Formatted: Subscript 1 2 3 An Improved BRDF Hotspot Model and its Use in VLIDORT to Study the Impact 4 of Atmospheric Scattering on Hotspot Directional Signatures in the Atmosphere 5 6 Xiaozhen Xiong1\*, Xu Liu1, Robert Spurr2, 7 Ming Zhao<sup>1,3</sup>, Qiguang Yang<sup>1,3</sup>, Wan Wu<sup>1</sup>, Liqiao Lei<sup>1,3</sup> 8 9 <sup>1</sup>NASA Langley Research Center, Hampton, VA, USA 10 <sup>2</sup> RT SOLUTIONS Inc., Cambridge, MA, USA 11 <sup>3</sup> Adnet Systems Inc., Bethesda, MD 20817, USA 12 13 Corresponding to: Xiaozhen Xiong (Xiaozhen.Xiong@nasa.gov) 14 15 Abstract 16 17 18 The term "hotspot" refers to the sharp increase of reflectance occurring when incident (solar) and Formatted: Justified, Space After: 0 pt, Don't adjust space between Latin and Asian text, Don't adjust space between 19 reflected (viewing) directions almost coincide in the backscatter direction. The accurate simulation Asian text and numbers 20 of hotspot directional signatures is important for many remote sensing applications. The 21 RossThick-LiSparse-Reciprocal (RTLSR) Bidirectional Reflectance Distribution Function 22 (BRDF) model is widely used in radiative transfer simulations, and the hotspot model mostly used 23 is from Maignan-Bréon but it typically requires large values of numerical quadrature and Fourier 24 expansion terms in order to represent the hotspot accurately for its use coupled with atmospheric Deleted: I 25 radiative transfer modelling (RTM). In this paper, we have developed a modified version based on Deleted: 26 the Maignan- Bréon's hotspot BRDF model that converges much faster numerically, making it Deleted: n improved more practical for use in the RTMs that require Fourier expansion of BRDF to simulate the top-27 **Deleted:** 28 of-atmosphere (TOA) hotspot signatures, such as in the RTM models using Doubling-Adding or 29 discrete ordinate method. Using the vector linearized discrete ordinate radiative transfer Deleted: s 30 model (VLIDORT), we found that reasonable TOA hotspot accuracy can be obtained with just 23 Deleted: atmospheric radiative transfer 31 Fourier terms for clear atmospheres, and 63 Fourier terms for atmospheres with aerosol scattering. Deleted: ions of 32 Deleted: . Using 33 In order to study to the impact of molecular and aerosol scattering on hotspot signatures, we carried Deleted: RT model 34 out a number of hotspot signature simulations with VLIDORT, We confirmed that (1) atmospheric Deleted: 35 molecules scattering and the existence of aerosol tend to smooth out the hotspot signature at the 36 TOA, but has no impact on hotspot width; and (2) the hotspot signature at the TOA in the near-Deleted: W 37 infrared is larger than in the visible, and its impact by surface reflectance is more significant. As Deleted: to study to the impact of molecular and aerosol scattering on hotspot signatures 38 the hotspot amplitude at the TOA with aerosol scattering included is smaller than that with 39 molecular scattering only, the amplitude of hotspot signature at the surface is likely underestimated Deleted: s 40 in the previous analysis based on the POLDER measurements, where the atmospheric correction Formatted: Strikethrough 41 was based on a single-scatter Rayleigh-only calculation. We also draw attention to a scaling factor Deleted: has an obvious increase with the solar zenith angle 42 of  $3\pi/4$  which has been applied to the Ross-Thick kernel with hotspot correction. This modified **Deleted:** attenuation 43 model can calculate the amplitude of hot spot accurately, and, as it agrees very well with the Formatted: Strikethrough 44 original RossThick model away the hotspot region, this model can be simply used in conditions Formatted: Strikethrough 45 with and without hotspot. However, there are some differences of this modified model with the

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original Maignan- Bréon model for the scattering angles close to the hot spot point, thus it may not be appropriate for those who need an exact representation of the Hot Spot angular signature.

Keywords: BRDF, Hot Spot, VLIDORT, RTLSR

#### 1. Introduction

76 Most land surfaces reflect incident light anisotropically. For a given incident sun angle, the surface 77 reflectance may vary by a factor of two in the near infrared [Kriebel et al., 1978]. An accurate 78 accounting of the anisotropic reflectance at the Earth's surface is very important for many remote 79 sensing applications, including monitoring of climate changes, mapping land covers, analyzing 80 vegetation densities, or inter-calibration between different satellite instruments (e.g. [Yang et al., 81 2020] and references therein). Lorente et al. [2018] investigated the importance of surface 82 reflectance anisotropy with regard to cloud and NO<sub>2</sub> retrievals from satellite measurements by the Global Ozone Monitoring Experiment 2 (GOME-2) and the Ozone Monitoring Instrument (OMI). 83 84 This study showed that retrieved cloud fractions have an east-west across-track bias of 10-50 %, 85 and under moderately polluted NO<sub>2</sub> scenarios with backward scattering geometry, clear-sky air 86 mass factors can be as much as 20% higher when surface anisotropic reflection is included in the calculations.

88 The angular distribution of reflected light by a surface is normally represented mathematically by 89 the Bidirectional Reflectance Distribution Function (BRDF) [Nicodemus et al., 1992], which is a 90 function of the incident solar zenith angle, the reflected viewing zenith angle, and the relative 91 azimuth angle between these two directions. Usually, there is a strong increase in BRDF toward 92 the backward-scatter direction, with much smaller BRDF variations seen around the opposite 93 forward-scatter direction. Peak BRDF values occur when backscatter incident and reflected 94 directions coincide; this sharp reflectance increase is usually referred to as the "hotspot" [Kuusk, 95 1985; Hapke, 1986]. The "hotspot" effect has been observed for a variety of planetary bodies, 96 including the Moon, Mars, asteroids, planetary satellites, as well as terrestrial vegetation [Bréon 97 et al., 2002]. The most widely accepted explanation for the hotspot effect is the so-called "shadow 98 hiding" effect. Here, particles at the surface (e.g. leaves, soil grains) cast shadows on adjacent 99 particles; these shadows are visible at large phase angles but at zero phase angle the shadows are 100 hidden by the particles that cast them. Coherent backscatter is another physical explanation of 101 reflectance enhancement in the hotspot direction [Kuga and Ishimaru, 1984; Hapke et al., 1993].

102 The bidirectional reflective spectra of land surfaces have been measured in laboratories, fields and 103 airborne experiments, or derived from satellite observations. The two most widely used 104 hyperspectral bidirectional reflective spectra of land surfaces are (1) the U.S. Geological Survey 105 (USGS) Spectral Library (Version 7) [Kokaly et al., 2017], comprising a very diverse land surface 106 BRDF data based with about 40,000 spectra in all, and (2) the ASTER Spectral Library from Formatted: Font: (Default) Times New Roman, 12 pt

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107 NASA's Jet Propulsion Laboratory, with a collection of over 2,000 measured spectra [Baldridge et al., 2009]. Using these two databases and RossThick-LiSparse-Reciprocal (RTLSR model), 108 109 Yang et al. [2020] went on to develop a Hyper-Spectral Bidirectional Reflectance (HSBR) model 110 for remote sensing applications. BRDF data derived from satellite observations have been used to 111 evaluate and correct for anisotropy in several instruments, including, for example, the Advanced Very High Resolution Radiometer (AVHRR) [e.g. Gutman, 1987; Roujean et al., 1992], the 112 113 Along-Track Scanning Radiometer (ATSR-2) located on board on the ERS-2 platform [Godsalve, 114 1995], and the MODerate resolution Imaging Spectrometer (MODIS) [Wanner et al., 1997; Lucht et al., 2000; Schaaf et al., 2002]. However, the AVHRR, ATSR and MODIS instruments have 115 limited viewing geometry options; in contrast, the POLarization and Directionality of Earth 116 117 Reflectances (POLDER) instrument on board the Advanced Earth Observing Satellite (ADEOS) 118 in August 1996 provided a much better directional sampling to measure the BRDF up to 65° VZA (viewing zenith angle) and for the full azimuth range [Deschamps et al., 1994]. So, these POLDER 119 120 reflectance measurements were used to examine the hotspot signature for different vegetated 121 surfaces [Bréon et al., 2002]. 122 Many BRDF models have been developed in order to simulate or reproduce directional signatures 123 of land surface reflectance. These include empirical models [Walthall et al., 1985], semi-empirical models [Hapke, 1981, 1986; Rahman et al., 1993; Roujean et al., 1992; Wanner et al., 1995; 1997; 124 125 Lucht et al., 2000], and physical models [Pinty and Verstraete, 1991]. In particular, kernel-driven 126 semi-empirical models have been used frequently to generate global BRDF and albedo products. 127 Several studies have identified the so-called Ross-Thick-Li-Sparse-Reciprocal (hereinafter

"RTLSR") kernel combination as the BRDF model best suited for the operational MODIS 128 129 BRDF/Albedo algorithm [Wanner et al., 1997; Lucht et al., 2000; Schaaf et al., 2002]. Using about 130 22,000 sets of the measured BRDFs derived from carefully selected cloud-free measurements with 131 large directional coverage from the spaceborne POLDER instrument [Bicheron and Leroy, 2000], Maignan et al. [2004] evaluated the efficacy of several analytical models to reproduce these 132 observed BRDF signatures. They found that a simple kernel-driven model with only three free 133 134 parameters can provide an accurate representation of the BRDF. One of the best such models is the three-parameter linear Ross-Li model. However, this model fails to capture the sharp 135 reflectance increase centered around the hotspot backscatter direction. From an analysis of 136 137 POLDER data, a correction to this model to capture the hotspot effect was proposed by [Bréon et 138 al., 2002]. By means of an explicit representation of the hotspot effect for a few degrees around 139 the backscattering direction, Maignan et al. [2004] found that the hot-spot modified RTLSR linear 140 BRDF model with three free parameters produced the best agreement with measurement. This 141 BRDF model from [Maignan et al., 2004] was referred to as the "Ross-Li-Maignan" model in 142 [Vermote et al., 2009].

143 With three linear parameters characterizing the Ross-Li model, it is a straightforward process to 144 invert the model by minimizing the Root Mean Square (hereafter RMS) difference between the 145 measurements and the modeled directional reflectances. This BRDF inversion technique has been 146 used to derive the MODIS BRDF/Albedo product [Schaaf et al., 2002]. An improvement was made 147 by Vermote et al. (2009) to correct the time series of surface reflectance derived from MODIS. 148 Using POLDER data, Bacour and Bréon [2005] retrieved the three parameters, using the modified 149 Ross-Li model, and further analyzed the variability of these parameters with vegetation cover 150 types. A common approach to derive the surface reflectance directional signatures from satellite 151 observations is to first remove the atmospheric absorption and scattering effects. This process,

152 which converts the top of the atmosphere (TOA) signal to a surface reflectance, is often called

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155 "atmospheric correction". The surface is generally taken to be Lambertian in such atmospheric

156 correction algorithms; however, it was found that without considering the BRDF effects,

157 atmosphere correction errors can reach up to 10% at certain geometries and under turbid conditions

[Vermote et al., 1997]. Since the mid-1980s, atmospheric correction algorithms have evolved from
 the earlier "empirical line" and "flat-field" methods to more modern approaches based on rigorous

radiative transfer modeling [Gao et al., 2009]. Clearly, the accurate simulation of atmospheric and

161 surface radiative transfer is a critical element in the derivation of surface BRDF from satellite

162 measurements.

163 Several key numerical radiative transfer models (RTMs) were developed in the 1980s, and the 164 most popular RTMs in use today are usually based on discrete ordinate methods or the doubling-165 adding technique. Following detailed mathematical studies made by Hovenier and others 166 [Hovenier and van der Mee, 1983; de Rooij and van der Stap, 1984], a general doubling-adding model was developed for atmospheric radiative transfer modeling, e.g. [de Haan et al., 1987; 167 168 Stammes et al., 1989]. DISORT is a discrete ordinate model developed by Stamnes and co-169 workers and released for public use in 1988 [Stamnes et al., 1988; Stamnes et al., 2000]; a vector 170 discrete ordinate model (VDISORT) was developed later on in the 1990s [Schulz et al., 1999]. In 171 the 1980s, Siewert and colleagues made a number of detailed mathematical examinations of the vector RT equations. The development of the scattering matrix in terms of generalized spherical 172 functions was reformulated in a convenient analytic manner [Siewert, 1981; Siewert, 1982; 173 174 Vestrucci and Siewert, 1984], and a new and elegant solution from a discrete ordinate viewpoint was developed for the scalar [Siewert, 2000a] and vector [Siewert, 2000b] single-layer slab 175 models. LIDORT [Spurr et al., 2001; Spurr, 2002] and VLIDORT [Spurr, 2006] are multiple-176 177 scattering multi-layer discrete ordinate scattering codes with simultaneous linearization facilities 178 for the generation of the radiation field and analytically-derived Jacobians (weighting functions or 179 partial derivatives of the radiation field with respect to any atmospheric or surface parameter). 180 SCIATRAN is a comprehensive software package for the modeling of radiative transfer processes 181 in the terrestrial atmosphere and ocean from the ultraviolet to the thermal infrared, including 182 multiple scattering processes, polarization, thermal emission and ocean-atmosphere coupling; the software package contains several radiative transfer solvers including discrete-ordinate techniques 183 184 [Rozanov et al., 2014]. The Second Simulation of the Satellite Signal in the Solar Spectrum (6S) 185 [Vermote et al., 1997] RTM is widely used in the atmospheric correction community; 6S is based 186 on the successive orders of scattering approach (SOS) [Lenoble et al., 2007]. In this study, we will 187 use the VLIDORT RTM, which has a fully-developed supplemental code package for the generation of surface BRDFs. This supplement includes a variety of BRDF kernel models (semi-188 empirical BRDF functions developed for particular types of surfaces) that can be combined 189 190 linearly to that provide total BRDFs required as input for the full VLIDORT RTM calculations. 191 These kernels include the Ross-Li model both with and without the hotspot correction.

192 In the first part of this study (Section 2) we discuss the Ross-Li kernel hotspot correction in detail, 193 and present an alternative model of the hotspot correction; this new formulation is designed to 194 improve the hotspot convergence with respect to the number of cosine-azimuth Fourier terms 195 needed to represent the BRDF and also to the number of azimuth quadrature angles needed for the 196 numerical derivation of these Fourier terms. In Section 3, we investigate accuracies for 197 reconstructed BRDFs in the hotspot region, comparing our new model with older hot-spot corrections. Then, using VLIDORT and the new hotspot correction model, we examine the impact 198 199 of atmospheric scattering on the simulated TOA-hotspot signature. Summary and conclusions are 200 given in Section 4.

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#### 2. Hotspot BRDF Models 203

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#### 2.1. RossThick-LiSparse-Reciprocal (RTLSR) BRDF model 204

205 Land surfaces possess complicated structural elements, making the reflective properties of such 206 surfaces very hard to model. The geometric structure of a given land surface greatly influences its 207 reflectance, thanks to shadowing and multiple scattering effects [Roujean et al., 1992]; this angle-208 dependent scattering component is called "geometric scattering". Another structure-related 209 scattering effect is called "volumetric scattering", which usually consists of multiple reflections 210 from different components within a volume and produces a minimum reflectance near nadir 211 212 213 viewing. Scattering by trees, branches, soil layers, and snow layers are typical manifestations of volumetric scattering. These two scattering processes are usually used to characterize the surface BRDF. For example, the operational Moderate Resolution Imaging Spectroradiometer (MODIS) 214 BRDF/Albedo product is derived based on semi-empirical kernel-driven linear BRDF models that 215 composes of three components: an isotropic scattering term, a geometric scattering kernel, and a 216 volumetric scattering kernel. The RossThick-LiSparse-Reciprocal (RTLSR) kernel combination 217 has been identified as the best model suited for the operational MODIS BRDF/Albedo retrieval 218 ([Schaaf et al., 2002] and references therein), in which the land surface reflectance function 219  $B(\theta_i, \theta_r, \Delta \varphi)$  is represented as:

$$B_{(\theta_i,\theta_r,\Delta\varphi)} = P_1 K_{Lamb} + P_2 K_{geo}(\theta_i,\theta_r,\Delta\varphi,P_4,P_5) + P_3 K_{vol}(\theta_i,\theta_r,\Delta\varphi).$$
(1)

Here,  $\theta_i$  and  $\theta_r$  are the incident (solar) and reflected (viewing) zenith angles, and  $\varphi_i$  and  $\varphi_r$  the 221 222 corresponding azimuth angles, with  $\Delta \varphi = \varphi_r - \varphi_i$  the relative azimuth angle.  $P_1$  is the Lambertian 223 kernel amplitude with  $K_{Lamb} \equiv 1$ , while  $P_2$  and  $P_3$  are the weights of the Li-Sparse-Reciprocal 224 geometric scattering kernel Kgeo and the Ross-Thick volume scattering kernel Kvol respectively. 225 Parameters P4 and P5 characterize Kgeo and are discussed below. This 3-kernel semi-empirical 226 model has shown surprising ability to reproduce with high accuracy the measured directional 227 signatures of the main land surfaces; the RTLSR model is significantly better than other analytical 228 models or combinations thereof [Maignan et al., 2004]

229 The Li-Sparse-Reciprocal geometric scattering kernel was derived from surface scattering and the 230 theory of geometric shadow casting by [Li and Strahler, 1992], and is given by

231 
$$K_{geo}(\theta_i, \theta_r, \Delta \varphi, P_4, P_5) = \frac{1 + sec\theta'_r sec\theta'_i + tan\theta'_r tan\theta'_i cos\Delta \varphi}{2} + \frac{t-sintcost}{\pi} - 1 (sec\theta'_r + sec\theta'_i).$$
(2)

$$\left(\frac{1-\sin(t)\delta t}{\pi}-1\right)(\sec\theta'_r+\sec\theta'_i).$$

233 
$$\cos^2 t = \left(\frac{P_4}{\sec\theta'_r + \sec\theta'_i}\right)^2 \left[G(\theta'_r, \theta'_i, \Delta\varphi)^2 + (\tan\theta'_r \tan\theta'_i \sin\Delta\varphi)^2\right];$$
(3)

234 
$$G_{(\theta'_r, \theta'_i, \Delta \varphi)} = \sqrt{\tan^2 \theta'_r + \tan^2 \theta'_i - 2\tan \theta'_r \tan \theta'_i \cos \Delta \varphi};$$
(4)  
235 
$$\tan \theta'_r = P_5 \tan \theta_r; \qquad \tan \theta'_i = P_5 \tan \theta_i.$$
(5)

236 We note also the following expression for the scattering angle 
$$\zeta$$
:

$$237 \qquad \cos\zeta = \cos\theta_r \cos\theta_i + \sin\theta_r \sin\theta_i \cos\Delta\phi \qquad (6)$$

238 Assuming a dense leaf canopy, and tree crowns that are spheroids with vertical length 2b,

Formatted: Font: Times New Roman, 12 pt Formatted: Font: Times New Roman, 12 pt Formatted: Font: Times New Roman, 12 pt horizontal width 2*r*, and centroid distance *h* above the ground, then  $P_4 = h/b$  and  $P_5 = b/r$  are two parameters representing the crown relative height.  $P_4$  and  $P_5$  can be obtained empirically, and they are usually assumed to take values 2 and 1 respectively.

242 The Ross-Thick volume scattering kernel  $K_{vol}$  was derived from volume scattering radiative 243 transfer models by [Ross, 1981], and it is often referred to as "*Ross thick*" [Wanner et al., 1995]:

$$K_{vol}(\theta_i, \theta_r, \Delta \varphi) = \frac{\left(\frac{\pi}{2} - \zeta\right) \cos\zeta + \sin\zeta}{\cos\theta'_r + \cos\theta'_i} - \frac{\pi}{4}.$$
(7)

245 Since we are using the RTLSR linear model to reproduce natural target BRDFs, it follows that the 246 three parameters will contain most of the reflectance directional information for view angles of 247 less than 60°. Theoretically, parameter  $P_1$  and  $P_2$  in Eq. (1) can be derived, but due to the extensive 248 variability of surface cover and biome types, there remains the practical question as to the 249 determination of the free parameters [Vermote et al., 2009], and for the MODIS BRDF/Albedo 250 product,  $P_1$ ,  $P_2$  and  $P_3$  are derived from MODIS measurements in a few channels. A hyperspectral 251 bidirectional reflectance (HSBR) model for land surface was developed by [Yang et al., 2020]. 252 The HSBR model includes a diverse land surface BRDF database with about 40,000 spectra, stored 253 in terms of the three Ross-Li parameters. The HSBR model has been validated using the USGS 254 vegetation database and the AVIRIS reflectance product, and can be used to generate hyperspectral 255 reflectance spectra at different sensor and solar observation geometries.

#### 256 2.2. Hot-Spot models, including an improved formulation

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Based on an analysis of POLDER measurements, Bréon et al.[2002] found that the hotspot directional signature is proportional to  $(1 + \zeta/\zeta_0)^{-1}$ , where  $\zeta_0$  is the hotspot halfwidth that can be related to the ratio of scattering element size and canopy vertical density. This hotspot modeling has been validated against measurements acquired with the spaceborne POLDER instrument with a very high directional resolution, i.e. on the order of 0.3° [Bréon et al., 2002]. Maignan et al.[ 2004] brought this hotspot correction into the Ross-Li model, and re-wrote the Ross thick kernel with hotspot correction as:

$$K_{vol} = \frac{4}{3\pi} \frac{\binom{\pi}{2} - \zeta \cos\zeta + \sin\zeta}{\cos\theta'_r + \cos\theta'_i} \left(1 + \frac{1}{1 + \zeta/\zeta_0}\right) - \frac{1}{3}.$$
 (8)

We note here that there is a difference of a factor of  $\frac{4}{3\pi}$  between Eqs. (7) and (8). Bréon et al. [2002] 265 266 indicated that  $\zeta_0$  is generally in a small range between 0.8° to 2°, while some dispersion occurs in 267 the range 1°-4° for scenarios classified as forest and desert types in the International Geosphere-268 Biosphere Program (IGBP) system. For the sake of simplicity, and to avoid the addition of a free 269 parameter in the BRDF modeling, Maignan et al.[2004] suggested setting a constant value of  $\zeta_0 =$ 270 1.5°. The version of the RTLSR model which accounts for the hotspot signature using Eq. (8) will 271 be denoted as RossThickHT-M in this paper. Using multidirectional PARASOL (Polarization & 272 Anisotropy of Reflectances for Atmospheric Sciences coupled with Observations from a 273 Lidar) data at coarse resolution (6 km) over a large set of representative targets, Maignan et 274 al.[2004] showed that the simple three-parameter model permits accurate representation of the 275 BRDFs.

276 Another hotspot correction was developed by Chen and Cihlar[1997] as a negative exponential

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278 function, and Jiao et al. [2013] brought this latter correction to the Ross-Li model, as follows:

$$K_{vol} = \frac{4}{3\pi} \frac{\binom{n}{2} - \zeta}{\cos\theta'_r + \cos\theta'_i} \frac{(1 + C_1 e^{\left(-\frac{\zeta}{\pi}\right)C_2}) - \frac{1}{3}}{(1 + C_1 e^{\left(-\frac{\zeta}{\pi}\right)C_2}) - \frac{1}{3}}.$$
 (9)

Here,  $C_1$  is physically related to the difference between the spectral reflectance of foliage and the background, controlling the height of the hotspot;  $C_2$  is related to the ratio of canopy height to the size of the predominant canopy structure, determining the width of the hotspot. We found that we can simply set  $C_2$  to be  $\zeta_0$ . We remark that  $\zeta_0$  is given in radians in Eq. (8) and in degrees in Eq. (9). However, Bréon et al.[2002] determined that observed hotspot signatures are better fitted with a function of  $(1 + \zeta/\zeta_0)^{-1}$  rather than with a negative exponential that is often used for hotspot modeling.

In this paper, we denote the version of the RTLSR model that accounts for the Hot-Spot process using Eq. (9) as RossThickHT-C. Some validation to the RossThickHT-C model has been made by Jiao et al. [2013]. Although one advantage of RossThickHT-C model is the ability to use parameter  $C_1$  to adjust the amplitude of hotspot [Jiao et al., 2013], such an adjustment can be also easily made by adding one parameter in the correction term in Eq. (8), i.e. to change  $(1 + \zeta/\zeta_0)^{-1}$ to  $C_1/(1 + \zeta/\zeta_0)$ . With this in mind, our effort will focus on an improvement in the Ross-Thick BRDF kernel, starting with the baseline model of Maignan et al. [2004].

A number of kernel BRDF models have been incorporated in the LIDORT and VLIDORT RTMs, including the RTLSR model and the RossThickHT-M model. In VLIDORT (and this applies equally to other polarized radiative transfer models). It is necessary to develop solutions for the radiation fields in terms of Fourier cosine and sine azimuth series; the same considerations apply to the BRDFs. For scalar kernel models without polarization, only the Fourier cosine series is

299 needed. The Fourier components of the total BRDF are calculated through:

300 
$$B^{m}(\mu,\mu') = \frac{1}{2\pi} \int_{0}^{2\pi} B(\mu,\mu',\varphi) \cos m\varphi \, d\varphi \, .$$

301 Integration over the azimuth angle is done by double numerical quadrature over the ranges  $[0, \pi]$ 302 and  $[-\pi, 0]$ . The number of BRDF azimuth quadrature abscissa (N<sub>BRDF</sub>) should be set to at least 100 in order to obtain a numerical accuracy of 10<sup>-4</sup> for most kernels considered in the VLIDORT 303 304 BRDF supplement [Spurr, 2004]. However, at and near the hotspot region, many more quadrature 305 points and Fourier terms (N<sub>FOURIER</sub>) will be needed, as we will demonstrate below. Indeed, Lorente 306 et al. (2018) found that in order to reach an accuracy of  $10^{-3}$  over the hotspot region, 720 Gaussian 307 points were needed for the azimuth integration and 300 Fourier terms for the reconstruction of any 308 BRDF in terms of its Fourier components; they also determined that, in the final implementation 309 of the surface BRDF in the DAK radiative transfer model (Doubling-Adding KNMI, [Lorente et 310 al., 2017]) designed to perform with optimal simulation time, some 100 Fourier terms and 360 311 Gaussian points were necessary for proper hotspot characterization.

These values of  $N_{BRDF}$  and  $N_{FOURIER}$  are still unacceptably high, and in order to use VLIDORT to simulate the hotspot signature with a modest number of discrete ordinates, we have made an

- 314 empirical modification to the hotspot correction in the RossThickHT-M model by choosing the
- function with a smooth transition near the hotspot peak and considering  $\sin(\zeta)$  can be used to
- 316 replace  $\zeta$  approximately when the phase angle is a small value. We experimented with different
- powers of this function, finally coming up with a function of  $sin^{x}(\zeta) * \frac{1}{sin^{x}(\zeta_{0})}$  to replace  $\zeta/\zeta_{0}$ ,

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(10)

321 where  $x = 2 + \sin(\theta'_r)$ . Thus:

$$K_{vol} = \frac{4}{3\pi} \frac{(\frac{\pi}{2} - \zeta) \cos\zeta + \sin\zeta}{\cos\theta'_r + \cos\theta'_i} \left(1 + \frac{1}{1 + \sin^x(\zeta)^* \frac{1}{\sin^x(\zeta_0)}}\right) - \frac{1}{3}.$$
 (11)

323 We use the nomenclature RossThickHT-X to indicate the model with the hotspot correction given 324 in Eq. (11).

325 In the next section, we first examine the above sets of hotspot signatures, with particular emphasis

326 on the accuracy of reconstructed BRDFs in terms of the two numerical indices  $N_{BRDF}$  and  $N_{FOURIER}$ .

327 We then determine the impact of a scattering atmosphere, using these hotpot BRDF quantities as

inputs to VLIDORT calculations based on standard-atmosphere pressure/temperature profiles with

two cases, one is Rayleigh scattering only and another one with aerosols added. Aerosol is in the

form of an optically-constant layer from the surface to 3.0 km with the total optical depth of 0.2.

and aerosol optical properties are taken from a "continental pollution" aerosol type [Hess et al.,

328 329 330 331 332 333 1998], with lognormal poly-disperse size distribution. Please note that the use of an optical depth

of 0.2 for aerosol might be a little high than the background aerosol.

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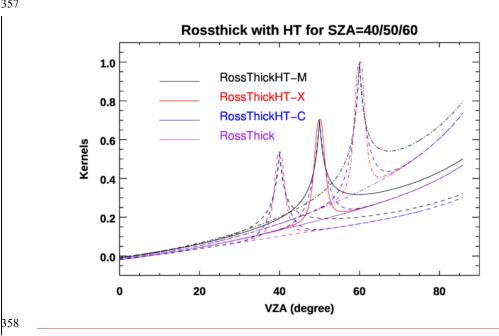
#### 337 3. Results and Discussion

#### 338 3.1 Hotspot Comparisons and BRDF reconstruction accuracy

339 Figure 1 shows a comparison of the volume-scattering kernel for the three hotspot models, 340 RossThickHT-X, RossThickHT-C and RossThickHT-M, with actual hotspots at three different 341 solar zenith angles in the principal-plane backscatter direction. For reference, the original 342 RossThick kernel is also plotted. The heights of Hotspot peaks from the three models are the same, 343 and the hotspot peak is higher and narrower at larger zenith angles. For model RossThickHT-X, 344 the angular shape around the hot spot peak (VZA=SZA) is not so sharp as the reference model 345 RossThickHT-M, thus, it may not be appropriate for those who need an exact representation of the 346 hot spot angular signature. However, from limited validation Jiao et al. [2013] found that 347 RossThickHT-M apparently overestimates the hot spot magnitude, and RossThickHT-M looks too 348 sharp from Figure 2 of Jiao et al. [2013]. Another major difference between the three models are 349 outside the hotspot region. As indicated by [Jiao et al., 2013], one asset of RossThickHT-C is that 350 it better matches the RossThick model in regions beyond the hotspot, while on the other hand, 351 there remain some differences between the RossThickHT-M and RossThick model away from the 352 hotspot. Our new model RossThickHT-X has the same advantage as RossThickHT-C, in that 353 agreement with the standard RossThick model beyond the hotspot region is accurate, thus 354 RossThickHT-X can be used automatically in conditions with and without hot spot impact and do 355 not to switch the BRDF models from RossThick to the one with HT correction, i.e. RossThickHT-356 M, when the hot spot occurs.

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Figure 1. Four Ross-Thick volume scattering kernels for a range of reflection zenith angles,
 and for three solar incident angles as indicated; reflectance is in the principal plane.

365 The major advantage of our new hotspot correction model is the rapid convergence for reconstruction. Table 1 lists values of N<sub>BRDF</sub> (number of azimuth quadrature abscissae) and 366 NFOURIER (number of Fourier Terms) that are needed to reconstruct the BRDF to different accuracy 367 368 levels; the accuracy is computed as the relative difference of the reconstructed BRDF to its exact 369 value at the hotspot. Compared to numbers required for the RossThickHT-M, values of NBRDF and 370 N<sub>FOURIER</sub> for the RossThickHT-X case are 10 to 60 times smaller (Table 1). These results show 371 that RossThickHT-X converges much faster than RossThickHT-M. We see also that convergence 372 of RossthickHT-C is somewhat faster than that for RossThickHT-M but still much slower than 373 that for RossThickHT-X. The computation time goes roughly as the third power of the number of 374 streams. Since the number of terms used in our hotspot model is more than 10 times less than that 375 specified for the original hotspot model (as shown in the Table 1), there would be a considerable 376 performance gain with the BRDF simulations. 377

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Table 1. Values of NBRDF and NFOURIER needed	ed to reconstruct a hotspot with $\zeta_0 = 1.5^\circ$ .
----------------------------------------------	----------------------------------------------------------

		RossThickHT-M		RossThickHT-X		RossThickHT-C	
#	Accuracy (%)	NBRDF	N_FOURIER	NBRDF	N_FOURIER	NBRDF	N_FOURIER
1	1	2810	1402	278	139	1578	789
2	0.5	5620	2807	324	162	3158	1579
3	0.4	7020	3509	338	169	3948	1974
4	0.3	9360	4679	356	178	5264	2632
4	0.2	14040	7019	382	191	7896	3948
5	0.1	28080	14039	428	214	15794	7897

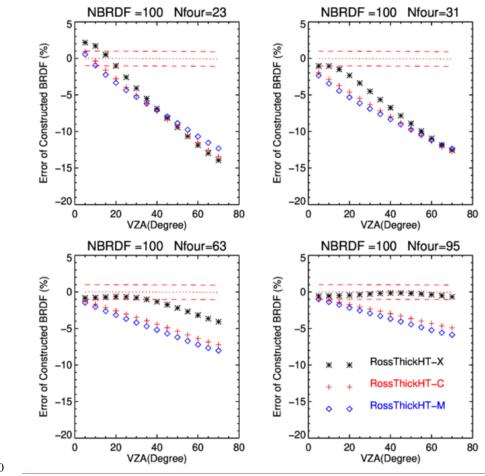
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379 While both numbers are necessary for the reconstructed BRDF accuracy, the main impact comes 380 from the number of Fourier terms N<sub>FOURIER</sub> used, when the value of N<sub>BRDF</sub> is twice (or more) that 381 of N<sub>FOURIER</sub> . In Figure 2, using a fixed value N<sub>BRDF</sub> =100 for the RossThickHT-M, RossThickHT-C and RossThickHT-X models, we show the dependence of the relative error of the reconstructed 382 BRDF on the solar zenith angle for four different values of NFOURIER. Choices of NFOURIER (23, 31, 383 384 63 and 95) correspond to values 12, 16, 32 and 48 for the number N<sub>STREAMS</sub> (number of half-space 385 polar discrete ordinates) used in VLIDORT (NFOURIER = 2NSTREAMS - 1). In this example, also used by [Lorente et al., 2018] (their Figure 6), the BRDF represents a vegetated surface over Amazonia 386 387 at wavelength 758 nm with free parameters  $[P_1, P_2, P_3] = [0.36, 0.24, 0.03]$  taken from MODIS band 2 (841-876 nm) to account for the increase in surface reflectivity near 700 nm. 388

389 Overall, the error decreases with increasing values of N<sub>FOURIER</sub>. The error also increases with those

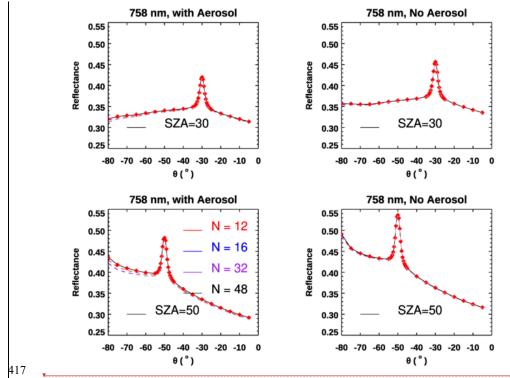
390 viewing angles at which the hotspot occurs, since the hotspot peaks are higher and narrower for 391 larger viewing angles. Errors for all three models are large when N<sub>FOURIER</sub> is as small as 23. The 392 advantage of RossThickHT-X starts to show when NFOURIER increases to 31, but this is not 393 significant when the hotspot viewing angle is larger than 45°. When N<sub>FOURIER</sub> is set to 95, the 394 performance of RossThickHT-X is much better than that for the other two models; the error is less 395 than 1% even for large viewing hotspot angles, whereas the corresponding errors using 396 RossThickHT-M or RossThickHT-C are still at the 5-8% level for hotspots at viewing angles 397 larger than 30°. Overall, the error with RossThickHT-C is slightly smaller than that for 398 RossThickHT-M.

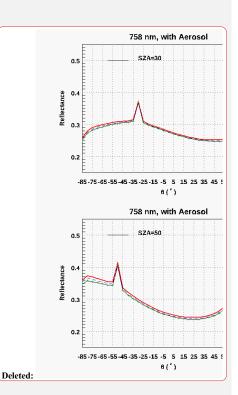




401Figure 2. Accuracy of Fourier-reconstructed BRDFs relative to their exact values, for the three402Ross-Li models.  $N_{BRDF} = 100$ , with  $N_{FOURIER}$  set to four different values as indicated. Surface403BRDF parameters represent a vegetated surface over Amazonia at 758 nm, with  $[P_1, P_2, P_3] =$ 404[0.36, 0.24, 0.03].

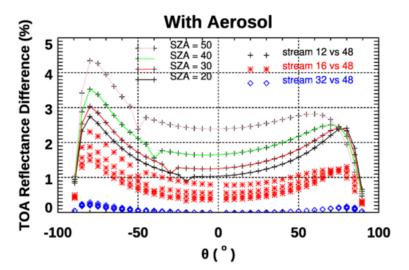
405 Next we examine simulated TOA reflectances at 758 nm with the three hotspot models providing 406 inputs to the main VLIDORT RT calculations. We again set  $N_{BRDF} = 100$  and  $N_{STREAMS} = 12, 16, 32$ 407 and 48. Results are shown in Figure 3 for two solar zenith angles. The hotspot signature is evident 408 at 30° (upper panels) and 50° (lower panels), and the peak signature with aerosols present is higher 409 than that without aerosol. The widths of the hotspots in Figure 3 are very similar, confirming the 410 argument of [Powers and Gerstl, 1988] that the hotspot width is expected to be relatively invariant 411 to atmospheric perturbations. Lines of different colors correspond to simulations using different 412 values of N<sub>STREAMS</sub>; in general, differences between these lines are pretty small, especially in the 413 atmosphere without aerosol and when the viewing angle is less than 60°. To better illustrate 414 patterns in TOA reflectance values using different values N<sub>STREAMS</sub>, we used the simulated 415 reflectances obtained with  $N_{\text{STREAMS}} = 48$  as the reference, and the results of this comparison are 416 shown in Figure 4.

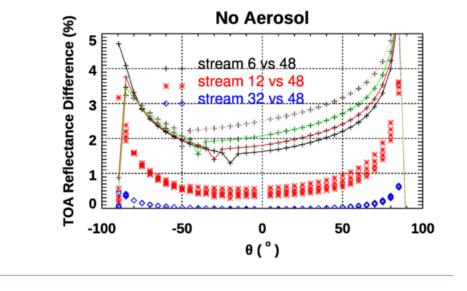




**Figure 3.** TOA reflectance as a function of viewing zenith angle, simulated by VLIDORT at 758 nm with a Ross-Li surface BRDF model with hotspot correction RossThickHT-X. Geometries

are in the principal plane for two solar zenith angles as indicated, and results were obtained with and without aerosol. Surface BRDF parameters represent a vegetated surface over Amazonia at 758 nm with (P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>) = (0.36, 0.24, 0.03). <u>The red solid line represents the simulation N<sub>STREAMS</sub></u> = 12, blue dashed line is for N<sub>STREAMS</sub> = 16, with the remaining lines for N<sub>STREAMS</sub> = 32 (green) and N<sub>STREAMS</sub> = 48 (dark); the latter two lines are almost aligned.





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428 **Figure 4**. Same set-ups as Figure 3, but now plotting the TOA reflectance differences with four 429 solar zenith angles as indicated.

430 From Figure 4 it is evident that relative differences in TOA reflectances for an atmosphere with 431 aerosols are larger than those for the atmosphere without aerosols. As the typical viewing angle 432 range for BRDF kernels is mostly within 60°, we will focus on these differences for viewing angles  $< 60^{\circ}$ . In the upper panel we see that TOA differences (comparing N<sub>STREAMS</sub> = 12 with N<sub>STREAMS</sub> 433 434 = 48) increase with solar zenith angle; the difference at SZA =  $50^{\circ}$  is almost double than that at 435  $SZA = 20^{\circ}$ . The relative difference in percentage at the hotspot region is smaller than beyond 436 hotspot, which is easy to understand as the absolute value of the TOA reflectance at the hotspot is 437 larger. In both cases with and without aerosol, TOA reflectance differences (comparing NSTREAMS 438 = 32 with  $N_{STREAMS}$  =48) are very small; VLIDORT simulations with  $N_{STREAMS}$  = 32 are accurate 439 enough in this case.

For the atmosphere with aerosol, the bias in simulated TOA reflectances using  $N_{\text{STREAMS}} = 16$ (relative to  $N_{\text{STREAMS}} = 48$ ) is 0.5-1.0%. In the clear atmosphere without aerosol, the bias of using  $N_{\text{STREAMS}} = 6$  can be in the region 2-3%, but the bias with  $N_{\text{STREAMS}} = 12$  is around 0.5%, suggesting that the setting for  $N_{\text{STREAMS}}$  should be 12 or higher in a Rayleigh atmosphere overlying a hotspot surface.

As noted already,  $N_{FOURIER} = 2N_{STREAMS} - 1$ . Compared to the value of  $N_{FOURIER}$  needed for 445 446 reconstruction of surface BRDFs near the hotspot (Table 1), that is, N<sub>FOURIER</sub> = 139-162 for an 447 accuracy of 0.5-1.0%, the values of  $N_{FOURIER} = 23$  (for the Rayleigh scenario) and  $N_{FOURIER} = 63$ 448 (for the atmosphere with aerosol) needed for full VLIDORT RT simulations are much smaller. 449 The reason for this reduction lies with the separation in VLIDORT between the first order (FO: 450 single scattering and direct reflectance) calculations and the multiple-scatter (MS) calculations in 451 VLIDORT. The first-order calculation in VLIDORT is always done with full accuracy with solar 452 beam and line-of-sight attenuations treated for a curved atmosphere, and with an exact value for the surface BRDF used to calculate the "direct-bounce" reflectance (which is very often the 453 454 dominant contribution from the surface). No Fourier reconstruction is necessary for this 455 contribution. For the MS contribution, multiple scatter is treated using Fourier cosine/sine azimuth 456 expansions and associated Fourier terms for both the truncated phase matrix for scattering and the diffuse-field BRDF contributions. The important point to note here is the use of the exact BRDF 457 458 for the direct-bounce contribution in VLIDORT; RT models without this FO/MS separation will 459 be constrained by the need to use a Fourier-expanded reconstruction for the direct-bounce BRDF 460 contribution.

461 The results shown in Figures 3-4 are confined to a single standard atmosphere and aerosol model. 462 In the next section below, we use VLIDORT simulations to investigate the impact of scattering on 463 hotspot signatures. For this study, we choose  $N_{BRDF} = 200$  and  $N_{STREAMS} = 32$ ; this should be 464 conservative enough to avoid any uncertainty associated with the use of surface BRDFs and the 465 choice of stream numbers in VLIDORT.

#### *3.2. Impact of scattering on the hotspot signature at TOA*

466

467 Here we use the three parameters  $(P_1, P_2, P_3) = (0.0399, 0.0245, 0.0072)$  for the RTLSR surface 468 BRDF model. These are the spatially averaged parameters from MODIS (BRDF/albedo product

469 MCD43A1) band 3 (459–479 nm) over Amazonia (latitude  $5^{\circ}$  N –  $10^{\circ}$  S, longitude  $60 - 70^{\circ}$  W)

470 for March 2008 [Lorente et al., 2018]. TOA reflectances are calculated as a function of viewing

471	zenith angle in the principal plane, with the solar zenith angle set at 30° (Figure 5). In this
472	experiment, we simulated two atmospheric conditions with and without aerosol and using the
473	new hotspot correction model, RossThickHT-X, and the RTLSR BRDF model without a hotspot
474	correction (RossThick). From the comparison of TOA reflectances at all angles between the left
475	and the right panels in Figure 5, we can see that the TOA reflectance in the atmosphere with
476	aerosol is overall larger than that without aerosol, indication the aerosol scattering increases the
477	TOA reflectance. Compared to the molecular scattering only, the addition of aerosol leads to an
478	increase of TOA reflectance near hot spot peak by ~ 8% and 17% at 469 and 645 nm
479	respectively. However, from a comparison of the TOA reflectances with and without hotspot
480	correction, i.e. using RossThickHT-X and RossThick, we found that at 469 nm the increase of
481	surface reflectance at hot spot results in an increase of TOA reflectance by ~ 4% for atmosphere
482	with molecular scattering only, while in the atmosphere with moderate aerosol the value of
483	increase is only 2%. At 645 nm, the values of reflectance increase at hot spot are about 12.5%
484	and 7% for atmosphere with and without aerosol, indicating that for the longer wavelength at 645
485	nm, the TOA-hotspot signature is much stronger than at 469 nm. The smaller TOA-hotspot
486	signature at 469 nm is due to the influence of stronger Rayleigh scattering. The inclusion of
487	aerosol scattering smooths out the hotspot signature at the TOA by ~44% to -50% compared to
488	the atmosphere with molecular scattering only in these two wavelengths, suggesting aerosol
489	scattering further smooths out the hotspot signature at the TOA, and makes it harder to
490	discriminate the TOA reflectance difference between the runs with and without hotspot
491	correction. This observation agrees with the results from [Bréon et al., 2002], in which it was
492	noted that no significant hotspot signature has been observed when the surface reflectance is very
103	small as in the blue channel or over the ocean

small, as in the blue channel or over the ocean.

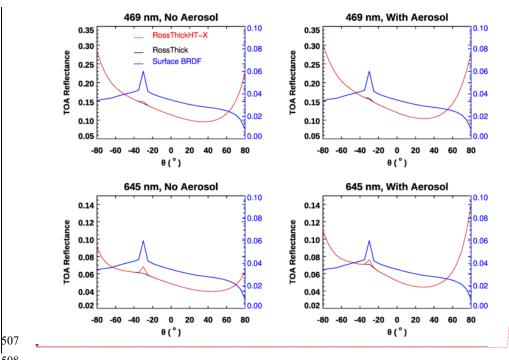
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**Figure 5.** VLIDORT TOA reflectances as a function of viewing zenith angle with solar angle 30° in the principal plane, at 469 and 645 nm using a Ross-Li surface BRDF model RossThick and RossThickHT-X, and with and without aerosol. The aerosol model used is the same as in Figure 3, with optical depth 0.2. Surface BRDF parameters represent a vegetated surface over Amazonia with (P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>) = (0.0399, 0.0245, 0.0072), and blue curves are surface reflectance.

514 We also examine the hotspot signatures in 765 and 865 nm, two wavelengths used in POLDER 515 data analysis. The three linear weighting parameters in the BRDF model are  $(P_1, P_2, P_3) = (0.36,$ 516 0.24, 0.03), which is the same set as that used by [Lorente et al., 2018]. As noted already, these 517 are taken from MODIS band 2 (841-876 nm) to account for the "red-edge" increase in surface 518 reflectivity near 700 nm (e.g. [Tilstra et al., 2017]). To test the representativeness of band 2 at 758 519 nm, Lorente et al. [2018] scaled the parameters from band 3 (459-479 nm) using the ratio of 520 reflectances at 772 nm and 469 nm; they found that differences with parameters taken from 521 MODIS band 2 were negligible. Since we would like to focus on the difference of the impact of 522 atmospheric scattering on the hotspot signatures at 758 and 865 nm, we have chosen to use the 523 same two sets of surface BRDF parameters. The results are plotted in Figures 6 and 7. To highlight 524 the differences caused by the  $3\pi/4$  factor normalizing the volume-scattering kernels  $K_{vol}$  (see note 525 in Section 2.2), we have added in Figure 7 two simulated TOA reflectances, one based on the 526 original hotspot correction model from Maignan et al. [2004] (RossThickHT-M) and the other 527 using the BRDF noted in the paper of Lorente et al. [2018] (indicated by "RossThickHT-L"). 528 Compared to Figure 5, much larger TOA-hotspot signatures at both 865 and 758 nm are evident 

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534 in Figures 6 and 7 respectively, and they are slightly larger at SZA=50° than at SZA=30°. As

535 expected, in the scattering region within 2° of hot spot there are some differences between

536 RossThickHT-M and RossThickHT-X, but beyond the hotspot (±5°), the TOA reflectance using

537 RossThickHT-X agrees very well with that using the original RossThick model. However, from

538 Figure 7, we see that the simulated reflectance using RossThickHT-M is slightly larger than that

539 using RossThick model even in a region of  $\pm 15^{\circ}$  beyond the hotspot, particularly in the large

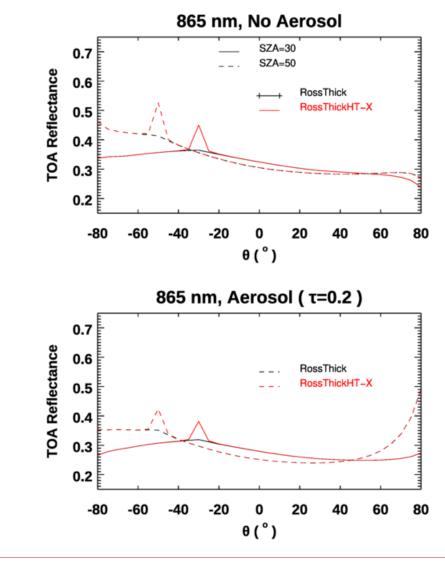
viewing angles in the forward direction. In the region of  $\pm 5^{\circ}$  to  $\pm 15^{\circ}$  beyond the hotspot, the 540

simulated reflectance using RossThickHT-M is clearly larger than that using RossThick and 541 RossThickHT-X.

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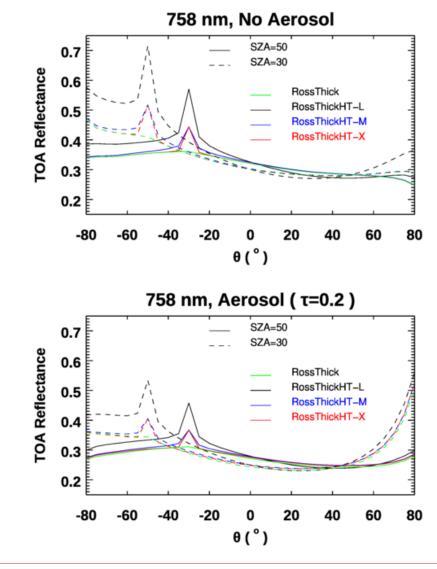
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**Figure 6**. Same as Figure 5 but results are calculated at 865 nm for solar zenith angles 30° and 50°. Surface BRDF parameters represent a vegetated surface over Amazonia with  $(P_1, P_2, P_3) = (0.36, 0.24, 0.03)$ .



**Figure 7**. Similar to Figure 6 but results calculated at wavelength758 nm. For comparison, we have added simulated TOA reflectances using the original hotspot correction model from [Maignan et al., 2004] (RossThickHT-M) and again using the model in [Lorente et al., 2018], which is a factor of  $4\pi/3$  times larger than RossThickHT-M in the hotspot region and is denoted here as RossThickHT-L.

To better quantify the hotspot effect and the impact due to scattering in the atmosphere, we define the "hotspot amplitude" as the difference between the TOA reflectance at the hotspot and the

556 corresponding TOA reflectance calculated without hotspot correction, namely:

557 
$$HT_{Amplitude} = \frac{R(\theta o, \theta, \phi = 180, \text{RossThickHT} - \text{Li})}{R(\theta o, \theta, \phi = 180, \text{RossThick} - \text{Li})}.$$

558 The impacts of molecular and aerosol scattering on these amplitudes are illustrated in Figure 8 for-559 a range of hotspot viewing angles and for four wavelengths. For comparison, the hotspot 560 amplitudes at the surface are also plotted. From Figure 8, it is evident that scattering in the 561 atmosphere smooths out the hotspot signature at TOA, and the impact of scattering is much larger 562 in the visible compare with that in the near-infrared part of the spectrum. Even in the visible, the 563 amplitude of the hotspot signature at 469 nm is much smaller than that at 645 nm. When the SZA 564 increases from 20<sup>o</sup> to 50°, the HS amplitude at 469 nm decreases by -1.34% and -1.08% for 565 atmospheric conditions without aerosol and with aerosol, respectively. The HS amplitude at 645 566 nm decreases by -1.24% and -2.14% similarly. In contrast, the HS amplitudes increase by 3.36 (0.03)% at 758 nm, and by 3.9 (1.5) % at 865 nm as SZA increases from 20° to 50°. Since 567 568 molecular scattering is much smaller than in the visible, the large difference in the amounts of HS 569 amplitude increase between no-aerosol and with-aerosol conditions indicates the impact of 570 multiple scattering, and the existence of aerosol smooths out the TOA hotspot signature. The 571 increase of HS amplitudes with SZA following with the increase of surface reflectance in the near 572 infrared, particularly in the no-aerosol condition, indicates that the HS amplitude is largely affected 573 by surface reflectance in the near infrared.

574 575 These simulated results agree well with the analysis of POLDER data by [Bréon et al., 2002]; at 440 nm, they found that the amplitude of the hotspot signature is very small. The much 576 larger amplitudes observed at 758 nm and 865 nm also confirm the findings by [Maignan et al., 577 2004], who showed that near-infrared measurements are preferred to those in the visible, not only 578 because of the larger-amplitude directional effects but also because of the lower atmospheric 579 perturbation. Indeed, Maignan et al. [2004] suggested that near-infrared measurement data is better 580 suited for the evaluation of different BRDF models. From Figure 8 we can also see that in the near-581 infrared, the amplitude of the hotspot signature increases with the zenith angle (right panel); 582 however, the angular dependencies in the surface hotspot and the TOA hotspot are almost opposite

583 in the visible, especially for an atmosphere without aerosols.

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	nfirming that the atmospheric contribution to be increase at the backscattering direction is

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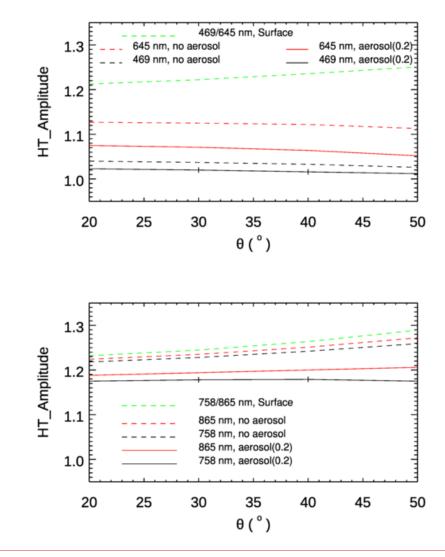


Figure 8. Comparison of hotspot amplitudes at the TOA for an atmosphere with and without
aerosols in visible (469 and 645 nm, left panel) and near-infrared (658 and 865 nm, right panel).
Hotspot amplitudes at the surface are computed using the differences between the RossThickHTLi and RossThick-Li BRDF models.

594 In the processing of POLDER data done by [Bréon et al., 2002] and [Maignan et al., 2004], only 595 molecular scattering to first order was taken into account for the atmospheric correction. As there 596 is no correction for the effects of aerosol scattering or the coupling of surface reflectance with 597 molecular scattering, absolute values of the reflectances may not be fully representative of the 598 surface for POLDER [Bréon et al., 2002]. From our simulations shown in Figure 8, the amplitude 599 of the hotspot signature with aerosol scattering included is smaller than that without aerosol, 600 suggesting that the results from POLDER [Bréon et al., 2002] might underestimate the amplitude 601 of hotspot signature at the surface. Based on the differences of the HS amplitudes between the 602 atmosphere with aerosol and without aerosol, we estimate that, on average, the HS amplitude is 603 underestimated by 4.0 ±1.7% when not considering aerosol for a moderately polluted atmosphere 604 with optical depth of 0.2, even though most satellite observations are less affected by the aerosols 605 than this simulation may suggest.

606

607 A final issue is related to a factor difference that exists between the equation of [Lorente et al., 608 2018] (i.e. their Eq. A1) with our Eq. (8), which is the one used in [Maignan et al., 2004]. The one 609 used by [Lorente et al., 2018] is  $3\pi/4$  times larger; this discrepancy results in a TOA-hotspot 610 signature more than twice as large, as shown in Figure 7. Since we used the same BRDF parameters 611 as [Lorente et al., 2018], this factor difference is the main reason that the TOA-hotspot signatures 612 shown by [Lorente et al., 2018] (their Figure 5) at 469 and 645 nm from their DAK model are 613 higher than our simulated results in this paper. In addition, in the paper of Lorente et al., 2018, the 614 615 616 617 618 authors obtained the VLIDORT result using an older version of the code, and this result showed the hotspot peak that was smaller than that generated with the other RT models. We think the reason for this lies with a scaling factor difference between the hotspot BRDF equation cited in [Lorente et al., 2018] and the equation used in the earlier VLIDORT model. Hence, we have added this simulation result here in order to bring attention to users when using scaling factor data from 619 the MODIS BRDF product, From the upper panel of Figure 7, it is evident that the hotspot peak 620 using RossThickHT-L seems too high, particularly for the hotspot occurring at 50°. From the 621 analysis of POLDER data, Bréon et al. [2002] found that the hotspot reflectance amplitude is 622 generally of the order 0.10 0.20 at 865 nm and 0.03 0.18 at 670 nm, although the full range of 623 values is wide. Therefore, we think that the use of an equation with a factor of  $3\pi/4$  discrepancy is 624 likely to overestimate the hotspot effect, and we caution users to be careful to check the equations 625 for the presence of this  $3\pi/4$  factor, <u>particularly</u> when using MODIS BRDF products.

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### 635 **4. Summary and Conclusions**

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In remote sensing, it is common practice to deploy a simple kernel-driven semi-empirical model with three free parameters to represent land surface BRDFs (excepting snow and ice); the commonly used model is the RossThick/LiSparse combination with a correction to account for the hotspot [Maignan et al., 2004]. In our study, we modified this BRDF model to improve convergence of the Fourier azimuth series decomposition. Furthermore, using this new hotspot model, we studied the impact of Rayleigh scattering and aerosol on the TOA atmospheric hotspot signature in the visible and near-infrared wavelengths using the VLIDORT RTM.

With the improved hotspot correction, we found that the numbers of Gaussian points (N<sub>BRDF</sub>) and Fourier Terms (N<sub>FOURIER</sub>) are more than 10 times smaller than those needed with the original hotspot model from Maignan et al. [2004]; this makes our BRDF model much more practical for use with VLIDORT to simulate the hotspot signature at the TOA. Another advantage of this modified model is that the new hotspot model agrees very well with the original RossThick model away the hotspot region, thus allowing the use of this single model in the conditions with and without hotspot in applications.

#### We carried out a number of investigations on the impact of molecular and aerosol scattering on the hotspot signature at the TOA. TOA reflectances were calculated for different solar and viewing angles and at four wavelengths. These simulations using VLIDORT show, that:

- 1. In agreement with previous analysis using POLDER measurement data, hotspot signatures in the near-infrared are larger than those in the visible <u>as it is less impacted by molecules</u> scattering, making it better to be used to derive the surface hotspot signature.
- Also in agreement with the POLDER study, the hotspot amplitudes at TOA and the surface
  both increase with solar zenith angle in the near-infrared; however, at 469 and 645 nm, this
  increase with solar zenith angle is not obvious at TOA, due to stronger Rayleigh scattering
  at shorter wavelengths, which is more pronounced for longer path lengths at larger solar
  zenith angles.
- Scattering by molecules and aerosols in the atmosphere tends to smooth out the hotspot signature at TOA, and the hotspot amplitude is reduced when aerosols are added to an otherwise clear (Rayleigh scattering only) atmosphere. <u>These results also showed that</u> atmospheric scattering does not generate hotspot-like signatures and does not change the width of the BRDF-induced hotspot.
- In VLIDORT, the direct-beam solar reflectance is calculated using the exact BRDF (rather than in a truncated Fourier-series form); this means that smaller values of N<sub>FOURIER</sub> (i.e. 23 and 63 for atmospheres without and with aerosol scattering) can be used in for the multiple scattering calculations in VLIDORT to obtain hotspot signature with acceptable accuracy.

Since atmospheric corrections in the POLDER data processing were performed using Rayleighonly single scattering without any consideration of aerosol. from our simulations we found that the amplitude of hotspot signature at the surface is likely underestimated by  $4.0 \pm 1.7\%$  in the analysis of hotspot signature using POLDER data [Bréon et al., 2002], highlighting the importance to consider the multiple scattering and to include aerosols in the retrievals of surface BRDF (hotspot),

Another issue related to the hotspot correction in the model used by Lorente et al. [2018] is the scaling by a factor of  $3\pi/4$ ; this may lead to the amplitude of hotspot too high in large solar zenith

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691 angle. It is recommended that users take care to check the kernel equations when using the three 692 parameters from MODIS BRDF products to generate the BRDF.

693 The agreement between our simulated results and observations from POLDER measurements. 694 enhances our understanding of the nature of the hotspot and the impact on it by atmospheric 695 scattering. It is also clear that VLIDORT makes accurate simulations of the hotspot effect, and the 696 results obtained here can be used as benchmarks. Our improved hotspot kernel is now a standard 697 feature in the latest version of the VLIDORT BRDF supplement code that significantly improve 698 the numerical efficiency. Since this new model has not been validated using any real observation 699 data, and considering the difference between this model and the original hotspot model from 700 Maignan et al. [2004] in scattering angles close to the peak of hotspot, it may not be appropriate 701 for those who need an exact representation of the hot spot angular signature around the peak of 702 hotspot,

703

#### 704 Description of author's responsibilities,

XX, XL and RS conceived of the idea. XX and RS led the writing. All authors edited themanuscript.

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#### 709 CRediT authorship contribution statement

- 710 Xiaozhen Xiong: Methodology, Writing original draft, Formal analysis, Investigation. Xu
- 711 Liu: Funding acquisition, Supervision, Writing review & editing, Conceptualization. Robert
- 712 Spurr: Methodology, Writing review & editing, Formal analysis. Ming Zhao: Coding,
- 713 Analysis. Wan Wu, Qiguang Yang, Liqiao Lei: Writing review & editing.

#### 714 Declaration of Competing Interest

- 715 The authors declare that they have no known competing financial interests or personal
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   Advanced Supercomputing (NAS) Division at NASA Ames Research Center.
- 721

## **Deleted:** Our results highlight the importance of the including aerosol scattering in the retrievals of surface BRDF (hotspot).

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