



**Evaluation of the operational Aerosol Layer Height retrieval algorithm for Sentinel-5 Precursor**

A. F. J. Sanders

**Evaluation of the operational Aerosol Layer Height retrieval algorithm for Sentinel-5 Precursor: application to O<sub>2</sub> A band observations from GOME-2A**

A. F. J. Sanders<sup>1,a</sup>, J. F. de Haan<sup>1</sup>, M. Sneep<sup>1</sup>, A. Apituley<sup>1</sup>, P. Stammes<sup>1</sup>, M. O. Vieitez<sup>1</sup>, L. G. Tilstra<sup>1</sup>, O. N. E. Tuinder<sup>1</sup>, C. E. Koning<sup>1</sup>, and J. P. Veefkind<sup>1</sup>

<sup>1</sup>Royal Netherlands Meteorological Institute, De Bilt, the Netherlands

<sup>a</sup>now at: Institute of Environmental Physics, University of Bremen, Bremen, Germany

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Correspondence to: A. F. J. Sanders (asanders@iup.physik.uni-bremen.de)

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## Abstract

An algorithm setup for the operational Aerosol Layer Height product for TROPOMI on the Sentinel-5 Precursor mission is described and discussed, applied to GOME-2A data, and evaluated with lidar measurements. The algorithm makes a spectral fit of reflectance at the O<sub>2</sub> A band in the near-infrared and the fit window runs from 758 to 770 nm. The aerosol profile is parameterized by a scattering layer with constant aerosol volume extinction coefficient and aerosol single scattering albedo and with a fixed pressure thickness. The algorithm's target parameter is the height of this layer. In this paper, we apply the algorithm to observations from GOME-2A in a number of systematic and extensive case studies and we compare retrieved aerosol layer heights with lidar measurements. Aerosol scenes cover various aerosol types, both elevated and boundary layer aerosols, and land and sea surfaces. The aerosol optical thicknesses for these scenes are relatively moderate. Retrieval experiments with GOME-2A spectra are used to investigate various sensitivities, in which particular attention is given to the role of the surface albedo.

From retrieval simulations with the single-layer model, we learn that the surface albedo should be a fit parameter when retrieving aerosol layer height from the O<sub>2</sub> A band. Current uncertainties in surface albedo climatologies cause biases and non-convergences when the surface albedo is fixed in the retrieval. Biases disappear and convergence improves when the surface albedo is fitted, while precision of retrieved aerosol layer pressure is still largely within requirement levels. Moreover, we show that fitting the surface albedo helps to ameliorate biases in retrieved aerosol layer height when the assumed aerosol model is inaccurate. Subsequent retrievals with GOME-2A spectra confirm that convergence is better when the surface albedo is retrieved simultaneously with aerosol parameters. However, retrieved aerosol layer pressures are systematically low (i.e., layer high in the atmosphere) to the extent that retrieved values are not realistically representing actual extinction profiles anymore. When the surface albedo is fixed in retrievals with GOME-2A spectra, convergence deteriorates as ex-

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pected, but retrieved aerosol layer pressures become much higher (i.e., layer lower in atmosphere). The comparison with lidar measurements indicates that retrieved aerosol layer heights are indeed representative of the underlying profile in that case. Finally, subsequent retrieval simulations with two-layer aerosol profiles show that a model error in the assumed profile (two layers in the simulation but only one in the retrieval) is partly absorbed by the surface albedo when this parameter is fitted. This is expected in view of the correlations between errors in fit parameters and the effect is relatively small for elevated layers (less than 100 hPa). In case one of the scattering layers is near the surface (boundary layer aerosols), the effect becomes surprisingly large such that the retrieved height of the single layer is above the two-layer profile.

Furthermore, we find that the retrieval solution, once retrieval converges, hardly depends on the starting values for the fit. Sensitivity experiments with GOME-2A spectra also show that aerosol layer height is indeed relatively robust against inaccuracies in the assumed aerosol model, even when the surface albedo is not fitted. We show spectral fit residuals, which can be used for further investigations. Fit residuals may be partly explained by spectroscopic uncertainties, which is suggested by an experiment showing the improvement of convergence when the absorption cross section is scaled in agreement with Butz et al. (2012) and Crisp et al. (2012) and a temperature offset to the a priori ECMWF temperature profile is fitted. Retrieved temperature offsets are always negative and quite large (ranging between  $-4$  and  $-8$  K), which is not expected if temperature offsets absorb remaining inaccuracies in meteorological data. Other sensitivity experiments investigate fitting of stray light and fluorescence emissions. We find negative radiance offsets and negative fluorescence emissions, also for non-vegetated areas, but from the results it is not clear whether fitting these parameters improves the retrieval.

Based on the present results, the operational baseline for the Aerosol Layer Height product currently will not fit the surface albedo. The product will be particularly suited for elevated, optically thick aerosol layers. In addition to its scientific value in climate research, anticipated applications of the product for TROPOMI are providing aerosol



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SCanning Imaging Absorption spectroMeter for Atmospheric CHartography) has been built up over the past years (e.g., Lelli et al., 2012, 2014; Wang and Stammes, 2014; Wang et al., 2008; Loyola et al., 2007; Kokhanovsky et al., 2006a, b; Koelemeijer et al., 2002, 2001).

Various instrument requirement and sensitivity studies investigating the potential of spectral measurements of the O<sub>2</sub> A band for aerosol retrieval have appeared in the past. These studies include the ones by Geddes and Bösch (2015), Hollstein and Fischer (2014), Sanders and De Haan (2013), Hollstein et al. (2012), Hasekamp and Sidans (2009), Siddans et al. (2007), Corradini and Cervino (2006), and Gabella et al. (1999). Overall, these studies show, among other things, that retrieval precision is typically better when the aerosols are optically thicker or more elevated, or when the solar zenith angle is larger. The amount of aerosol profile information from such a passive satellite measurement is however limited (Geddes and Bösch, 2015; Corradini and Cervino, 2006; Timofeyev et al., 1995).

Case studies based on satellite data have been performed by Koppers and Murtagh (1997) for GOME data, and by Sanghavi et al. (2012) and Kokhanovsky and Rozanov (2010) for SCIAMACHY data. Koppers and Murtagh (1997) show retrieved aerosol optical thickness from GOME for two months of global observations and for several months of observations over two AEROSOL ROBOTIC NETWORK (AERONET) stations near the Saharan desert. Sanghavi et al. (2012) analyse retrievals for a year of SCIAMACHY observations over an AERONET station in the Indo–Gangetic Plain, and Kokhanovsky and Rozanov (2010) demonstrate their retrieval technique using a SCIAMACHY observation of a Saharan dust outbreak over the Atlantic Ocean. Koppers and Murtagh (1997) fit aerosol optical depth in five atmospheric layers, Sanghavi et al. (2012) parameterize the aerosol extinction profile by a lognormal function for which they retrieve the peak height and the width in addition to optical thickness, while Kokhanovsky and Rozanov (2010) fit the optical thickness and the top of a scattering layer that extends to the ground and has a constant aerosol volume extinction coefficient inside the layer. Only in the retrieval scheme proposed by Koppers and Murtagh (1997) is the surface

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albedo retrieved simultaneously with aerosol parameters. The issue of selecting cloud-free pixels is explicitly addressed by Koppers and Murtagh (1997), who devised a cloud mask based on sub-pixel information from GOME's Polarization Measurement Devices (PMDs). Kokhanovsky and Rozanov (2010) use visual inspection of a MEdium Resolution Imaging Spectrometer's (MERIS) RGB image to select a cloud-free SCIAMACHY pixel and Sanghavi et al. (2012) dissociate aerosols from clouds in a post-retrieval analysis of retrieved optical thickness. Finally, a comparison of retrieved aerosol optical thickness with AERONET aerosol optical thickness is provided by Koppers and Murtagh (1997) and Sanghavi et al. (2012). None of these studies compared the retrieved height distribution with independent measurements.

This brief summary of previous case studies already illustrates a number of issues involved when setting up an O<sub>2</sub> A band aerosol retrieval: the choice of the vertical profile assumed in retrieval, masking of pixels containing clouds, and validation of the retrieval results. We continue these case studies using data from GOME-2A. Our primary goal is to retrieve aerosol layer height (see below). Based on the case studies discussed above and on our own experiences we pay special attention to the following three aspects when setting up the experiments. Firstly, we put effort in accurate cloud masking and in cirrus masking in particular. Even though cirrus clouds are optically thin, their optical thickness is similar in magnitude to aerosol optical thicknesses and, as a consequence, any undetected cirrus may significantly bias retrieved aerosol height (e.g., Sanders and De Haan, 2014; see also Sect. 9 of this paper). We use an Advanced Very High Resolution Radiometer (AVHRR) cloud mask accurately collocated to the respective GOME-2A pixel that includes a dedicated cirrus test using AVHRR's thermal infrared channels. Secondly, we apply our algorithm to observations of aerosol scenes covering different aerosol types and height distributions as well as covering sea and land surfaces. The aerosol scenes concern desert dust near the coast of West-Africa and over the Iberian Peninsula, volcanic ash over Europe, smoke from forest fires in North-America transported across the Atlantic Ocean, aerosols over the Aegean Sea, and various boundary layer aerosol and multi-layered aerosol cases over the Nether-



cloud retrieval schemes discussed above one of the two parameters is indeed fixed or retrieved in a separate step.

The work presented in this paper is part of an on-going effort to develop a dedicated Aerosol Layer Height (ALH) product for TROPOMI on the Sentinel-5 Precursor mission. Its main purpose is to retrieve and report the height of (vertically localized) aerosol layers in the free troposphere. Observations of aerosol height are of scientific interest, for example, for improving estimates of injection heights for transport modeling, for calculating direct radiative effects, or for better understanding effects on local atmospheric stability related to aerosol absorption. An important intended application of the TROPOMI product is providing aerosol height information for aviation safety. Furthermore, aerosol height information can be used to improve interpretation of the Absorbing Aerosol Index (AAI; De Graaf et al., 2005), as this index is strongly height-dependent. Currently, Aerosol Layer Height and Absorbing Aerosol Index are the two operational TROPOMI aerosol products. Science requirements for the Aerosol Layer Height product are defined in Van Weele et al. (2008). The target requirement on accuracy and precision of retrieved Aerosol Layer Height is 0.5 km or 50 hPa; the threshold requirement is 1 km or 100 hPa. A minimum aerosol optical thickness for which these requirements should be met is not indicated. Also note that requirements are not specified for the accuracy and precision of retrieved aerosol optical thickness from the O<sub>2</sub> A band. Dedicated retrievals of spectral aerosol optical thickness are provided by separate algorithms foreseen for TROPOMI or already operational for the Visible Infrared Imaging Radiometer Suite (VIIRS) on the Suomi National Polar-orbiting Partnership (Suomi NPP) mission. (TROPOMI is planned to fly in loose formation with Suomi NPP.) These aerosol optical thickness retrievals typically cover wavelength ranges that are much broader than the fit window used in our O<sub>2</sub> A band retrieval (currently 12 nm). The Algorithm Theoretical Basis Document for the Aerosol Layer Height product has been delivered as Sanders and De Haan (2014), which is expected to be released after publication of this paper.

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lations showing the effect of profile shape on retrieved aerosol layer height. Section 9 describes a simulation study investigating this effect in more detail. A discussion and conclusions are given in Sect. 10.

Throughout this paper, height is used as a general indication of vertical location, which can be expressed in terms of pressure in units of hPa or in terms of altitude (above ground level) in units of km. Finally, we remark that a companion paper (Lelli et al., 2015) in this issue describes a science verification of the Aerosol Layer Height algorithm using observations of an optically thick volcanic ash plume near Iceland in May 2010.

## 2 Should the surface albedo be a fit parameter?

In this section, we discuss in some detail why in one of the two experimental conditions for the GOME-2A scene retrievals we also fit the surface albedo when retrieving aerosol properties from the  $O_2$  A band. It is difficult to separate effects of the surface albedo and aerosol optical thickness from continuum reflectances, but independent information about the two parameters is available from the spectral shape of the absorption band: in case of single scattering, photons backscattered by aerosols follow shorter paths through the atmosphere than photons reflected by the surface and they will thus have a smaller chance of being absorbed. Indeed, two different combinations of surface albedo and aerosol optical thickness that give the same continuum reflectance may be distinguished from their reflectance spectra inside the absorption band, as is illustrated in Fig. 1 (left panel). The spectrum plotted in red corresponds to the scenario of an aerosol layer between 700 and 600 hPa ( $P_{\text{mid}}$  of 650 hPa) with an optical thickness ( $\tau$ ) at 760 nm of 0.3 over a ground surface with albedo ( $A_g$ ) of 0.2. The spectrum plotted in green corresponds to the scenario of an aerosol layer with the same height and pressure thickness but with a different optical thickness and for a surface with a different albedo. The combination of aerosol optical thickness and surface albedo is chosen such that the continuum reflectance remains the same as in the first scenario. Note

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that the two spectra show differences inside the absorption band. For comparison, the spectrum plotted in blue corresponds to the scenario of an aerosol layer moved to a different height but with optical thickness and surface albedo kept the same as in the first scenario. This spectrum differs from the first two also inside the absorption band.

Spectra are calculated for TROPOMI's resolution in the near-infrared band of 0.38 nm (anticipated at the time of writing). Also illustrated in Fig. 1 (right panel) are derivatives with respect to aerosol layer mid pressure ( $P_{\text{mid}}$ ), aerosol optical thickness ( $\tau$ ) and surface albedo ( $A_s$ ) for the example scenario. We cannot simultaneously fit surface albedo and aerosol optical thickness when the spectral shape of the derivatives is the same. The question of whether derivatives for a particular scenario are eventually sufficiently different has to be answered by actually doing the (non-linear) retrieval and by subsequently performing an error analysis.

Of course, in order to simplify the retrieval problem one may ask whether it is possible to retrieve aerosol properties while fixing the surface albedo at values provided by climatologies. We have done retrieval simulations investigating the effect on retrieved aerosol properties of uncertainties typically associated with surface albedo climatologies. Figure 2 shows representative results for an aerosol layer over land (the example scenario mentioned above). We assume the climatological (a priori)  $1-\sigma$  error to be 0.02 for land surfaces. The forward model and inversion scheme are the same as used in the GOME-2A retrievals (described in detail in Sect. 5), except for the instrument model (here: TROPOMI spectral response function and noise model). Also, for simplicity we take the surface albedo to be independent of wavelength. The left panel shows biases in retrieved aerosol layer pressure when the true surface albedo deviates from the value assumed in retrieval (“climatology”). The three plot lines correspond to retrievals in which the surface albedo is not fitted (a priori error of 0.0), the surface albedo is fitted with an a priori error equal to the climatological error, and the surface albedo is fitted when unconstrained by a priori information (large a priori error of 0.2). When the surface albedo is fixed in the retrieval, small deviations of the true surface albedo cause pressure biases well above 100 hPa and non-convergent retrievals (miss-

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ing data points). For darker surfaces, the effect is more moderate but still significant. For example, when the true surface albedo is 0.04 but the albedo assumed in retrieval is 0.03, retrieved aerosol layer pressure for the example scenario is almost a 100 hPa too high (not shown). The right panel of Fig. 2 illustrates the situation in a different way. In this plot we show precision of retrieved aerosol layer pressure and optical thickness as a function of the a priori error in the surface albedo. The three plot lines of the left panel thus correspond to three distinct points on the  $x$  axis of the plot in the right panel. One can see that auxiliary information about the surface albedo should have a  $1-\sigma$  error smaller than about  $10^{-3}$  to  $10^{-4}$  before it starts constraining the retrieval of aerosol properties, which is a very small number. In other words, the  $O_2$  A band contains independent information about the surface albedo and aerosol optical thickness. Of course, this information is more pronounced the more elevated aerosols are (i.e., the larger the pressure difference between the aerosols and the surface is).

Thus, when the surface albedo is fixed, aerosol height retrieved from the  $O_2$  A band will be biased or the retrieval will not converge for typical uncertainties in surface albedo climatologies. This is the first reason why we include an experimental condition for the GOME-2A scene retrievals in which the surface albedo is fitted. The second reason to do so is explained in the following. Retrieval of aerosol pressure and optical thickness from the  $O_2$  A band requires of course an assumed aerosol model. As discussed above, the target parameter of the TROPOMI  $O_2$  A band Aerosol Layer Height product is, however, aerosol pressure. In retrieval simulations we have observed that this parameter becomes quite insensitive to the assumed aerosol model if we simultaneously fit the surface albedo (see Sanders and De Haan, 2013). This is illustrated for the example scenario in Fig. 3. We investigate the bias in retrieved aerosol layer pressure as a function of a model error in the single scattering albedo. The value assumed in retrieval is 0.95 (“model value”). This time we show results for a sea surface (left panel) and a land surface (right panel). One can see that in case of a model error in the single scattering albedo, aerosol layer pressure is biased significantly and retrievals do not converge when the surface albedo is fixed in retrieval. Aerosol optical thickness and the surface

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albedo are biased as well (not shown). This effect is more moderate for the darker surface. For example, if the true single scattering albedo is 1.0 while the assumed value is 0.95, retrieved aerosol pressure is too high by about 20 hPa for aerosols over sea and by about 180 hPa for aerosols over land. Biases in retrieved aerosol layer pressures and non-convergences almost disappear when the surface albedo is included in the fit. Aerosol optical thickness and surface albedo, however, remain biased (not shown) and as a consequence retrieved values depend on the particular aerosol model assumed in retrieval (one might call them effective quantities). Since aerosol height is the target parameter, this finding is an important reason why at this stage of algorithm development we do not put effort in defining the most realistic aerosol model for every aerosol scene. Instead, in all retrievals presented in this paper we simply model the aerosol with a single scattering albedo of 0.95 and a Henyey–Greenstein phase function with asymmetry parameter of 0.7.

As an important caveat, we mention that correlations between errors in fit parameters for an O<sub>2</sub> A band aerosol retrieval are typically very high. Absolute values of correlation coefficients ( $r$ ) are often well above 0.9 and can sometimes become as high as 0.999. As an example, Table 2 lists correlation coefficients for retrieval of the example aerosol layer over land and over sea. The corresponding a posteriori errors, however, are small, as was shown in the right panel of Fig. 2. Apparently, parameters can be fitted with small precision errors in case errors are as highly correlated as this. Derivatives of reflectance with respect to the various fit parameters are similar, yet there are small but significant differences (see right panel of Fig. 1), which cause correlation coefficients to be smaller than one and make it possible to simultaneously fit parameters. Still, we should anticipate retrieval becoming sensitive to the many other systematic and quasi-random model and instrument errors present in real data when moving from the retrieval simulations reported in this section to the GOME-2A retrievals reported in the next sections. Finally, we remark that we are not aware of previous studies on O<sub>2</sub> A band cloud or aerosol retrieval reporting a posteriori correlation coefficients.

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We mention that more extensive retrieval simulations investigating the effects discussed above and many other retrieval sensitivities are presented in Sanders and De Haan (2014). In this paper, we present a number of sensitivity experiments using GOME-2A spectra, rather than simulated spectra, to further investigate the retrieval.

In conclusion, from simulation studies we learn that the surface albedo should be a fit parameter when retrieving aerosol properties from the O<sub>2</sub> A band. In the following sections we investigate whether this conclusion also holds for retrievals with real spectra.

### 3 GOME-2 instrument characteristics

The GOME-2 instruments are in polar orbits with local equator crossing times of about 9.30 h (descending node). In this paper, we only consider observations by GOME-2 on Metop-A (GOME-2A). The swath of GOME-2A had been 1920 km until mid July 2013 at which point it was reduced by a factor of two. In nadir scanning mode, the scanning mirror has a return time of 6 s, taking 4.5 s for the forward scan (east to west) and 1.5 s for the backward scan (west to east). In this work, only forward pixels are considered. The scan speed profile is such that the across track pixel size is approximately constant. The across track pixel size is mainly determined by the integration time, which generally is 0.1875 s for spectrometer Band 4 for the sunlit part of the orbit track. Thus, the across track forward pixel size is 80 km for the nominal 1920 km swath and 40 km in reduced swath mode (aerosol scene 06 in this work). The along track pixel size at nadir is 40 km and is primarily determined by the instrument's along track instantaneous field of view. Band 4 runs from 584 to 798 nm and has a spectral sampling of about 0.21 nm. The instrument spectral response function in Band 4 has a full width at half maximum (FWHM) of approximately 0.53 nm, which is coarser than TROPOMI's resolution (FWHM of 0.38 nm). Finally, we mention that GOME-2 has so-called Polarization Measurement Devices (PMDs), which measure P-polarized and S-polarized light in a number of wavelength bands. These measurements are used to correct radiance spectra for the instrument's polarization sensitivity. They can also

provide sub-pixel information for spectrometer measurements, because PMD ground pixels are eight times smaller in the across track direction (e.g., 10 by 40 km for a spectrometer ground pixel of 80 by 40 km). More information can be found in EUMETSAT (2014a). Without further clarification, the GOME-2A ground pixel refers to the ground pixel of the spectrometer throughout this paper.

#### 4 Selection of aerosol scenes and masking of clouds

We first compiled a list of sixteen aerosol scenes that served as an input for the GOME-2A retrieval experiments. In this paper, we define a scene as a three-minute granule of GOME-2A observations, which covers an area of about 1920 km across track by 1200 km along track (at nadir) for ground pixel sizes of 80 by 40 km (at nadir). Scenes were selected not only for the presence of aerosols but also for the availability of lidar measurements within the scene. We initially focussed on ground-based measurements because we might find good spatiotemporal collocation with the GOME-2A overpass for these lidar measurements. Ground-based measurements from the Cabauw Experimental Site for Atmospheric Research (CESAR) and the EARLINET station at Cabauw (Netherlands), from EARLINET stations at Evora (Portugal) and Granada (Spain), and from the Micro Pulse Lidar NETwork (MPLNET) station at Santa Cruz (Canary Islands) are included in this study. We also used airborne measurements taken aboard the Facility for Airborne Atmospheric Measurements's (FAAM) Atmospheric Research Aircraft during two dedicated campaigns over the North Sea (Eyjafjallajökull eruption) and the Aegean Sea (the European Space Agency's CARBONEXP campaign). Finally, we took satellite-based lidar measurements from CALIPSO into account. The initial checking of the presence of significant amounts of aerosols and of cloud conditions was done using AERONET aerosol optical thickness plots, lidar quicklooks and RGB images from the MODerate resolution Imaging Spectroradiometer (MODIS). Table 3 provides a short description of the sixteen aerosol scenes that were eventually selected.

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Having lidar measurements available within the geographical area of the aerosol scene that are also reasonably close in time to the GOME-2A overpass is a severe constraint, because of the sparse spatiotemporal sampling of lidar measurements. For example, exceptionally thick ash plumes close to an erupting volcano, which may have been an easy starting point for our case studies, were not included as there are no such aerosol cases (to our knowledge) for which there are nearby lidar measurements. As a consequence, the aerosol scenes have aerosol optical thicknesses that are moderate (see Table 3).

GOME-2A aerosol scenes were cloud-cleared using four conventional AVHRR threshold tests (EUMETSAT, 2011). These tests are (i) a brightness temperature test in the 11  $\mu\text{m}$  channel to detect medium to high clouds, (ii) a brightness temperature difference test for the 11 and 12  $\mu\text{m}$  channels to detect thin cirrus clouds, (iii) an albedo test using the two visual channels (one for land, the other for sea) to detect bright low clouds, and (iv) a spatial coherence test for the 11  $\mu\text{m}$  channel to detect broken clouds over sea. For every AVHRR pixel, if one of the tests indicated the presence of a cloud, the AVHRR pixel was considered cloudy. Then, a cloud fraction for the GOME-2A ground pixel was derived by dividing the number of cloudy AVHRR pixels by the total number of AVHRR pixels falling within the spectrometer's footprint. Aerosol height retrievals in this paper are only attempted for GOME-2A pixels with zero AVHRR cloud fraction. Table 3 lists the number of cloud-free pixels for every aerosol scene.

We mention here that we did not take AVHRR cloud information directly from the AVHRR level-1b product but used the European organisation for the exploitation of Meteorological SATellite's (EUMETSAT) new Polar Multi-sensor Aerosol product (PMAp) instead (EUMETSAT, 2014b). This product provides spectral aerosol optical thickness derived from GOME-2's PMD broadband radiances. As a support field, PMAp also provides an AVHRR cloud fraction for PMD ground pixels using the approach described above. AVHRR pixels are accurately collocated to PMD ground pixels (EUMETSAT, 2014b). We used cloud fractions for PMD ground pixels to calculate cloud fractions for spectrometer ground pixels.

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Finally, we also selected a target GOME-2A pixel for every scene resulting in a set of sixteen pixels. This set serves two purposes: first, it is used in extensive retrieval experiments investigating a number of retrieval sensitivities and second, it is used for comparison against lidar measurements. Sensitivity experiments are limited to a set of sixteen target pixels because computation time currently renders difficult investigating sensitivities for entire aerosol scenes. Target pixels were carefully selected according to the following criteria: (i) spatiotemporal collocation with lidar measurement, (ii) cloud-free conditions (AVHRR cloud mask), (iii) high aerosol optical thickness (Absorbing Aerosol Index; PMAp aerosol optical thickness; MODIS Terra aerosol optical thickness), (iv) homogeneous pixel (no coastal pixel, low variability of surface elevation inside pixel); and (v) outside sun glint region (threshold of  $18^\circ$  on sun glint angle, i.e., the angle between viewing direction and direction of specular reflection). These criteria could not be fulfilled all at the same time and a qualitative trade-off had to be made. An overview of the sixteen target pixels is shown in Fig. 4 (the numbering of the target pixels corresponds to the numbering of the scenes in Table 3).

Also shown in Fig. 4 are the locations of the corresponding lidar measurements. Often, the lidar profile showed cloud-free conditions while the AVHRR cloud mask unfortunately indicated the significant presence of clouds for the overlapping GOME-2A pixel. The high chance of cloud contamination due to the large GOME-2A ground pixel size is one of the reasons why good spatial collocation with the lidar measurement was not achieved for every target pixel. Sometimes, there was also a significant time difference between the lidar measurement and the GOME-2A observation (e.g., in case of a Raman lidar measurement in the early evening). For several cases, two lidar measurements were included in the analysis. Table 4 gives a description of each lidar measurement and lists the spatiotemporal distance to the target pixel.

We emphasize here that we are not attempting a comprehensive lidar validation of our results in this study but only do a first comparison. A validation is beyond the scope of this paper and given the present GOME-2A retrieval results it is not needed for our purposes at this point (to be discussed in detail in Sect. 8). We will primarily use

lidar measurements to better understand the difference in retrieval outcome when the surface albedo is retrieved simultaneously with aerosol parameters or when it is fixed in the retrieval.

## 5 Description of the retrieval setup

Here, we summarize main aspects of the forward model and the inversion scheme and describe the implementation for retrievals with GOME-2A as presented in this paper. The forward model and related modules are part of a software package developed at the Royal Netherlands Meteorological Institute (KNMI) called DISAMAR. The abbreviation DISAMAR stands for Determining Instrument Specifications and Analyzing Methods for Atmospheric Retrieval.

### 5.1 Forward model

Monochromatic reflectances in the O<sub>2</sub> A band are calculated online using the doubling-adding method (e.g., De Haan et al., 1987; Hovenier et al., 2004). Multiple scattering is included in the calculations, but polarization and rotational Raman scattering are ignored. An efficient high-resolution wavelength grid is constructed by defining small wavelength intervals bounded by strong O<sub>2</sub> line positions and using Gaussian division points for each interval. This results in about 3000 line-by-line calculations for a fit window extending from 758 to 770 nm and an oxygen absorption cross section that includes the three major isotopologues. The atmosphere is divided into 24 homogeneous layers, the distribution of which is not equidistant but again follows a Gaussian integration scheme. Finally, nine Gaussian points (eighteen streams) are used for integration over the polar angle. Derivatives are calculated in a semi-analytical manner using reciprocity (equivalent to the adjoint method, e.g., Landgraf et al., 2001).

In addition to line absorption by O<sub>2</sub>, first-order line mixing and collision-induced absorption by O<sub>2</sub>-O<sub>2</sub> and O<sub>2</sub>-N<sub>2</sub> are included in the oxygen absorption cross section

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according to Tran et al. (2006) and Tran and Hartmann (2008). Line parameters for the three major isotopologues are taken from the Jet Propulsion Laboratory database in agreement with Tran and Hartmann (2008). In the baseline retrieval setup, the resulting absorption cross section is multiplied by 1.03 following Butz et al. (2012) and Crisp et al. (2012).

Temperature profiles and surface pressures were taken from the European Centre for Medium-range Weather Forecasts' (ECMWF) Interim reanalysis fields. Reanalysis data are available every six hours (model times: 00:00, 06:00, 12:00 and 18:00 UTC) with a native spatial resolution of about 80 km. We used data on a 0.5° by 0.5° regular latitude–longitude grid. Note that this resolution is comparable to the size of the GOME-2 pixel. In the spatial dimension we took meteorological data for the model grid point closest to the center coordinate of the GOME-2A pixel. In the temporal dimension, we used linear interpolation between the two closest model times to determine meteorological parameters at the time of the GOME-2A observation.

Next to oxygen absorption and Rayleigh scattering, scattering and absorption by aerosols takes place in the atmosphere. In the baseline retrieval setup, we assume a single aerosol layer that is modelled as a layer of particles with a constant particle volume extinction coefficient and particle single scattering albedo. Also the pressure thickness is assumed constant and taken to be 50 hPa in all GOME-2A retrievals. By default, aerosols have a single scattering albedo of 0.95 and a Henyey–Greenstein phase function with asymmetry parameter of 0.7. There is no particular reason for choosing these values of single scattering albedo and asymmetry parameter other than that they are intermediate to values typically observed (Dubovik et al., 2002). In a similar fashion, we choose a phase function that is smooth and can serve as an approximate phase function for many aerosol types.

The ground surface is modelled as a Lambertian surface and we allow the surface albedo to depend linearly on wavelength. Albedo values at two wavelength nodes located at the end points of the fit window (758 and 770 nm) are specified and intermediate values are determined by interpolation. A priori values for the albedo at

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the two nodes are taken from the MERIS black-sky albedo climatology (Popp et al., 2011). Note that for sea pixels this climatology is filled with values from the GOME Lambertian-equivalent reflectivity climatology (Koelemeijer et al., 2003). In one of the sensitivity experiments of Sect. 7, we investigate the effect of fitting fluorescence emissions. Chlorophyll fluorescence from terrestrial vegetation is modeled as an isotropic contribution to the upwelling radiance field at the surface. Also fluorescence emissions are allowed to depend linearly on wavelength and they are specified at the same two wavelength nodes as the surface albedo. We assume fluorescence emissions to be absent a priori.

Finally, we use the measured GOME-2A spectral response functions as described and analysed by Siddans et al. (2007) and the high-resolution solar irradiance spectrum from Chance and Kurucz (2010) to simulate measured reflectance spectra and their derivatives. Instrument stray light can be included in the forward model as a spectrally smooth (i.e., low-order polynomial in wavelength) additive offset to the simulated measured radiance spectrum. In one of the sensitivity experiments of Sect. 7, we include a spectrally constant stray light offset in the fit and assume the offset to be absent a priori. We specify the additive radiance offset as a percentage of the continuum radiance at 758 nm.

### 5.2 Inversion

GOME-2A level-1b files provide radiance spectra and a daily irradiance measurement. The product also provides a noise spectrum for each radiance measurement, which we call the nominal noise in this paper. Level-1b files from the latest processor version 5.3 are used.

The atmospheric state vector is determined through a spectral fit of reflectance across the fit window running from 758 to 770 nm and using the Optimal Estimation framework (Rodgers, 2000). The state vector contains in any case aerosol layer mid pressure ( $P_{\text{mid}}$ ) and aerosol optical thickness ( $\tau$ ) at 760 nm. Depending on the experimental condition, the state vector may contain other parameters as well. State vector

elements, a priori values and a priori errors are summarized in Table 5. A positive temperature offset means that the entire a priori ECMWF temperature profile is shifted by the offset amount to higher temperatures in the retrieval.

Gauss–Newton iteration is used to find a minimum in the cost function, which is an efficient method if the forward model is only moderately non-linear. However, in case of non-linear behaviour of the forward model, convergence and the retrieval solution itself may depend on the starting values for the iteration. For example, it has been noted in simulation experiments that the cost function for O<sub>2</sub> A band aerosol retrieval may have multiple local minima (e.g., Fig. 19 in Hollstein et al., 2012; Fig. 6-1 in Sanders and De Haan, 2014). One of the aims of the retrieval experiments reported in this paper is therefore to systematically investigate convergence and stability of the retrieval. For that reason, we now discuss in somewhat more detail the implementation of the Gauss–Newton method in our retrieval setup.

Gauss–Newton iteration is embedded in an iterative scheme with two modifications. First, when the initial state differs strongly from the true state, it is known that the update of the state vector in case of Gauss–Newton iteration can become very large and lead to a point in state space far from the correct solution. Therefore, if the update of the state vector becomes larger than a pre-defined threshold, we reduce the size of the update. We do this by temporarily decreasing the signal-to-noise ratio of the measurement until the update falls below the threshold. In our GOME-2A retrieval experiments, reduction of the state vector update occurs almost every run, particularly during the first few updates. Second, parameters can attain non-physical values during iteration (e.g., negative optical thickness). For various parameters we have therefore defined boundaries. If a state vector element crosses such a boundary, we simply reset the element to that boundary value. We prefer this method to transformations that make such boundary crossings impossible (e.g., fitting of the logarithm of the optical thickness) because we have experienced that such transformations tend to make the model more non-linear. In our GOME-2A retrieval experiments, we see that boundary resets occur regularly during iteration, also for retrievals that subsequently converge. Exam-

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Figure 7 shows PMAp aerosol optical thickness at 550 nm against retrieved aerosol optical thickness (at 760 nm) for both experimental conditions. PMAp retrieves spectral aerosol optical thickness for PMD ground pixels. The theoretical basis is described in EUMETSAT (2014b) and a first validation with AERONET aerosol optical thickness is reported in EUMETSAT (2014c). Eight PMD ground pixels make up one spectrometer ground pixel. In Fig. 7, the mean of valid PMD subpixel PMAp aerosol optical thicknesses is compared against the aerosol optical thickness retrieved from the O<sub>2</sub> A band. Thus, PMAp aerosol optical thickness is spatiotemporally collocated with the spectrometer measurements that we use for our O<sub>2</sub> A band retrievals. Note that at the time of writing PMAp aerosol optical thickness was only available for sea pixels. We have also compared retrieved aerosol optical thickness with MODIS Terra aerosol optical thickness, which is available for land surfaces as well, but the correlation was worse. This is probably due to the different overpass times of the Metop-A and Terra satellites.

It is important to remark that an absolute validation of retrieved aerosol optical thickness is neither attempted here nor expected, because PMAp aerosol optical thickness is reported at a different wavelength and our optical thickness is an effective quantity, which holds for the aerosol model assumed in the retrieval (see Sect. 2). However, if our O<sub>2</sub> A band retrieval is indeed picking up an aerosol signal, we do expect a significantly positive correlation with PMAp aerosol optical thickness when many different aerosol scenes are included in the comparison. PMAp aerosol optical thickness correlates significantly with retrieved O<sub>2</sub> A band aerosol optical thickness when not fitting the surface albedo (left panel of Fig. 7). When fitting the surface albedo, the situation becomes less clear. The data appear to separate into two clusters (which is the reason why a linear regression is not performed) and retrieved O<sub>2</sub> A band aerosol optical thickness for the denser one is significantly lower than PMAp aerosol optical thickness. We come back this observation in Sect. 10.

## 7 Algorithm sensitivities for GOME-2A target pixels

In this section, we illustrate a number of algorithm sensitivities using real data retrievals. Because the radiative transfer calculations are time-consuming, we select a target GOME-2A pixel for every scene and perform sensitivity experiments for this set of pixels only. We discuss the effect on convergence and the retrieval solution of the assumed aerosol model, scaling of the oxygen absorption cross section and fitting of a temperature offset, fitting of the surface albedo, and fitting of a stray light offset or a fluorescence emission.

In the first experiment we investigate the effect of the assumed aerosol model. The retrieval setup is the same as in Sect. 6 and the surface albedo is fixed in retrieval (as in Fig. 5) or it is retrieved (as in Fig. 6). Figure 8 shows the fraction of converged runs, retrieved aerosol layer mid pressure, aerosol optical thickness and surface albedo (only wavelength node 758 nm is shown) for three different aerosol models assumed in retrieval when the surface albedo is fitted. Figure 9 shows retrieved aerosol layer mid pressure and aerosol optical thickness for the same three aerosol models when the surface albedo is not fitted. These aerosol models are (i) a particle with a single scattering albedo of 0.95 and a Henyey–Greenstein phase function with asymmetry parameter of 0.7 (the default model), (ii) a particle with a single scattering albedo of 1.0 and a Henyey–Greenstein phase function with asymmetry parameter of 0.8, and (iii) a Mie particle with single scattering albedo at 760 nm of 0.97 and a phase function with asymmetry parameter of 0.58. The latter model is the weakly absorbing fine-mode aerosol type as defined within the aerosol project of ESA’s Climate Change Initiative program and described in De Leeuw et al. (2015). These aerosol models are chosen for no other reason than that they show some variability in microphysical properties. In this experiment and in all other sensitivity experiments described in Sect. 7, retrieval is attempted for four initial values of the aerosol layer mid pressure and three initial values of the optical thickness (twelve runs in total). The fraction of converged runs is thus defined as the number of converged runs divided by twelve. Finally, retrieved

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In the second experiment we investigate the effect of scaling the oxygen absorption cross section and fitting of a temperature offset. Recall that in the default retrieval setup, the calculated oxygen absorption cross section is increased by 3 % in agreement with Butz et al. (2012) and Crisp et al. (2012), and an offset to the a priori ECMWF temperature profile is fitted. Figure 12 shows the fraction of converged runs and retrieved aerosol layer mid pressure for three experimental conditions. In the first condition, neither the oxygen absorption cross section is scaled nor a temperature offset is fitted. In the second condition, the oxygen absorption cross section is increased by 3 %. In the third condition, also a temperature offset is fitted. This latter condition then corresponds to the default retrieval setup.

We observe that convergence for the set of target pixels improves when the oxygen absorption cross section is scaled and when a temperature offset is fitted. In fact, for two target pixels none of the twelve runs converges in the base condition while all twelve runs converge when the absorption cross section is scaled and a temperature offset is fitted. The significant improvement of convergence is the reason why we did both in the default retrieval setup for the scene retrievals. There are small but systematic effects on retrieved parameter values, which is in general expected in view of the high correlations between errors in fit parameters discussed above. Furthermore, we find that retrieved temperature offsets are always negative and ranging from about  $-4$  to  $-8$  K (not shown). This means that for every GOME-2A pixel the entire a priori temperature profile, which we constructed from ECMWF reanalysis data at high spatial resolution, is shifted to lower temperatures by this amount in the retrieval. Apparently, fitting a temperature offset compensates for model errors other than remaining inaccuracies in meteorological data, as the temperature offset would have been random and much smaller in magnitude in that case. (Note that we are retrieving aerosol in cloud-free, hence meteorologically stable, conditions.) Finally, we remark that, although convergence improves, retrievals that converged in all three conditions do not show an overall and systematic decrease in spectral fit residuals. Some peaks slightly decrease but other peaks slightly increase.

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We have also experimented with fitting stray light (i.e., additive top-of-atmosphere radiance offset) and a fluorescence emission (i.e., additive contribution to the upwelling radiance field at the surface). The actual spectral shape of a presumed stray light offset at the O<sub>2</sub> A band, or rather stray light that remains after corrections have been applied in the level-1b processor, is unknown and can be quite variable because of the large dynamic range of the radiance spectrum. In these first investigations, we have therefore simply assumed that the stray light offset is spectrally constant. A fluorescence emission is typically spectrally smooth and here allowed to depend linearly on wavelength across our fit window.

When fitting the surface albedo, including a stray light offset in the state vector does not show a systematic improvement of the retrieval. The fraction of converged runs stays the same or perhaps slightly decreases. At the same time we do not observe a systematic decrease of fit residuals. Interestingly, we find that the retrieved radiance offset is typically quite large and negative (ranging from 0 to −5% and on average −2.5% of the continuum radiance). A negative offset means that light is removed from the spectrum. At the same time, we see that retrieved mid pressure is systematically lower by on average 85 hPa (range: 0 to 150 hPa). The relative contribution of spectrally constant stray light to the reflectance spectrum is largest inside the absorption band. Any errors in retrieved spectral stray light (for example, because the spectral model is inaccurate) may thus easily interfere with retrieved aerosol layer mid pressure. Since there is no systematic improvement of convergence or residuals, and because the spectral shape of possible stray light is presently unknown to us, we have decided to not fit stray light in the default algorithm setup for the scene retrievals of Sect. 6.

A similar observation is made when including fluorescence emissions in the state vector instead of a stray light offset. There is no systematic effect on convergence. For some pixels the fraction of converged runs increases, for others it stays the same, and for again others it decreases. Also, no effect on spectral fit residuals is found. Interestingly, retrieved fluorescence emissions are always negative. The emission at 758 nm ranges from 0 to  $-2 \times 10^{12}$  photons s<sup>-1</sup> cm<sup>-2</sup> sr<sup>-1</sup> nm<sup>-1</sup> and





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sponding ECMWF (a priori) temperature profiles rather than the retrieved (a posteriori) temperature profiles because the former are probably more accurate (see discussion of retrieved temperature offsets in Sect. 7). Finally, error bars indicate the a posteriori  $1-\sigma$  error in retrieved altitude. Errors are only occasionally large enough to be visible in these plots. We remark that precision errors are calculated from the nominal level-1b noise errors (see Sect. 5.2). It can be anticipated based on the discussion of correlations in Sect. 2 that the total error budget is dominated by accuracy errors.

Typical collocation criteria used by EARLINET stations for correlative measurements with CALIPSO are on the order of 100 km and 2 h (e.g., Mona et al., 2009; Pappalardo et al., 2010). Spatiotemporal collocation of GOME-2A target pixels with lidar measurements (Table 4) is then already quite reasonable for most (but not all) extinction profiles considering the size of GOME-2A pixels. However, as mentioned before, we are not attempting a full validation of our retrieval results but only do a first comparison to better understand the effects that we have found, in particular the effect of treatment of the surface albedo. In Sect. 6, we saw that retrieved aerosol pressures are often very low and can attain unrealistic values when the surface albedo is fitted. On the other hand, retrieved aerosol pressures are much more realistic when the surface albedo is not fitted (although convergence is worse in that case). Retrieved aerosol heights can now be compared against a number of example lidar profiles that are to some extent representative of general aerosol conditions in the respective aerosol scene. The main observation in Fig. 13 is that retrieved mid altitudes when fitting the surface albedo are indeed too high for most cases. However, retrieved mid altitudes when not fitting the surface albedo typically show values that are probably representative of actual aerosol extinction profiles. Thus, the observations made in Sect. 6 are supported by the comparison with lidar measurements.

In detail, focusing on retrieved mid altitudes when not fitting the surface albedo (blue horizontal lines), we see that altitudes are usually inside the corresponding extinction profile (cases 03, 04-a and 04-b, 07-a and 07-b, 08, 10-a and 10-b, 13-a and 13-b). For two cases they are somewhat near the top of the profile (cases 01 and 14), for another



## 9 Retrieved layer pressure when two scattering layers are present

In the previous sections, we found on the one hand that treating the surface albedo as a model parameter, whose value is taken from a climatology, leads to many non-converging retrievals. Interestingly, we also observed that retrievals that did converge showed retrieved aerosol layer mid pressures that appear representative of the actual aerosol extinction profiles. Of course, next to noise errors also systematic errors, such as an error in the assumed aerosol model, contribute to the total error budget. On the other hand, including the surface albedo in the state vector led to a fraction of converged retrievals close to one, but retrieved aerosol layer mid pressures in that case were very low and often the layer appeared to be retrieved above the aerosols. In this section, we show results from retrieval simulations investigating the effect of a second interfering scattering layer on retrieved pressure of a target aerosol layer to further understand these findings.

The forward model is the same as used for the GOME-2A retrievals, except that now the TROPOMI instrument model is used. Also, the target layer (in simulation and retrieval) and the interfering layers contain purely scattering particles for ease of interpretation, but other settings are the same as in the simulation study of Sect. 2. The elevated target layer is between 700 and 600 hPa and has an optical thickness at 760 nm of 0.3. Aerosols have a single scattering albedo of 1.0 and a Henyey–Greenstein phase function with asymmetry parameter of 0.7. The surface has a constant albedo of 0.03 (sea) or 0.20 (land). Fit parameters are the pressure of an assumed single aerosol layer with fixed pressure thickness (here: 100 hPa), the aerosol layer’s optical thickness and sometimes also the surface albedo. We illustrate the effect of two scattering layers on retrieved layer pressure with two representative examples. The left column of Fig. 14 shows retrieved layer mid pressure when an interfering cirrus layer is present. The cirrus layer is between 500 and 440 hPa (about 6 to 7 km) and has a cloud fraction of one, and cirrus particles have a single scattering albedo of 1.0 and a Henyey–Greenstein phase function with asymmetry parameter of 0.8. The right column of Fig. 14 shows

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retrieved layer mid pressure when an interfering boundary layer is present. Boundary layer aerosols, which have the same properties as the aerosols in the target layer, are between the surface and 100 hPa above the surface.

When above the elevated target layer an interfering scattering layer is present, such as a cirrus layer for example (left column of Fig. 14), retrieved aerosol layer mid pressure is between the target layer and the interfering layer. The higher the optical thickness of the interfering layer, the more retrieved aerosol layer pressure tends towards this second layer. Although both layers are elevated, whether the surface albedo is fitted (solid lines) or not (dashed lines) affects retrieved layer pressure. This is perhaps surprising but it is understandable in view of the high correlations between errors in fit parameters (Sect. 2): a model error in the assumed aerosol profile (one vs. two scattering layers) affects retrieved surface albedo and this in turn has an effect on retrieved aerosol layer pressure. Here, the surface albedo is retrieved at a value slightly higher than its true value. One may argue that retrieved aerosol layer pressure when the surface albedo is not fitted but held at its model value is the true average pressure. Then, in the left column of Fig. 14 fitting the surface albedo causes biases in retrieved aerosol layer pressure up to 50 hPa (cirrus optical thickness of 0.2, sea) and 90 hPa (cirrus optical thickness of 0.2, land), which is the difference between dashed and solid lines.

When boundary layer aerosols are added to the scene (right column of Fig. 14), retrieved layer pressure is between the two layers if the surface albedo is not retrieved. However, if the surface albedo is fitted, retrieved layer pressure moves away from the boundary layer. Fitting the surface albedo now causes large biases in retrieved aerosol layer pressure. For example, for a boundary layer optical thickness of 0.05 to 0.1, which are common values, retrieved pressure of the target layer (optical thickness of 0.3) is biased by about 115 to 155 hPa (difference between dashed and solid lines). Biases are larger and non-convergences occur more often for the brighter surface. Also, the retrieved surface albedo is above its true value while the retrieved optical thickness is

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biased low. Finally, we remark that residues in both conditions increase when more and more boundary layer aerosols are added to the scene (not shown).

We hypothesize that the following mechanism is at work. Although the two columns of Fig. 14 seemingly show such diverging results, the effects of a second interfering scattering layer, be it cirrus or boundary layer aerosols, are actually similar in a qualitative sense. Yet quantitatively, the effect is much more pronounced for boundary layer aerosols. Suppose we start the simulations with only one scattering layer (i.e., the elevated target layer). The forward model used in retrieval captures this situation well of course and all parameters are retrieved at their true values. Now we begin adding cirrus or boundary layer aerosols. Remember that we consider purely scattering aerosols throughout. To get agreement in the continuum, the aerosol optical thickness of the single layer assumed in the retrieval is increased when the surface albedo is held fixed at its true value. In case the surface albedo is fitted, also this parameter will increase to a certain extent, because errors are correlated. But the penalty for increasing the surface albedo is that the absorption band becomes too deep. To also fit reflectances inside the absorption band then, the aerosol layer has to be moved to lower pressures to compensate for this in the retrieval. Hence, retrieved pressures in Fig. 14 are lower when the surface albedo is fitted. The particular combination of aerosol optical thickness, surface albedo and aerosol layer pressure that eventually results depends on the fit. However, it is easier to attribute aerosol scattering to surface reflection when aerosols are closer to the surface (indeed, the surface albedo reacts more strongly in that case). The pressure difference between boundary layer aerosols and the surface has still to be compensated for and this causes the aerosol layer to be retrieved above the elevated target layer.

## 10 Discussion and conclusions

In this paper, we have presented and discussed an algorithm setup for retrieval of aerosol layer height from spectral measurements of the oxygen A band. The algorithm

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has been applied to GOME-2A spectra in a number of systematic and extensive case studies, retrieved aerosol layer height has been compared against lidar measurements and subsequent retrieval simulations have been performed to further understand the GOME-2A retrieval results. Retrieval of aerosol height information from the O<sub>2</sub> A band is challenging, as becomes clear also in this paper, and algorithm development will continue in the coming time. In this work, we have identified many starting points for further investigations. We believe that we have made a step ahead from the sensitivity studies and the limited number of case studies on O<sub>2</sub> A band aerosol retrieval that have appeared so far. The definitive answer to the question of what an O<sub>2</sub> A band aerosol height retrieval is eventually capable of, however, has yet to be given. The following main observations and conclusions emerge from the GOME-2A retrievals and the retrieval simulations.

Whether or not the surface albedo is retrieved simultaneously with aerosol layer height and optical thickness can have a significant impact on the retrieval outcome. When the surface albedo is fitted, convergence of the GOME-2A scene retrievals is good but we find that retrieved aerosol layer pressures are very low. With this in mind, we have applied a very strict filtering on cirrus using, among other tests, a dedicated test in the thermal infrared. Therefore, we can rule out cirrus contamination of the relatively large GOME-2A pixel as an explanation for the systematically low aerosol pressures and we hypothesize that these are more likely linked to a characteristic of the retrieval algorithm itself. Indeed, retrieved aerosol layer heights attain realistic values when the surface albedo is removed from the state vector. The observation of realistic aerosol layer heights in case the surface albedo is fixed in retrieval is further supported by the comparison of retrieved aerosol layer heights with lidar profiles for a selected set of GOME-2A target pixels. The drawback of not fitting the surface albedo, however, is a decrease in convergence, which is probably caused by, among other things, inaccuracies in climatological values.

In subsequent retrieval simulations we investigated the effect of the shape of the aerosol extinction profile in isolation. As a first step, we used realistic extinction profiles

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to simulate measured spectra while assuming the single-layer model in the retrieval. Again, we find that retrieved aerosol layer pressures are typically biased low when fitting the surface albedo compared to when not fitting this parameter. As a second step, we narrowed down the retrieval simulations to investigating the effect of two scattering layers. Particles are now taken purely scattering in both simulation and retrieval so that results can be interpreted more easily. From these retrieval simulations, we learn that a model error in the extinction profile is partly absorbed by the surface albedo. This is expected as errors in fit parameters are correlated. We see that the retrieved particle optical thickness underestimates the true total particle optical thickness and that the retrieved surface albedo overestimates the true surface albedo. At the same time, the aerosol layer is retrieved at lower pressures in agreement with the GOME-2A retrievals. In case of boundary layer aerosols, however, the corresponding effect on retrieved aerosol layer height is substantial to the extent that the aerosol layer is eventually retrieved above the two-layer system. This is perhaps unexpected given previous cloud validation studies investigating multiple-layer clouds (e.g., Wang and Stammes, 2014; Joiner et al., 2010, 2012; Lelli et al., 2012; Snee et al., 2008; Vasilkov et al., 2008). These studies show, using both retrieval simulations and validation data, that in many realistic conditions the height of the Lambertian surface or the (middle) height of the scattering layer is in between the two scattering layers assumed in the simulation or somewhere inside the actual extinction profile measured for example with radar. Moreover, the retrieved height tends toward the height of the layer with the higher optical thickness or to the height with the highest extinction coefficient. Retrieved cloud pressures may then be interpreted as an average cloud pressure weighted, for example, by the contribution of each atmospheric layer to the top-of-atmosphere reflectance (see Joiner et al., 2012). Interestingly, however, for optically thin clouds or clouds with a small cloud fraction, the Lambertian surface can be retrieved above the actual cloud top height (see Wang and Stammes, 2014). For these clouds, as for aerosols, the contribution of the surface is large. We have discussed a possible mechanism that might explain why in our retrieval simulations the aerosol layer is retrieved above the elevated

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target layer when aerosols close to the surface are present and the surface albedo is fitted. Note at this point that the clustering of aerosol optical thicknesses in the right panel of Fig. 7 and particularly the decrease in magnitude of retrieved  $O_2$  A band aerosol optical thicknesses compared to the left panel could be related to this mechanism, but this needs to be further investigated. To conclude, optical thicknesses at the  $O_2$  A band for boundary layer aerosol of about 0.1 are quite common and retrieved aerosol layer pressure can be significantly biased (Fig. 14) when the surface albedo is fitted.

Throughout all GOME-2A retrieval experiments, we have explicitly addressed the issue of stability of retrieval. By running retrievals for different sets of starting values for the fit (six in case of the scene retrievals), we could estimate the dependence on starting values of both convergence and the retrieval solution. When the surface albedo is not fitted, 56 % of all GOME-2A pixels had at least one converging retrieval, and in fact, in that case retrievals for all starting values typically converged (i.e., the fraction of converged runs usually was either zero or one; not shown). When the surface albedo is fitted, 94 % of all GOME-2A pixels had at least one converging retrieval, but in this case, there is a dependence of convergence on starting values (i.e., the fraction of converged runs varied more smoothly between zero and one; not shown). In contrast to reports of multiple minima in the cost function observed in simulation studies (e.g., Hollstein et al., 2012; Sanders and De Haan, 2014), we find for the GOME-2A retrievals that multiple minima hardly seem to occur. Once retrieval converges, it typically converges to the same retrieval solution independent of starting values (see Fig. 8). Also, the average number of iterations needed for convergence is acceptable (3.9 when not fitting and 6.5 when fitting the surface albedo). The iterative scheme is based on Gauss–Newton iteration with two modifications to better account for possible non-linear behavior of the forward model. Because we presently have no clear indications that multiple minima in the cost function occur regularly, an efficient retrieval approach would be to attempt retrieval for different starting values until a run converges or a pre-defined maximum number of runs is reached. In the former case, it is assumed that the first converged run gives the global retrieval solution.

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An important question in aerosol height retrieval is which aerosol model to assume. The simulation studies of Sect. 2 indicate that the retrieved height parameter (here: the height of a scattering layer with constant particle extinction coefficient) is quite robust against model errors in the assumed aerosol type. This finding agrees with Hollstein and Fischer (2014), who show in a similar simulation study that the retrieved center height of a lognormal aerosol profile is also quite stable with respect to aerosol type. The simulations of Sect. 2 furthermore show that it helps in this respect to fit the surface albedo. Subsequent sensitivity experiments with GOME-2A spectra corroborate these findings. They show that the effect of the aerosol model is indeed modest, particularly when compared to other model errors and even when not fitting the surface albedo. This observation simplifies the retrieval problem considerably and it is the reason why at this stage of algorithm development we do not give much priority to optimizing the retrieval with respect to aerosol type.

In the selection of GOME-2A pixels, we have applied a strict filtering on clouds. The reason for doing so was twofold. First, we wanted to exclude pixels that are contaminated by cirrus to rule out that this might explain the low retrieved layer pressures. Second, since we are evaluating an aerosol height retrieval algorithm, we wanted to ensure that the scenes for which we investigate algorithm performance are truly aerosol scenes. Cloud filtering criteria can perhaps be more relaxed in the future. Considering the previous discussion of the effect of aerosol model, one could argue that our algorithm setup eventually is an algorithm optimized for retrieving the height of optically thin scattering layers, while a dedicated cloud retrieval algorithm such as SACURA is optimized for retrieving the height of optically thick scattering layers (e.g., with optical thicknesses larger than about five; Kokhanovsky and Rozanov, 2004). Thus, cloud contamination is not a fundamental problem from the perspective of algorithm performance per se.

We find that fit residuals have a distinct and systematic spectral structure. Previous case studies reporting residuals for retrievals comparable to ours include the studies by Van Diedenhoven et al. (2007) and Kokhanovsky and Rozanov (2010). Van Dieden-

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hoven et al. (2007) present an improved method for cloud retrieval using O<sub>2</sub> A band measurements and simultaneous measurements in the UV. Their Fig. 15 depicts the mean and standard deviation of fit residuals at the O<sub>2</sub> A band for 3400 retrievals with GOME spectra. The study by Kokhanovsky and Rozanov (2010) has been discussed above. Their Fig. 11b depicts residuals for the single SCIAMACHY retrieval. Note that residuals in these two figures are defined as  $(R_{\text{fit}} - R_{\text{meas}})/R \cdot 100\%$ . Thus, they should be multiplied by  $-1$  before they can be compared with ours. Overall, the residuals that these authors report are comparable in magnitude to the residuals shown in Fig. 10. The residuals also peak inside the deepest part of the O<sub>2</sub> A band, where they are about  $8\% \pm 8\%$  (Van Diedenoven et al., 2007) and about 16% (Kokhanovsky and Rozanov, 2010). Residuals in the continuum near 758 nm in the left panel of Fig. 10 are perhaps somewhat larger than reported by these authors. Future research should look more closely into fit residuals and investigate to what model and instrument errors spectral characteristics of residuals can be traced back. In this respect, we mention uncertainties in the oxygen absorption cross section, including line-mixing effects and collision-induced absorptions. The improvement of convergence when the absorption cross section is scaled and a temperature offset is fitted as well as the observation that the retrieved temperature offset is systematically negative and quite large in that case supports the hypothesis that spectroscopic uncertainties may indeed be significant.

In the sensitivity experiments for the GOME-2A target pixels, we have also looked into the effect on retrieval of fitting stray light or fluorescence emissions. In both cases, no systematic improvement of convergence or residuals was found. At the same time, negative stray light offsets, meaning that light is removed from the radiance spectrum, and negative fluorescence emissions are found for both land and sea pixels. Therefore, we suspect that retrieved fluorescence emissions have the same origin as stray light offsets. Retrieval simulations in Sanders and De Haan (2013) indicate that fluorescence emissions may be fitted simultaneously with aerosol parameters with only a moderate loss of precision and accuracy of retrieved aerosol layer pressure. The spectral shape of fluorescence emission is known quite well, but for stray light this is not the case. The

present experiment then indicates that it is needed in this respect that stray light is well characterized. For example, scenes free of clouds and aerosols may be identified to retrieve additive and multiplicative offsets including their spectral shape provided the surface albedo and absorption cross sections are well known.

We adopted a fit window running from 758 to 770 nm. GOME-2A covers a much wider spectral range, so this fit window can in principle be complemented with other wavelengths to obtain more information about aerosols. However, inter-band and intra-band co-alignment errors will become more pronounced in that case. Alternatively, careful selection of channels at the O<sub>2</sub> A band (see Siddans et al., 2007) may be worth investigating in order to decrease the computation time.

Algorithm development may now proceed into two main directions. On the one hand, the retrieval simulations of Sect. 9 suggest that the retrieved height of an assumed single layer is most meaningful as a height parameter when the surface albedo is not fitted. In that case, however, the accuracy of the model for the surface reflectivity becomes more important. More effort should then be put into improving characterization of the surface reflectivity. We have done some preliminary investigations using the ADAM-BRDF database (ESA, 2013). Perhaps a dynamic surface reflectance map (e.g., Sanghavi et al., 2010) rather than a monthly climatology based on multi-year averages can improve the retrieval. On the other hand, the retrieval simulations of Sect. 9 also suggest that the single-layer model does not represent well particularly aerosol scattering near the surface, leading to large biases if the surface albedo is fitted. Alternative profile parameterizations that better account for boundary layer aerosols, may ameliorate these biases. For example, one could try to fit optical thickness of a boundary layer with prescribed height in addition to the optical thickness and height of an elevated aerosol layer. The observation that residues increase and retrieved layer pressure decreases when boundary layer aerosols are added to the scene suggests that some information about boundary layer aerosols is contained in the spectrum. Alternatively, profile parameterizations using empirically determined orthogonal functions (e.g., Hollstein and Filipitsch, 2014) could also be worth investigating in this respect. In view of the limited

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information content, we strongly doubt however whether adding many more profile parameters to the state vector will improve the retrieval. The problem of limited information is then merely shifted to finding better a priori information on aerosol profiles.

The main purpose of the TROPOMI Aerosol Layer Height product is to retrieve the height of localized aerosol layers in the free troposphere. Based on the results and the discussions presented in this paper, we currently (at the time of writing) decide to not fit the surface albedo in the operational baseline adopted for the Aerosol Layer Height product. Further efforts are taken to increase the computational speed of the algorithm. At this stage we prefer online calculations for their flexibility when improvements to the forward model are made. A correlated  $k$ -distribution method as described in Hasekamp and Butz (2008) is being implemented. At a later stage, efficient look-up table approaches, such as for example described in Hollstein and Lindstrot (2014), may be investigated.

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**Table 1.** Characteristics of operational satellite cloud retrieval schemes using spectral measurements of the O<sub>2</sub> A band.

Retrieval scheme	Satellite instruments	Cloud model	Cloud fraction	Surface albedo	References
Fast REtrieval Scheme for Clouds from the Oxygen A band (FRESCO)	Global Ozone Monitoring Experiment-2 (GOME-2), Global Ozone Monitoring Experiment (GOME), SCanning Imaging Absorption spectroMeter for Atmospheric CHartography (SCIAMACHY)	Lambertian surface with albedo of 0.8; the height of the Lambertian surface is a fit parameter.	Cloud fraction is a fit parameter.	From climatology	Wang et al. (2008); Koelemeijer et al. (2001)
Semi-Analytical Cloud Retrieval Algorithm (SACURA)/ SACURA – Next Generation for GOME (SNGome)	GOME-2, GOME, SCIAMACHY	Scattering layer with constant particle volume extinction coefficient; cloud top height, cloud geometrical thickness and cloud optical thickness are fit parameters.	Cloud fraction is determined from an analysis of the Polarization Measurement Devices' (PMDs) broadband reflectances (OCRA: Optical Cloud Recognition Algorithm; Loyola et al., 2007) and used as an input for retrieval.	From climatology	Kokhanovsky and Rozanov (2004); Rozanov and Kokhanovsky (2004)
Retrieval Of Cloud Information using Neural Networks (ROCINN)	GOME-2, GOME	Lambertian surface; the albedo and the height of the Lambertian surface are fit parameters.	Cloud fraction is determined from an analysis of PMD broadband reflectances (OCRA; Loyola et al., 2007) and used as an input for retrieval.	From climatology	Loyola et al. (2007)

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**Table 2.** A posteriori correlation coefficients ( $r$ ) for a simulated retrieval of an aerosol layer between 700 and 600 hPa with optical thickness at 760 nm of 0.3 located over land and over sea. Either mid pressure and optical thickness or mid pressure, optical thickness and surface albedo are fitted. Other details are the same as in Figs. 1 and 2.

Correlation coefficient ( $r$ )	$P_{\text{mid}} - \tau$	$P_{\text{mid}} - A_s$	$\tau - A_s$
land/fit $P_{\text{mid}}, \tau, A_s$	-0.992	0.957	-0.975
sea/fit $P_{\text{mid}}, \tau, A_s$	-0.989	0.985	-0.999
land/fit $P_{\text{mid}}, \tau$	-0.917	-	-
sea/fit $P_{\text{mid}}, \tau$	-0.612	-	-

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**Table 3.** Description of the sixteen aerosol scenes used in the GOME-2A retrieval experiments. Here, an aerosol scene is a three-minute granule of GOME-2A observations, which consists of 720 pixels in total.

Scene	Date	Scene description: geographical location; surface type; aerosol type and vertical distribution	Mean/maximum MODIS Terra aerosol optical thickness <sup>4</sup>	Maximum Absorbing Aerosol Index (AAI)	Number of cloud-free GOME-2A pixels (out of 720) <sup>5</sup>
01	3 Sep 2011	Eastern Mediterranean region; land and sea; (polluted) dust up to about 5 km	0.29/0.90	2.3	135
02	6 Sep 2011	Eastern Mediterranean region; land and sea; polluted dust up to about 3 km	0.21/0.63	2.7	136
03	20 Apr 2011	Northwest Europe; land and sea; continental pollution, mainly in boundary layer	0.28/2.07	1.2	109
04	9 Jul 2013	Northwest Europe; land and sea; elevated smoke transported across the Atlantic from forest fires in North America, continental pollution in boundary layer	0.21/0.64	1.5	167
05	2 Jul 2009	Northwest Europe; land and sea; continental pollution, multi-layered, up to about 2 km	0.24/0.82	1.4	87
06 <sup>1</sup>	18 Jul 2013	Northwest Europe; land and sea; continental pollution, multi-layered, can extend up to 5 km	0.16/0.53	1.0	73
07	12 May 2011	Northwest Africa; land and sea; Saharan dust outbreak, elevated dust layers up to 5 km	0.63/1.34	5.0	27
08	31 Jul 2011	Atlantic Ocean off the coast of Northwest Africa; sea; Saharan dust outbreak, elevated dust layers up to 6 km	0.33/1.75	3.1	17
09	10 Aug 2011	Atlantic Ocean off the coast of Northwest Africa; sea; Saharan dust outbreak, elevated dust layers up to about 5 km	0.58/1.27	3.4	54
10	28 Jun 2012	Atlantic Ocean off the coast of Northwest Africa; sea; Saharan dust outbreak, elevated dust layers up to 6 km	0.18/1.20	3.8	53
11	28 Jun 2012	Western Mediterranean region; land and sea; Saharan dust transported to Southern Europe, dust layer up to 5 km	0.54/1.55	4.2	126
12	7 Apr 2011	Western Mediterranean region; land and sea; Saharan dust transported to Southern Europe, dust up to 5 km, sometimes also continental pollution in boundary layer	0.12/0.82	3.5	226
13 <sup>2</sup>	7 Apr 2011	Atlantic Ocean west of Gibraltar; mainly sea; Saharan dust transported to Southern Europe, dust up to 5 km	0.58/3.25	4.2	89
14	18 Apr 2010	Northwest Europe; land and sea; volcanic ash from Eyjafjallajökull eruption, dense plume passes over Cabauw at about 2 km around noon that day	0.18/0.78	2.4	184
15	19 May 2010	Northwest Europe; land and sea; volcanic ash from Eyjafjallajökull eruption, geometrically thin layer around 2 km is present over Cabauw	0.19/0.65	2.1	4
16 <sup>3</sup>	17 May 2010	Northwest Europe; land and sea; volcanic ash from Eyjafjallajökull eruption, plume over North Sea between about 4 and 6 km	0.28/0.93	2.4	6

<sup>1</sup> Reduced swath for GOME-2 on Metop-A: ground pixels are 40 km by 40 km.

<sup>2</sup> This dust outbreak is described in detail in Preißler et al. (2011).

<sup>3</sup> The flight of the FAAM aircraft and measurements taken aboard are described in Johnson et al. (2012).

<sup>4</sup> Mean and maximum of MODIS Terra aerosol optical thicknesses (at 550 nm) for MODIS ground pixels collocated with GOME-2A pixels in the scene. MODIS aerosol optical thicknesses are from Dark Target Land and Ocean algorithms. Note that the Terra platform lags Metop-A by about one hour.

<sup>5</sup> For a description of the cloud mask applied to the GOME-2A spectrometer pixels, see main text.

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**Table 5.** State vector elements, a priori values and a priori ( $1-\sigma$ ) errors. In the default retrieval setup for the GOME-2A scene retrievals (Sect. 6), only the first three or five parameters are fitted. Fitting stray light or fluorescence emissions is only done in sensitivity experiments reported in Sect. 7.

Element	A priori value	A priori error
Aerosol layer mid pressure ( $P_{\text{mid}}$ )	[varying]	500 hPa
Aerosol optical thickness ( $\tau$ ) at 760 nm	[varying]	1.0
Temperature offset ( $\Delta T$ )	0 K	3 K
Surface albedo ( $A_s$ ) at 758 and 770 nm (two nodes)	Climatology	0.2
Stray light (additive radiance offset expressed as a percentage of the continuum radiance at 758 nm)	0 %	3 %
Fluorescence ( $F_s$ ) at 758 m and 770 nm (two nodes)	0 photons $\text{s}^{-1} \text{cm}^{-2} \text{sr}^{-1} \text{nm}^{-1}$	$10^{12}$ photons $\text{s}^{-1} \text{cm}^{-2} \text{sr}^{-1} \text{nm}^{-1}$

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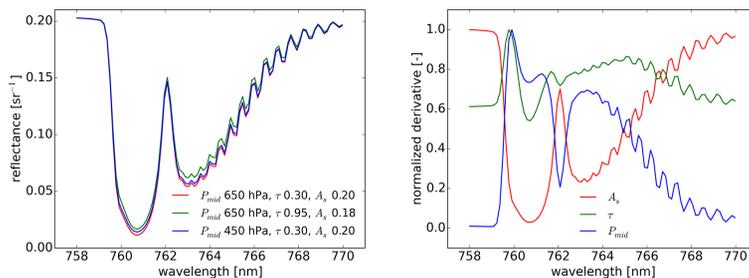
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**Figure 1.** Left panel: simulated top-of-atmosphere reflectance spectra for three different aerosol scenarios at a resolution of 0.38 nm. The solar zenith angle is  $50^\circ$  and the viewing direction is nadir. The spectrum plotted in red corresponds to the example scenario of an aerosol layer between 700 and 600 hPa with an optical thickness at 760 nm of 0.3 over a ground surface with albedo of 0.2. The spectrum plotted in green corresponds to the scenario of an aerosol layer with the same height and pressure thickness but with a different optical thickness and for a surface with a different albedo such that the continuum reflectance remains the same. For comparison, the spectrum plotted in blue corresponds to the scenario of an aerosol layer moved to a different height but with optical thickness and surface albedo the same as in the example scenario. Signal-to-noise ratios for these reflectance levels expected for TROPOMI are about 1000 in the continuum to about 250 in the deepest part of the absorption band. Right panel: derivatives of reflectance with respect to surface albedo, aerosol optical thickness and aerosol layer mid pressure for the example aerosol scenario. Derivatives are normalized to 1.0 at their respective maximums. Both panels: the aerosol has a single scattering albedo of 0.95 and a Henyey–Greenstein phase function with asymmetry parameter of 0.7. The forward model for these calculations is the same as the forward model used in the GOME-2A retrievals. For simplicity, we assume the surface albedo to be independent of wavelength. Furthermore, the temperature profile corresponds to a mid-latitude summer atmosphere and the surface pressure is 1013 hPa.

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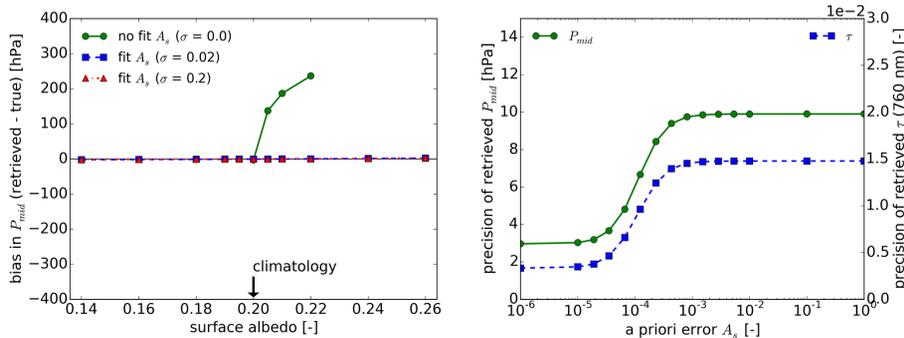
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**Figure 2.** Left panel: results of retrieval simulations showing the bias in retrieved aerosol layer mid pressure as a function of the true surface albedo for three different a priori errors. The a priori value for the surface albedo is 0.20 (“climatology”). Results are shown for the example aerosol scenario (aerosol layer between 700 and 600 hPa with optical thickness at 760 nm of 0.3, surface albedo of 0.2). Missing data points indicate non-converging retrievals. Right panel: results of retrieval simulations showing precision of retrieved aerosol layer mid pressure and optical thickness as a function of the a priori error in the surface albedo. Both panels: a TROPOMI noise model is used which assumes shot noise throughout and a signal-to-noise ratio of 500 at 758 nm for a reference radiance of  $4.5 \times 10^{12}$  photons  $s^{-1} cm^{-2} sr^{-1} nm^{-1}$ . The a priori error for aerosol layer mid pressure is 500 hPa and for aerosol optical thickness is 1.0. Other details are the same as in Fig. 1.

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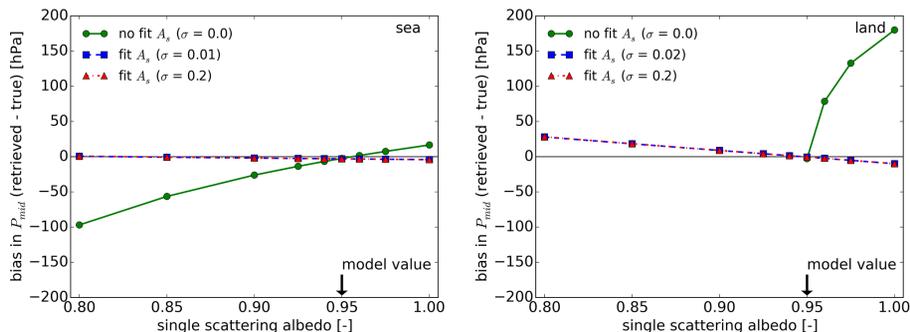
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**Figure 3.** Results of retrieval simulations showing the bias in retrieved aerosol layer mid pressure as a function of the true single scattering albedo for three different a priori errors in the surface albedo used in retrieval simulations. The single scattering albedo assumed in retrieval is 0.95 (“model value”). The aerosol layer is over sea (albedo of 0.03, left panel) or over land (albedo of 0.2, right panel). Missing data points indicate non-converging retrievals. Other details are the same as in Figs. 1 and 2.

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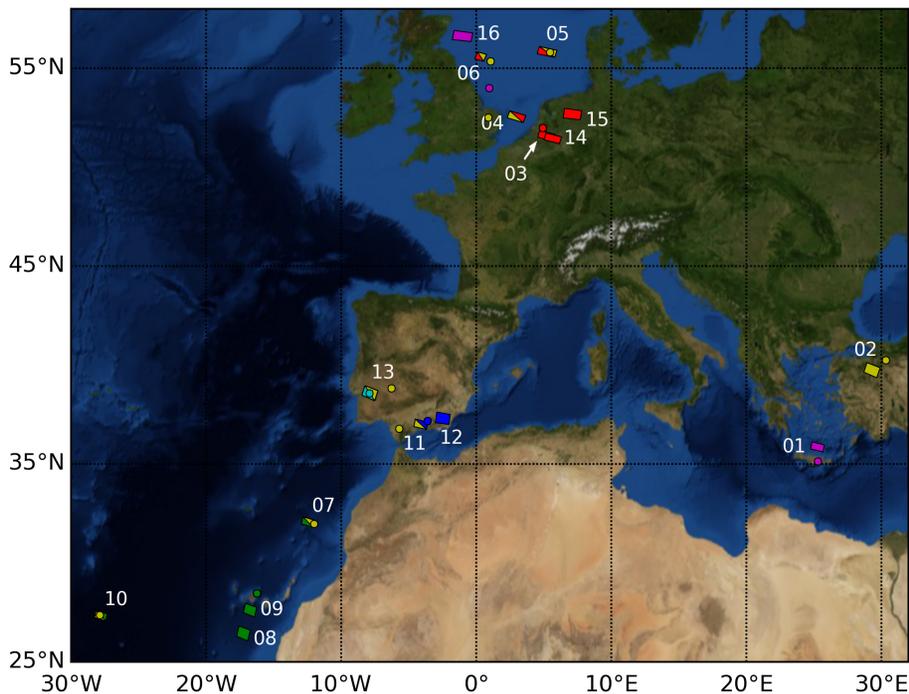
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**Figure 4.** Overview of GOME-2A target pixels (numbered quadrangles) and corresponding lidar measurements (circles). The lidar measurements are described in Table 4. Color code for lidar measurements: FAAM aircraft (magenta), CALIPSO (yellow), Cabauw (red), Santa Cruz (green), Granada (blue), and Evora (cyan). For some pixels, two lidar measurements are available for evaluation. There are nine GOME-2A target pixels over sea (target pixels 01, 04, 05, 06, 07, 08, 09, 10, 16) and seven over land (target pixels 02, 03, 11, 12, 13, 14, 15). The aerosol scenes are described in Table 3.

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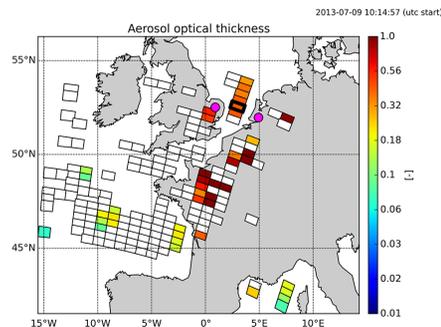
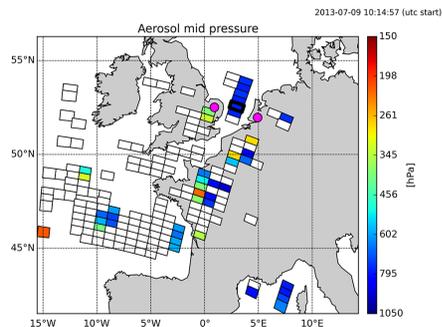
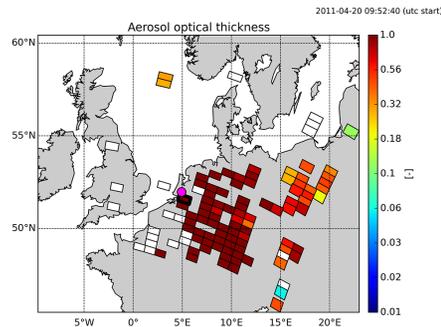
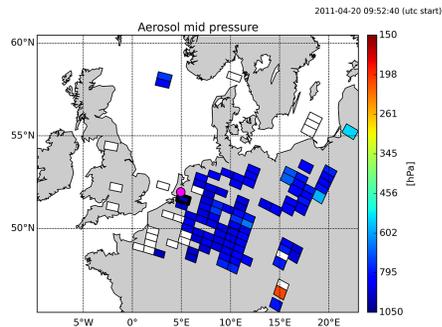
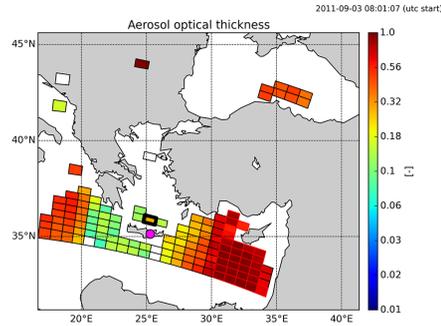
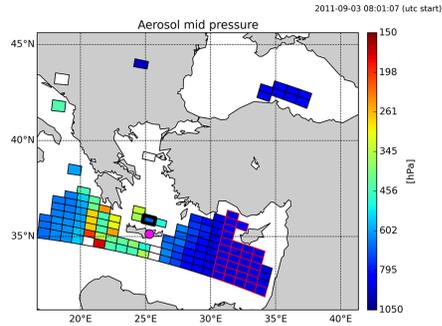
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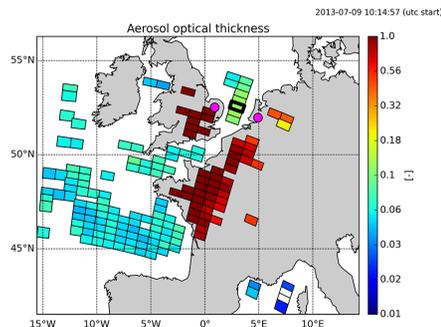
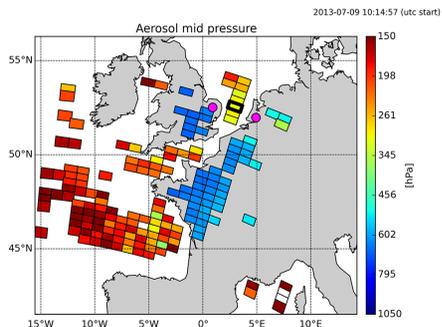
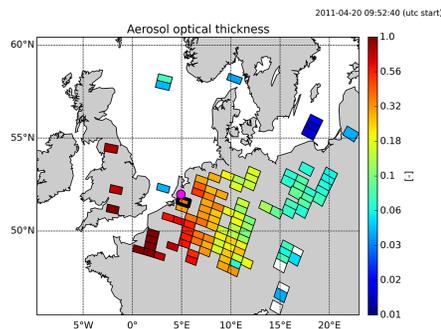
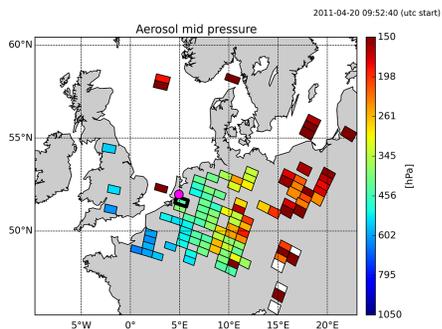
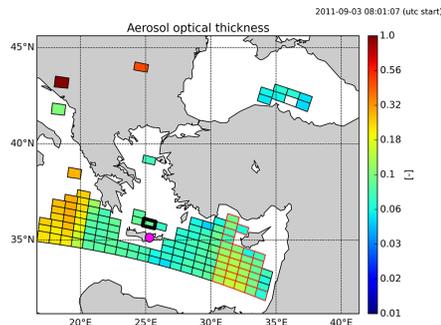
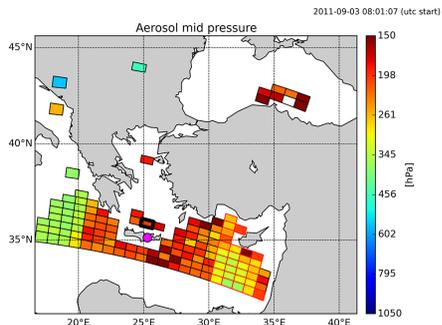


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**Figure 6.** Retrieved aerosol layer mid pressure (left column) and aerosol optical thickness (right column) for the same GOME-2A scenes (rows) as in Fig. 5 when including the surface albedo in the state vector. Next to  $P_{\text{mid}}$  and  $\tau$  (760 nm), the surface albedo  $A_s$  and a temperature offset  $\Delta T$  are fitted. Other settings are the same as in Fig. 5.

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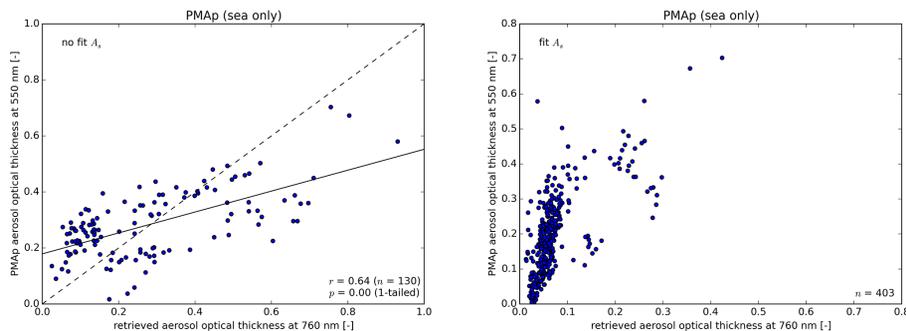
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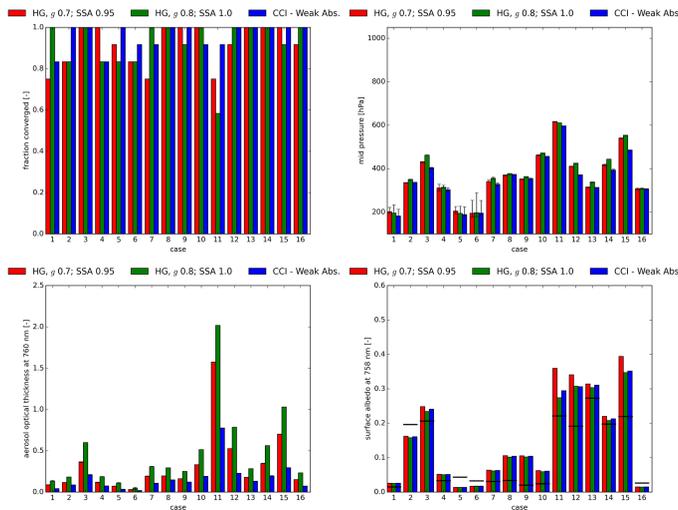


**Figure 7.** PMAp aerosol optical thickness at 550 nm against aerosol optical thickness retrieved from the  $O_2$  A band measured with GOME-2A when the surface albedo is not fitted (left panel) and when it is (right panel). In these plots, PMAp aerosol optical thickness is the mean of valid PMAp retrievals (at least one) for PMD subpixels within the GOME-2A spectrometer’s footprint.

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**Figure 8.** Fraction of converged runs (top left), retrieved aerosol layer mid pressure (top right), retrieved aerosol optical thickness (bottom left) and retrieved surface albedo at 758 nm (bottom right) for sixteen GOME-2A target pixels and three different aerosol models. For a description of these aerosol models, see the main text. The first aerosol model is the model also assumed in the scene retrievals. All other details of the retrieval setup are the same as in Sect. 6 and the surface albedo is fitted (as in Fig. 6). Thus, retrieval results for cases 01, 03 and 04 shown here with red bars are the same as retrieval results for highlighted target pixels in the scenes of Fig. 6. Also, retrieval is now attempted for twelve different sets of initial values (as opposed to six in the scene retrievals). Whiskers for retrieved parameter values indicate the maximum to minimum range of retrieval solutions. Often, the range of retrieval solutions for different initial values is so small that whiskers are not visible. Finally, black horizontal line segments in the bar plot for the surface albedo show the climatological (a priori) value from the MERIS black-sky albedo climatology.

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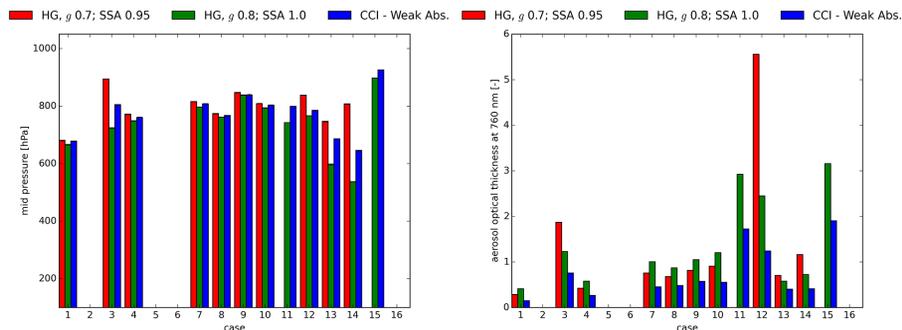
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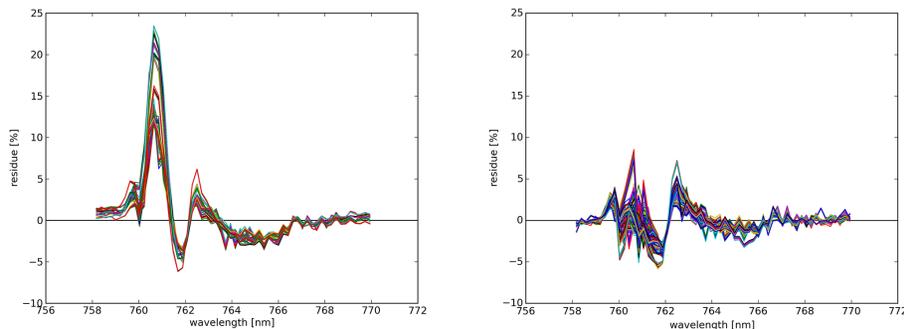
**Figure 9.** Retrieved aerosol layer mid pressure (left) and aerosol optical thickness (right) for sixteen GOME-2A target pixels and three different aerosol models. Details are the same as in Fig. 8, except that now the surface albedo is fixed in retrieval (as in Fig. 5).

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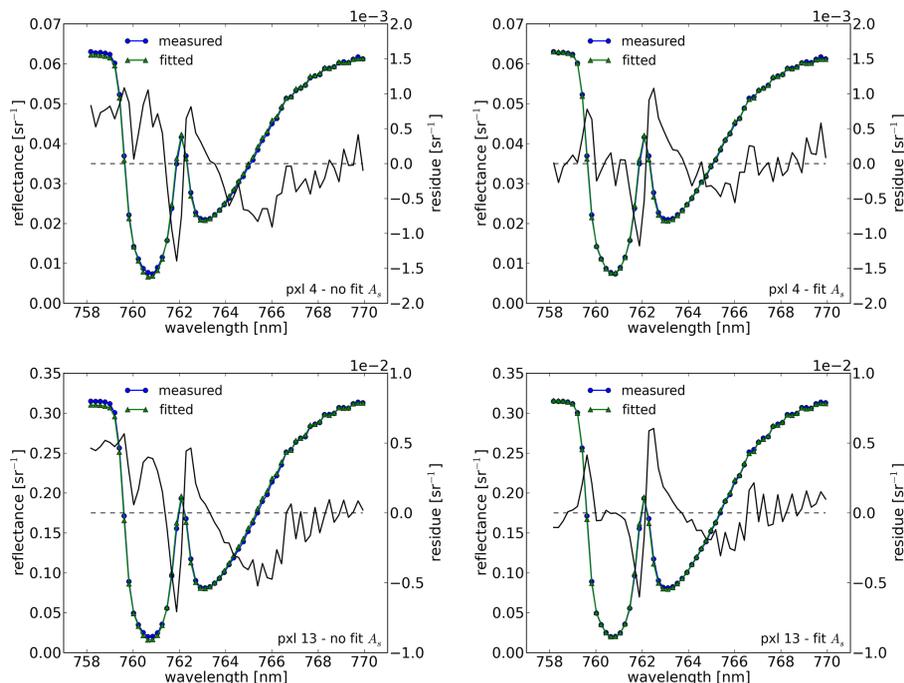


**Figure 10.** Fit residuals for all converged runs for the sixteen GOME-2A target pixels. The default retrieval setup of Sect. 6 is used. Left panel: surface albedo not fitted (see Fig. 5); right panel: surface albedo fitted (see Fig. 6). Relative residues are defined as  $(R_{\text{meas}} - R_{\text{fit}})/R_{\text{meas}} \cdot 100\%$ .

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**Figure 11.** Measured and modeled reflectance spectra for two example GOME-2A target pixels. Top row: pixel over sea (target pixel 04); bottom row: pixel over land (target pixel 13). Left column: surface albedo not fitted; right column: surface albedo fitted. Absolute residues are defined as  $R_{\text{meas}} - R_{\text{fit}}$ . The default retrieval setup of Sect. 6 is used and the run with the smallest  $\chi^2$ -value is shown.

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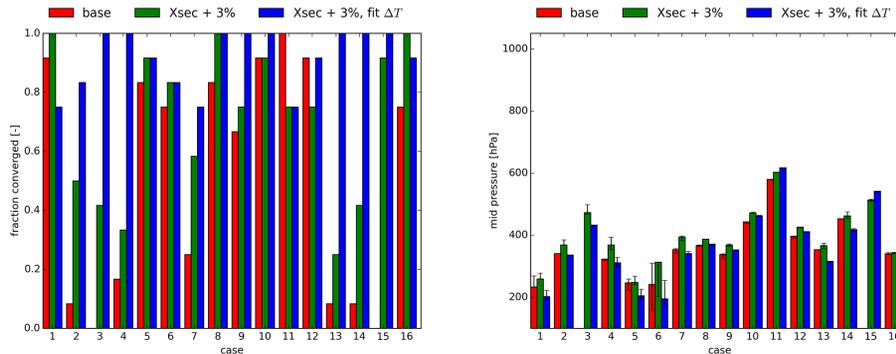
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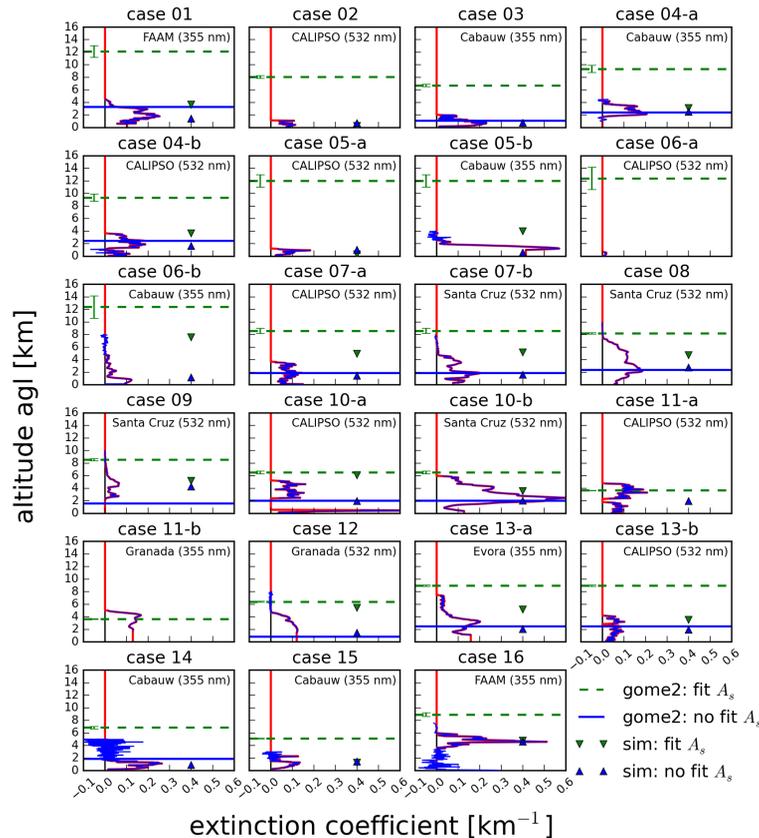
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**Figure 12.** Fraction of converged runs (left) and retrieved aerosol layer mid pressure (right) for sixteen GOME-2A target pixels and three experimental conditions. In the third experimental condition, the oxygen absorption cross section is increased by 3% and a temperature offset is fitted. This condition corresponds to the default retrieval setup used for the scene retrievals of Sect. 6. In the second experimental condition, only the oxygen absorption cross section is scaled, but the temperature profile is fixed in retrieval. In the first experimental condition, neither the oxygen absorption cross section is scaled nor a temperature offset is fitted. All other details of the retrieval setup are the same as in Sect. 6 and the surface albedo is fitted (as in Fig. 6).

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**Figure 13.** Comparison of retrieved aerosol layer mid heights for the sixteen GOME-2A target pixels with aerosol extinction profiles measured by the lidars listed in Table 4. For some target pixels, two lidar measurements are included in the comparison. An overview of the spatial layout of target pixels and locations of the lidar observations is depicted in Fig. 4. Aerosol extinction profiles are given at 355 or 532 nm for altitudes above ground level (a.g.l.). Profiles indicated with thin blue lines are the data provided by the lidar teams; profiles indicated with thick red lines are inter- and extrapolated and smoothed profiles used in the retrieval simulations. Horizontal lines are GOME-2A retrieved aerosol layer mid altitudes (green dashed: surface albedo is fitted; blue solid: surface albedo is fixed in retrieval). The retrieval setup is the same as in the scene retrievals of Sect. 6. Missing lines indicate that the GOME-2A retrieval did not converge. Finally, triangles indicate retrieved aerosol layer mid altitudes when the aerosol extinction profiles shown in red are used to simulate a measurement (green downward triangles: surface albedo is fitted; blue upward triangles: surface albedo is fixed in retrieval). Missing data points indicate that the simulated retrieval did not converge. For details of this simulation, see the main text.

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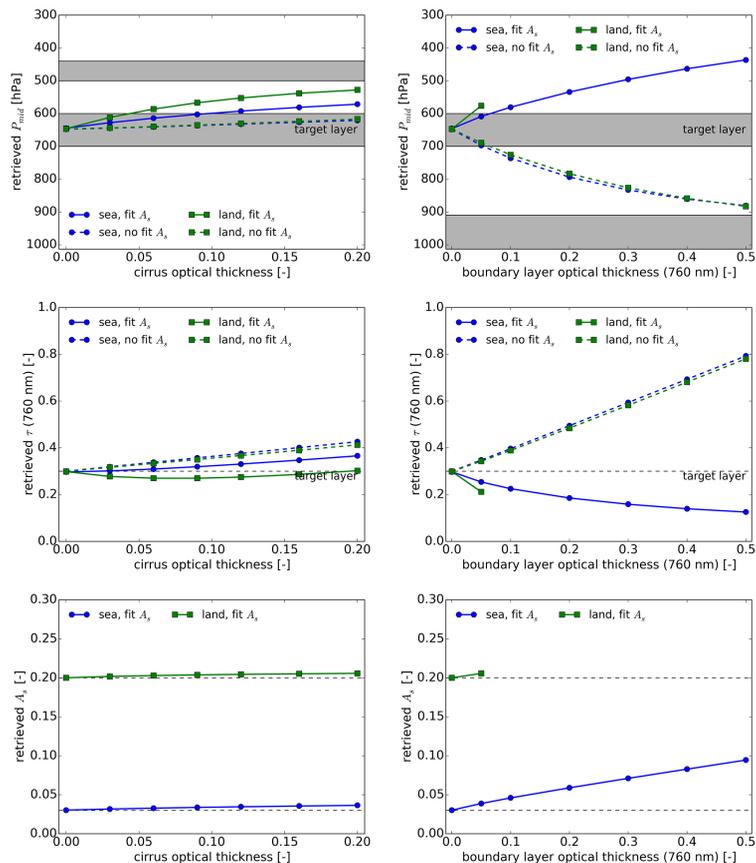
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**Figure 14.** Results of retrieval simulations showing retrieved mid pressure (top row) of an assumed single aerosol layer with fixed pressure thickness, the layer's retrieved optical thickness (middle row) and the retrieved surface albedo (bottom row) when in the forward simulation two scattering layers are present. Retrieved parameter values are shown as a function of the optical thickness of the interfering layer. The four plot lines correspond to sea (blue, circles) and land (green, squares) and to not fitting (dashed lines) and fitting (solid lines) the surface albedo. The target layer has an optical thickness of 0.3. Aerosols have a single scattering albedo of 1.0 and a Henyey–Greenstein phase function with asymmetry parameter of 0.7. The interfering layer is a cirrus layer (left column) or a boundary layer containing aerosols (right column). The cirrus layer has a cloud fraction of 1.0, and cirrus particles have a single scattering albedo of 1.0 and a Henyey–Greenstein phase function with asymmetry parameter of 0.8. Missing data points indicate non-converging retrievals. The solar zenith angle is 50° and the viewing direction is nadir. All other settings are the same as in the simulation study of Sect. 2 (see also Figs. 1 and 2).

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