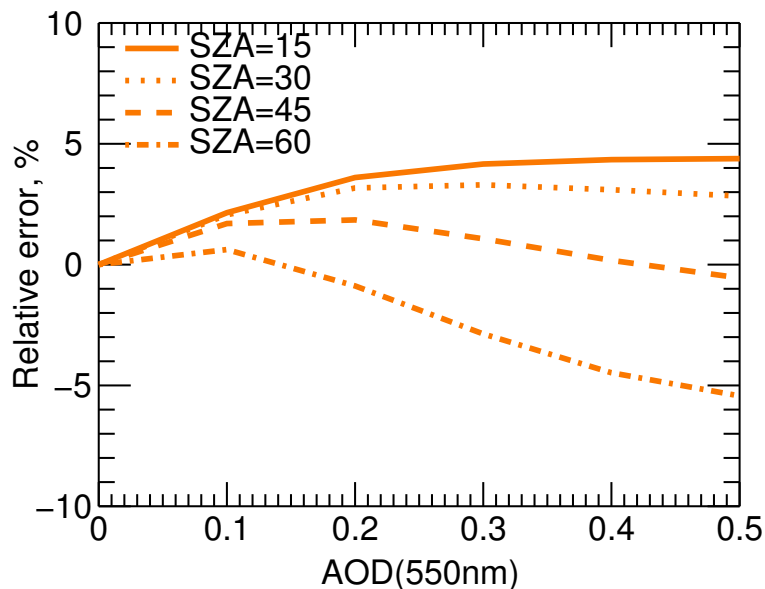


Fig. 5. $\delta R_{550 \text{ nm}}^{\text{aerMie}}(\tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Percent error of the SMART reflectance function due to aerosol scattering with respect to aerosol optical depth (AOD). SMART and 6S use the same phase function from Lorenz-Mie theory.

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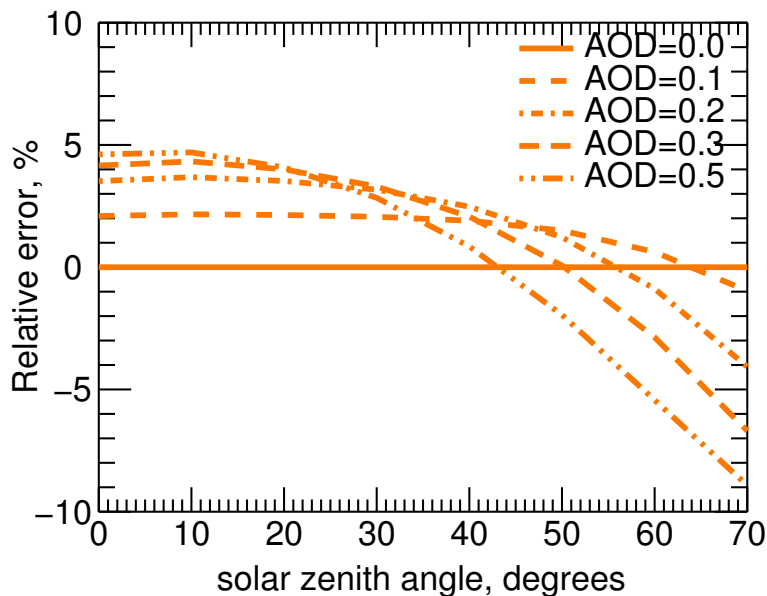


Fig. 6. $\delta R_{550\text{ nm}}^{\text{aer,Mie}}(\text{SZA}) \cdot 100$. Percent error of the SMART reflectance function due to aerosol scattering with respect to solar zenith angle (SZA). SMART and 6S use the same phase function from Lorenz-Mie theory.

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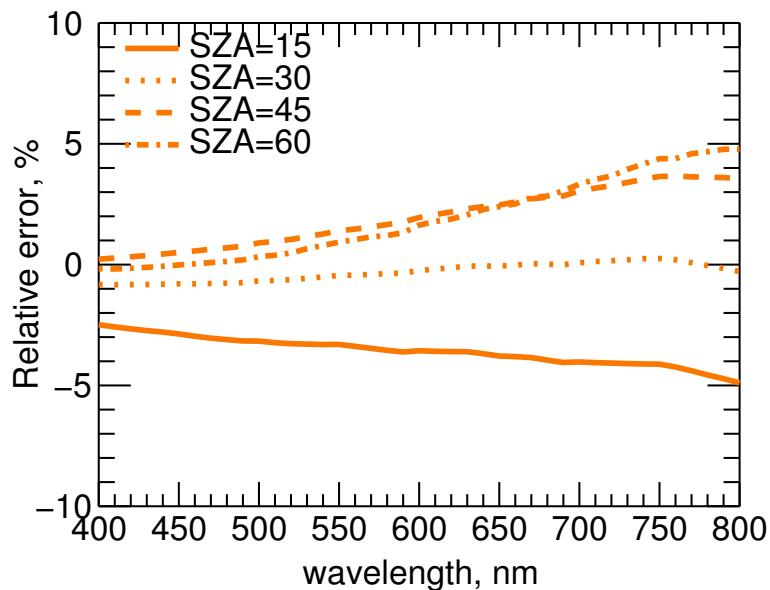


Fig. 7. $7\delta R^{\text{aerHG}}(\lambda) \cdot 100$. Percent error of the SMART reflectance function due to aerosol scattering with respect to wavelength. SMART uses the HG phase function, 6S the phase function from Lorenz-Mie theory.

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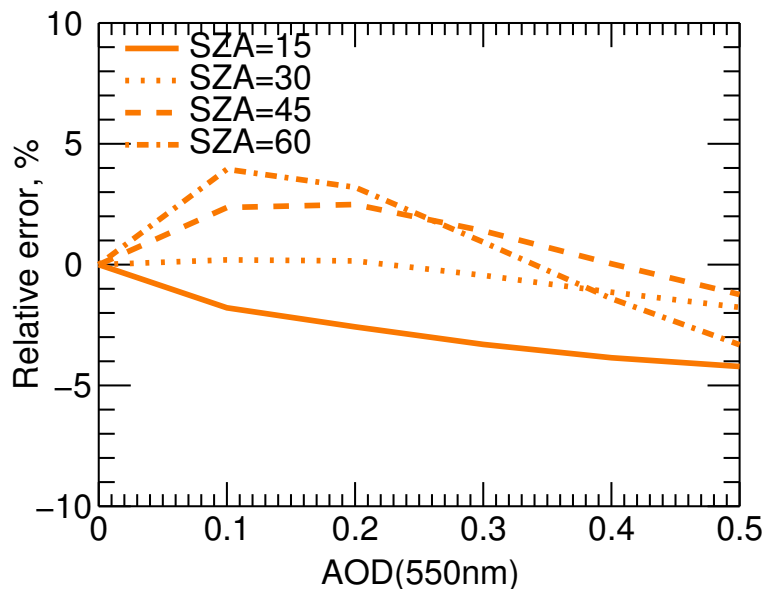


Fig. 8. $\delta R_{550 \text{ nm}}^{\text{aer,HG}}(\tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Percent error of the SMART reflectance function due to aerosol scattering with respect to aerosol optical depth (AOD). SMART uses the HG phase function, 6S the phase function from Lorenz-Mie theory.

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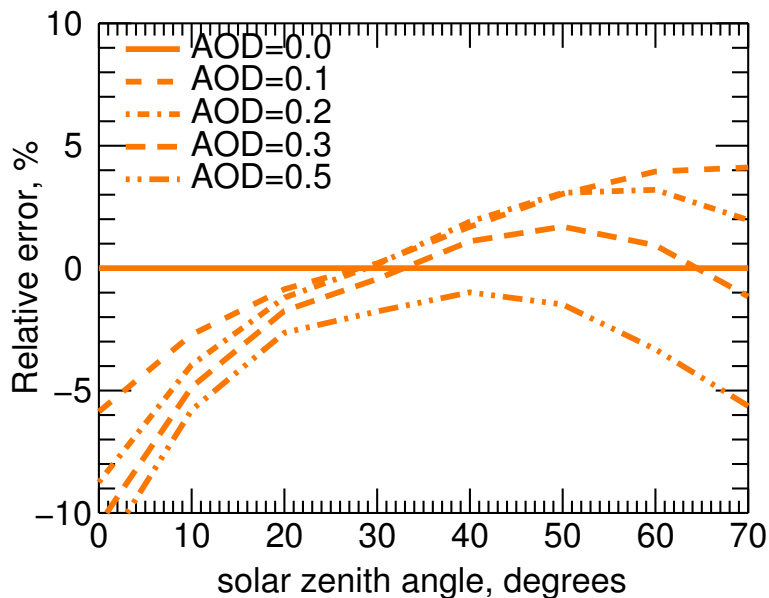


Fig. 9. $\delta R_{550\text{ nm}}^{\text{aerHG}}(\text{SZA}) \cdot 100$. Percent error of the SMART reflectance function due to aerosol scattering with respect to solar zenith angle (SZA). SMART uses the HG phase function, 6S the phase function from Lorenz-Mie theory.

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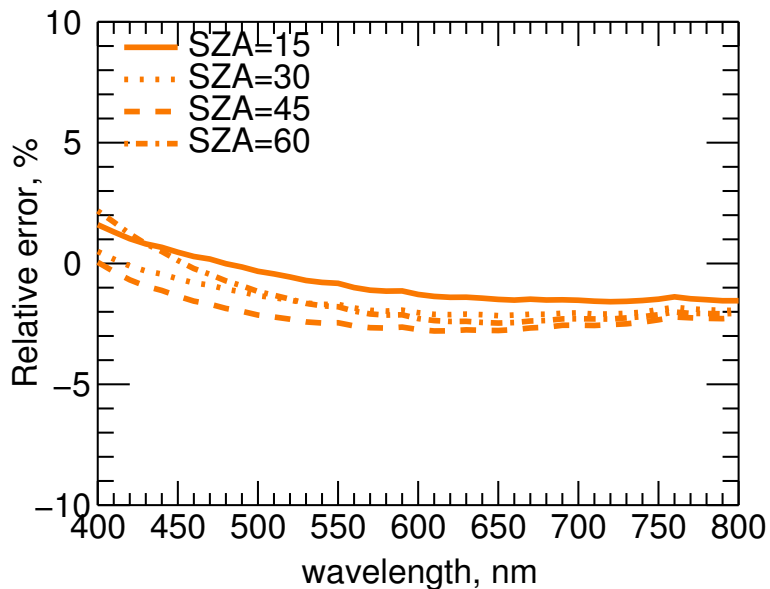


Fig. 10. $\delta R^{\text{mlc+aer}}(\lambda) \cdot 100$. Percent error due to the non-coupling approximation with respect to wavelength.

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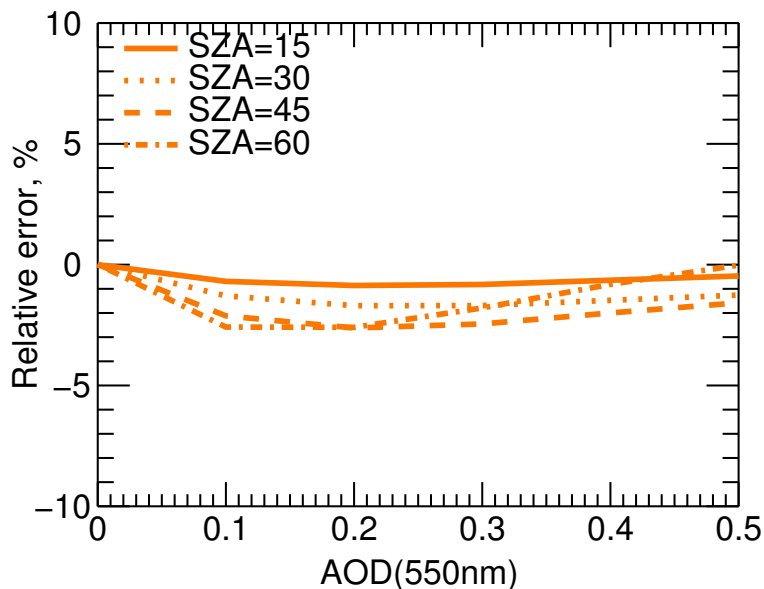


Fig. 11. $\delta R_{550\text{ nm}}^{\text{mlc+aer}}(\tau_{550\text{ nm}}^{\text{aer}}) \cdot 100$. Percent error due to the non-coupling approximation with respect to aerosol optical depth (AOD).

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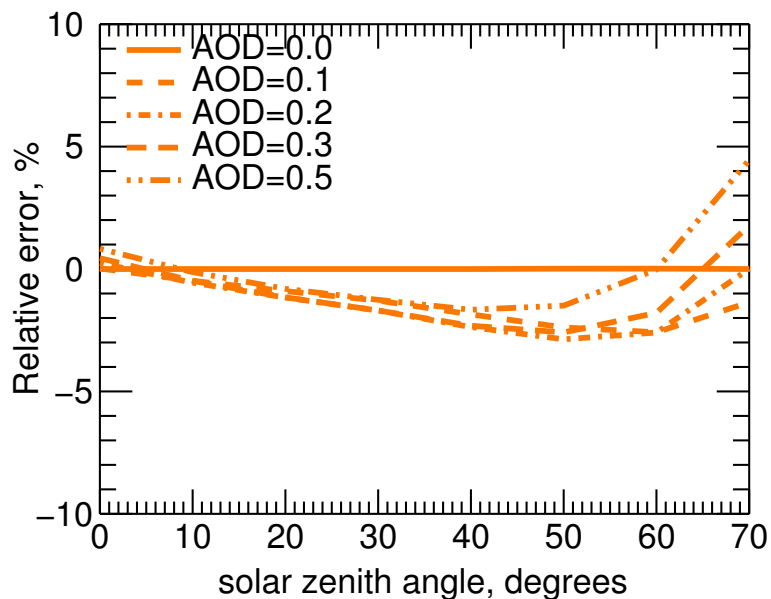


Fig. 12. $\delta R_{550 \text{ nm}}^{\text{mlc+aer}}(\text{SZA}) \cdot 100$. Percent error due to the non-coupling approximation with respect to solar zenith angle (SZA).

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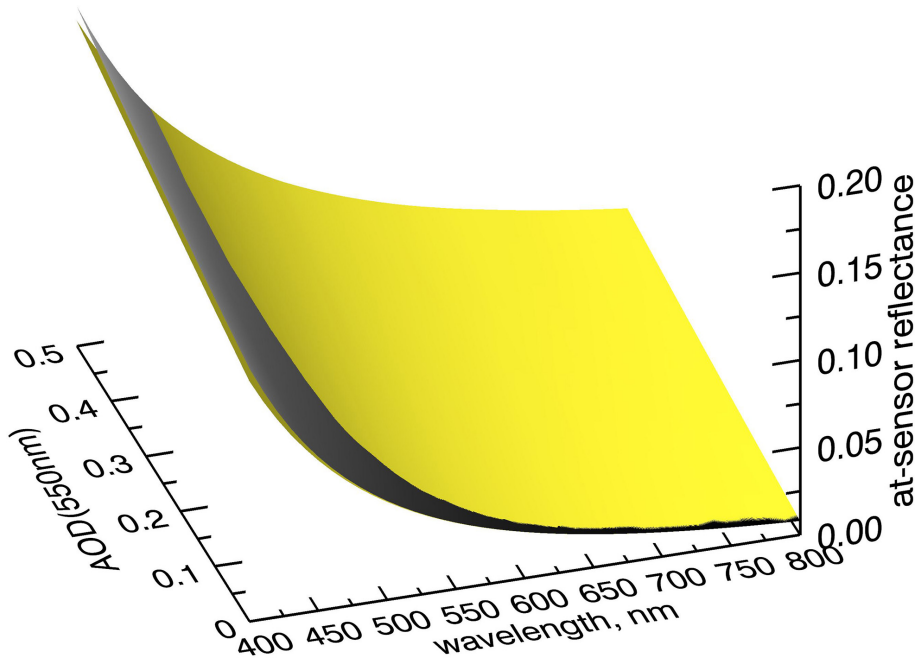


Fig. 13. Results of the at-sensor reflectance function $R_{\lambda}^{S,TOA}$ as computed by SMART (dark surface) and by 6S (bright yellow surface). Input parameters are given in Table 1 with $SZA=30^{\circ}$. SMART uses the HG phase function, while 6S uses the phase function from Mie theory.

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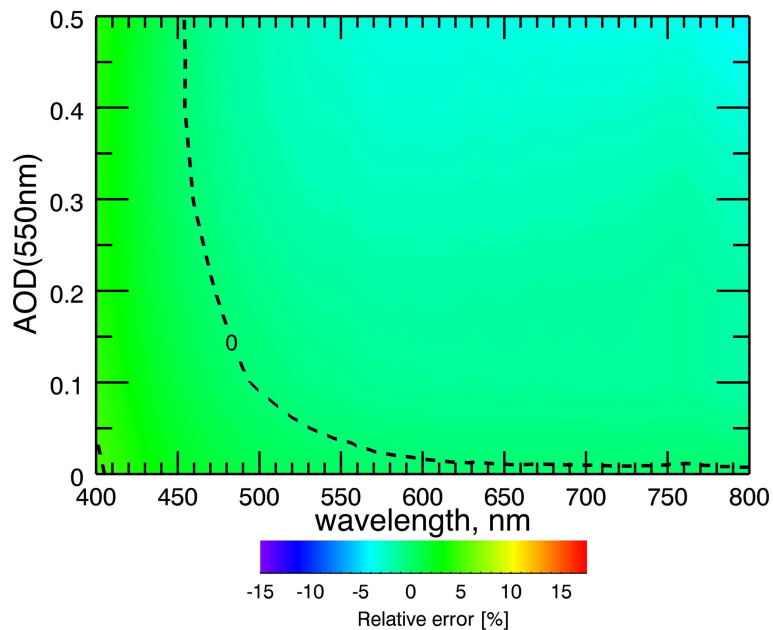


Fig. 14. $\delta R^{S,TOA}(\lambda, \tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Overall accuracy with a sensor at TOA and 30° SZA.

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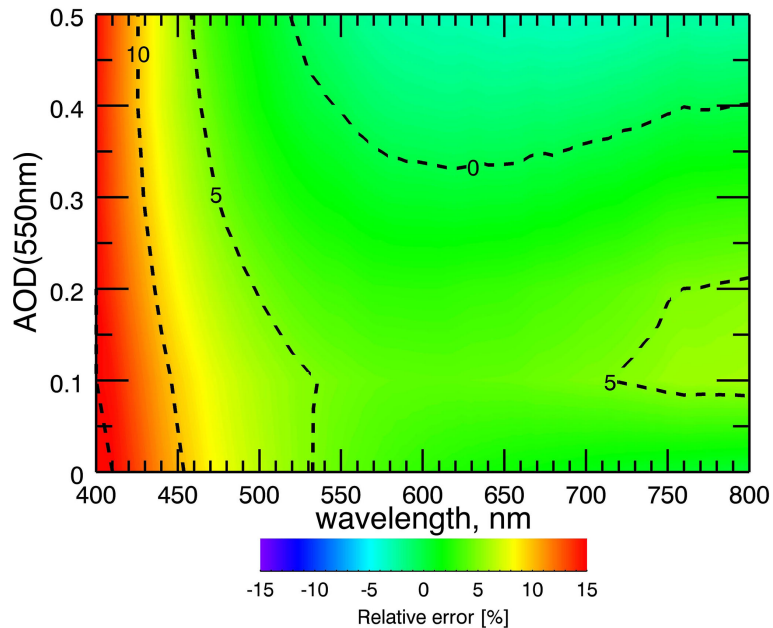


Fig. 15. $\delta R^{\text{S,TOA}}(\lambda, \tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Overall accuracy with a sensor at TOA and 60° SZA.

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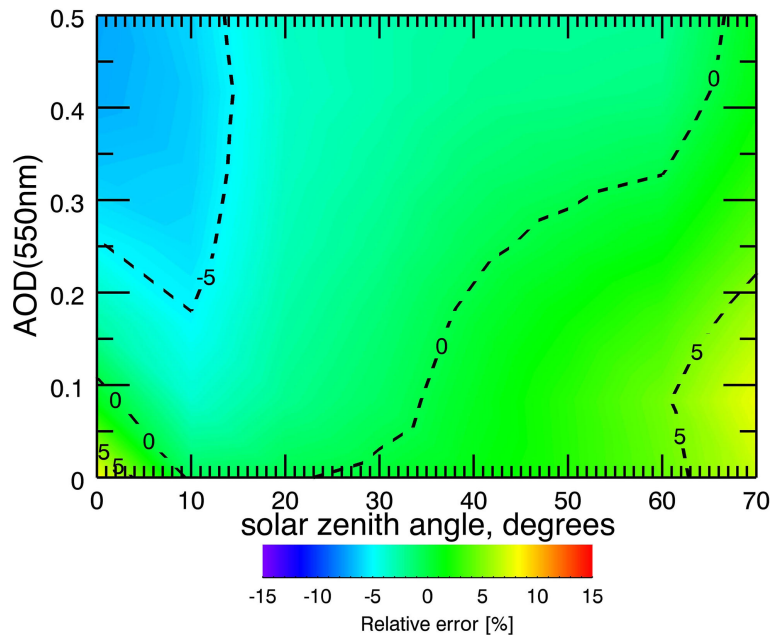


Fig. 16. $\delta R_{550 \text{ nm}}^{\text{S,TOA}}(\text{SZA}, \tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Overall accuracy with a sensor at TOA and $\lambda = 550 \text{ nm}$.

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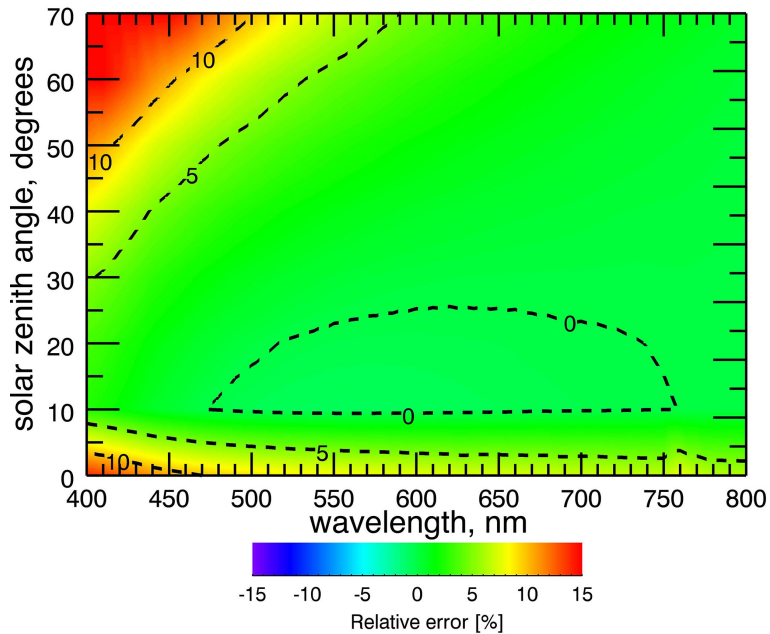


Fig. 17. $\delta R^{\text{S,TOA}}(\lambda, \text{SZA}) \cdot 100$. Overall accuracy with a sensor at TOA and $\tau_{550 \text{ nm}}^{\text{aer}} = 0.0$.

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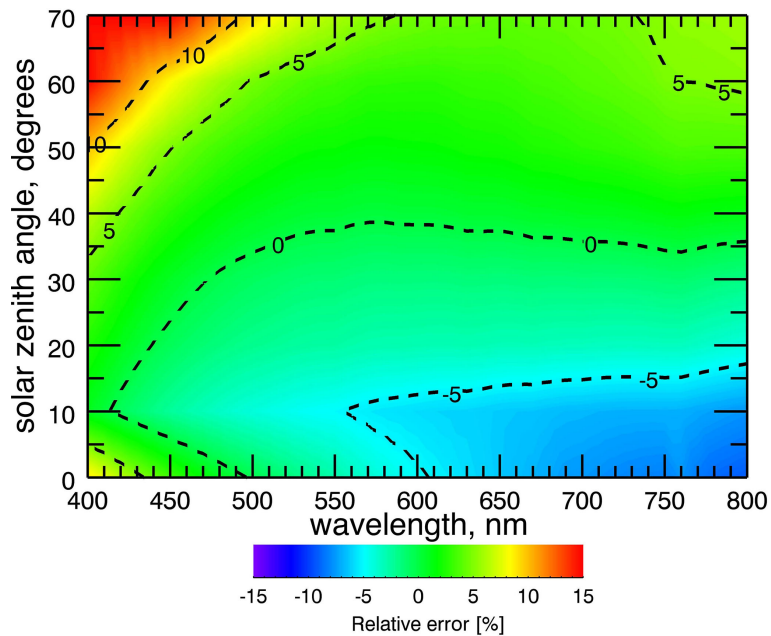


Fig. 18. $\delta R^{\text{S,TOA}}(\lambda, \text{SZA}) \cdot 100$. Overall accuracy with a sensor at TOA and $\tau_{550 \text{ nm}}^{\text{aer}} = 0.2$.

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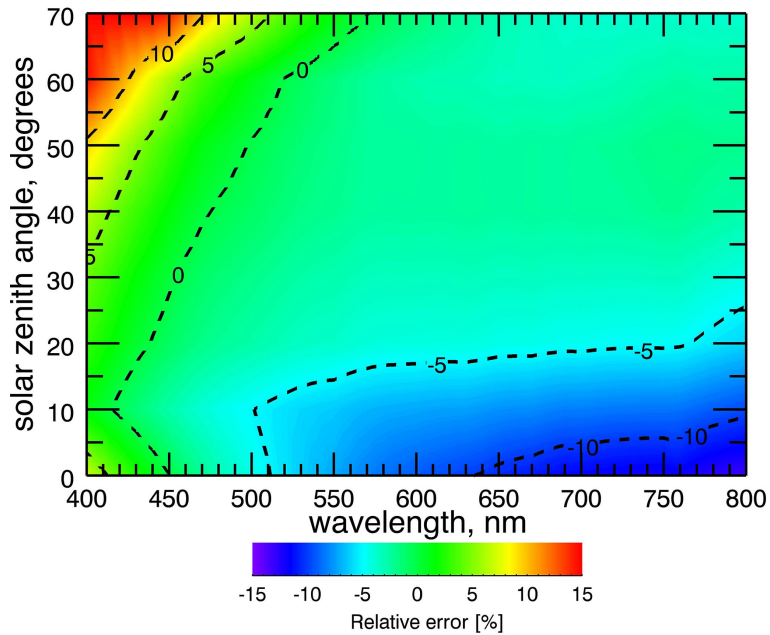


Fig. 19. $\delta R^{\text{S,TOA}}(\lambda, \text{SZA}) \cdot 100$. Overall accuracy with a sensor at TOA and $\tau_{550 \text{ nm}}^{\text{aer}} = 0.5$.

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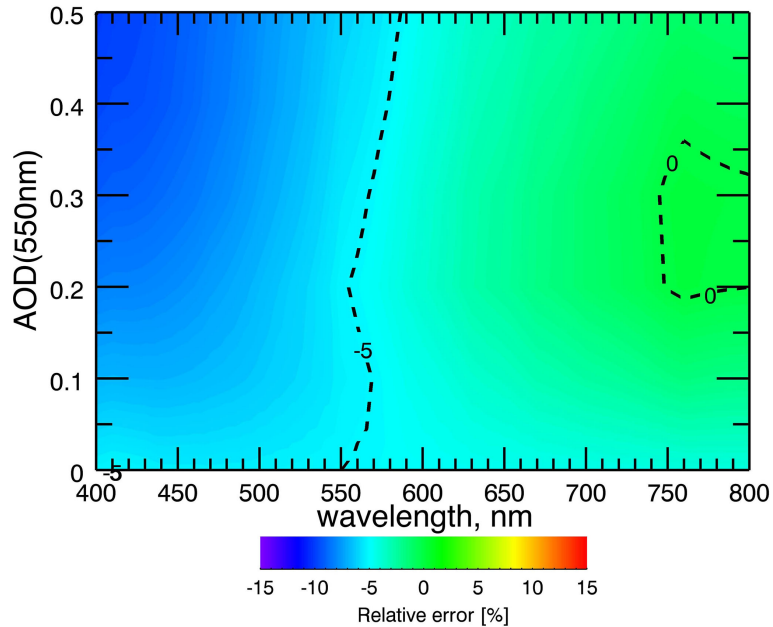


Fig. 20. $\delta R^{S, 5500 \text{ m}}(\lambda, \tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Overall accuracy with a sensor at 5500 m and 30° SZA.

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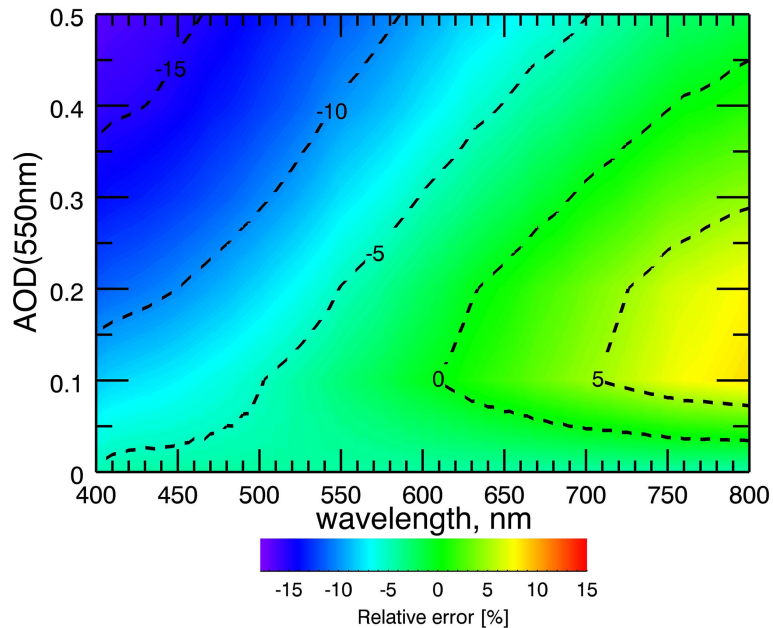


Fig. 21. $\delta R^{S, 5500 \text{ m}}(\lambda, \tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Overall accuracy with a sensor at 5500 m and 60° SZA.

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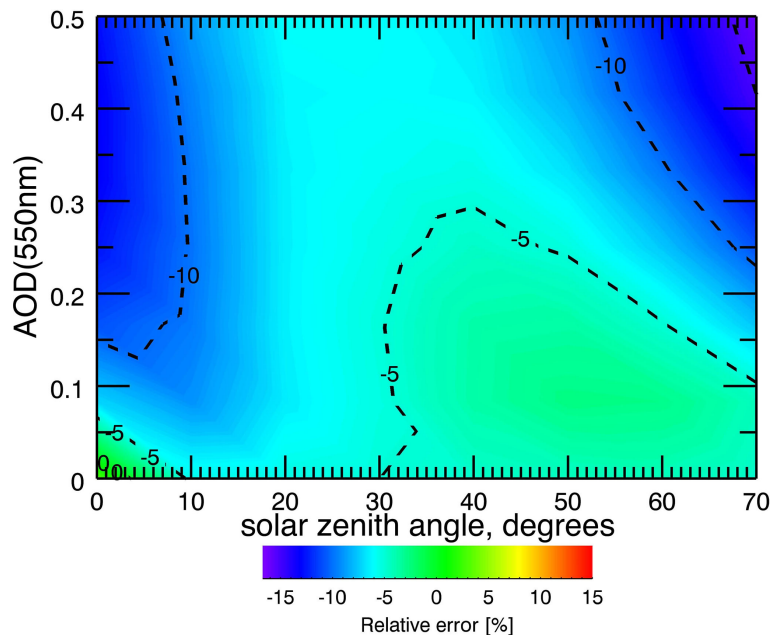


Fig. 22. $\delta R_{550 \text{ nm}}^{S, 5500 \text{ m}}(\text{SZA}, \tau_{550 \text{ nm}}^{\text{aer}}) \cdot 100$. Overall accuracy with a sensor at 5500 m and $\lambda = 550 \text{ nm}$.

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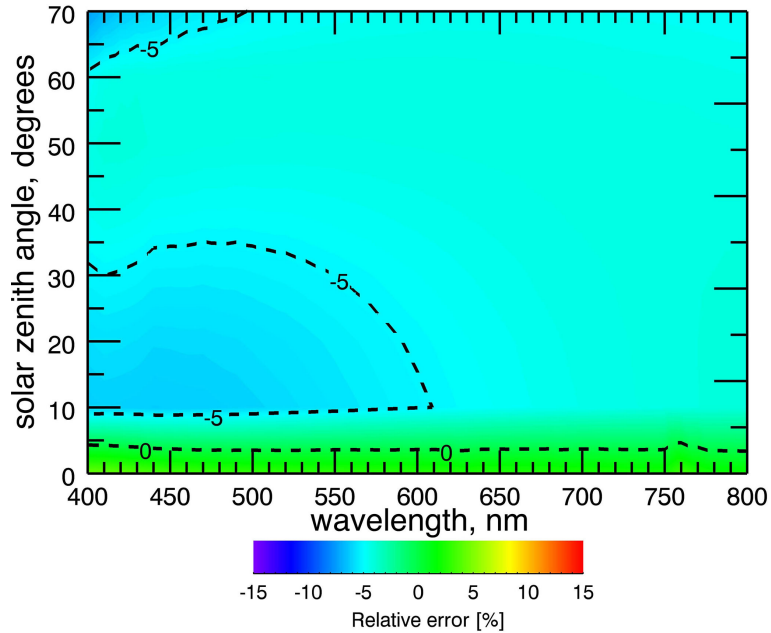


Fig. 23. $\delta R^{S, 5500 \text{ m}}(\lambda, \text{SZA}) \cdot 100$. Overall accuracy with a sensor at 5500 m and $\tau_{550 \text{ nm}}^{\text{aer}} = 0$.

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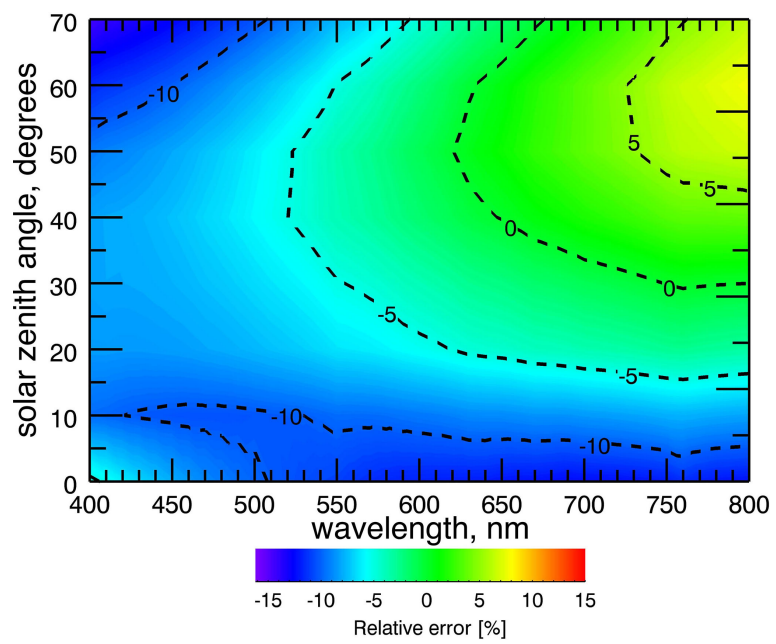


Fig. 24. $\delta R^{S, 5500 \text{ m}}(\lambda, \text{SZA}) \cdot 100$. Overall accuracy with a sensor at 5500 m and $\tau_{550 \text{ nm}}^{\text{aer}} = 0.2$.

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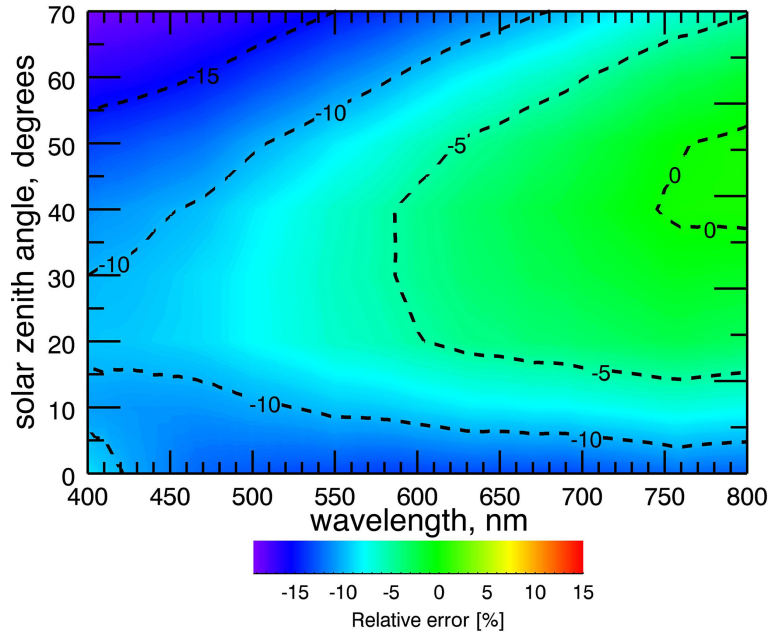


Fig. 25. $\delta R^{S, 5500 \text{ m}}(\lambda, \text{SZA}) \cdot 100$. Overall accuracy with a sensor at 5500 m and $\tau_{550 \text{ nm}}^{\text{aer}} = 0.5$.

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