RETRIEVAL OF AEROSOL HEIGHT FROM THE OXYGEN A BAND WITH *TROPOMI*

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ABSTRACT

The Tropospheric Monitoring Instrument (TROPOMI) will feature a new aerosol product that is specifically dedicated to retrieval of the height of tropospheric aerosol layers. The Aerosol Layer Height product will be based on the oxygen A band. The operational algorithm is currently being developed at KNMI. In this paper we will highlight the key aspects of the algorithm and present results from a sensitivity study.

1. AEROSOL HEIGHT

At present, daily global observations of aerosol height are not available on an operational basis. Aerosol profiles are provided by active sensors, such as the space-borne lidar system CALIOP. These sensors have a high vertical resolution, but they observe in narrow tracks only. However, passive sensors, such as TROPOMI, can cover the entire earth in a single day.
Observations of aerosol height will make a substantial improvement to the scientific understanding of aerosol interactions. For example, they will improve modeling of long-range transport. Furthermore, the aerosol profile is an important variable determining the radiative forcing related to scattering and absorption effects (e.g. [1]) and to indirect effects through microphysical interactions with cloud formation. In addition, effects due to local heating of the atmosphere in case of absorbing aerosol are also strongly dependent on the profile, particularly in the ultraviolet to blue wavelength range. Examples are semi-direct radiative effects ('cloud burn-off') and convective motion induced by local heating of absorbing aerosol layers ([2]). Finally, aerosol height helps to interpret the Absorbing Aerosol Index (AAI) as the index is strongly dependent on the height of the aerosol.
A set of global observations of aerosol height from TROPOMI will also contribute to improving ash-forecasting systems for aviation safety. We mention in this respect that TROPOMI's aerosol height product is intended to be delivered near real-time.

2. TROPOMI

TROPOMI is a spaceborne nadir viewing grating spectrometer with bands in the ultraviolet, visible, near-infrared and shortwave infrared wavelength range. Its purpose is to make global observations of atmospheric composition for air quality and climate monitoring ([3]). Launch of the satellite is planned for early 2015. TROPOMI is a collaboration between The Netherlands and the European Space Agency. It is the precursor to the Sentinel-5 mission, which is part of the European Global Monitoring for Environment and Security (GMES) program. TROPOMI continues measurement series by Aura/ OMI and ENVISAT/ SCIAMACHY.
The combination of a sun-synchronous orbit and a wide swath ensures that TROPOMI will have daily global coverage. Overpass is at ~13.30 local solar time. Its spatial resolution is an unprecedented 7 x 7 km^2. The spectral ranges are 270-500 nm, 675-775 nm and 2305-2385 nm. The spectral resolution near the oxygen A band is approximately 0.5 nm.

3. PRINCIPLE OF HEIGHT RETRIEVAL

Retrieval of aerosol height will be based on absorption by oxygen in the A band. The O_2 A band is located in the near-infrared wavelength range between 759 and 770 nm. It is a highly structured line absorption spectrum with strongest absorption lines occurring between 760 and 761 nm. The absorption band spans a wide range of absorption optical thicknesses: At some wavelengths, photons only reach the upper levels of the atmosphere. The O_2 A band can provide altitude information on scattering layers (clouds or aerosol) from the troposphere up to the stratosphere. Fig. 1 shows simulated reflectance spectra at the anticipated instrument specifications for TROPOMI for an aerosol layer at two different heights. The difference between the two spectra essentially provides the aerosol height

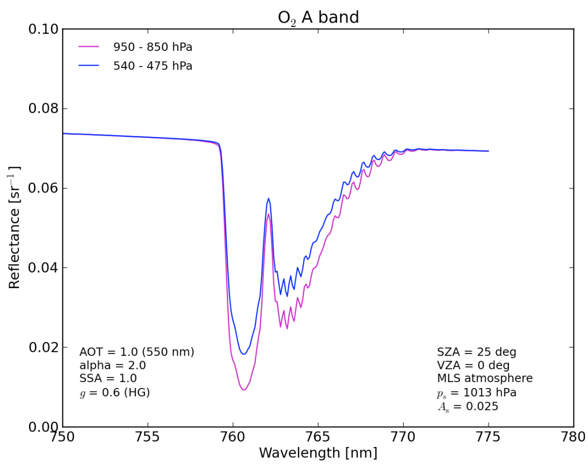

Figure 1. Reflectance spectra of the oxygen A band for a particular aerosol layer at two different heights at TROPOMI's spectral resolution. The signal-to-noise ratio is sufficient to distinguish between the two cases.

signal: Relative absorption depths are different for the two heights.

4. OPERATIONAL ALGORITHM

4.1. Retrieval method

The retrieval algorithm will make a spectral fit of reflectance across the entire O_2 A band (spectral resolution is ~0.5 nm). The retrieval technique is Optimal Estimation to ensure proper error propagation. An effort is made within the KNMI L1b team to supply the (ir)radiance products that serve as input for the L2 algorithms, with accurate estimates of the measurement error. The L2 aerosol height product will contain error estimates for its retrieval parameters as well as other relevant diagnostics so that the user can evaluate the retrieval result.

The basic fit parameters are aerosol pressure (p), aerosol optical thickness (AOT) and surface albedo (A_s) – the latter two parameters obviously for wavelengths at the O_2 A band. The surface albedo depends linearly on wavelength to account for spectral variations of the surface reflectivity over land.

It is important to note that since we are fitting an absorption spectrum, the surface albedo can be retrieved and we don't need climatological (a priori) information on the reflectivity of the surface. The contributions to reflectance from the surface and from the aerosol can be distinguished from absorption (see Fig. 2): Photons scattered by the surface have to pass through the atmosphere between the surface and the aerosol layer, in which additional oxygen absorption can take place.

4.2. Forward model

The forward model for retrieval calculates measured TOA reflectances for an atmosphere in which Rayleigh scattering, gas absorption and scattering and absorption by aerosol and clouds can take place. The atmosphere is bounded from below by an isotropically reflecting ground surface.

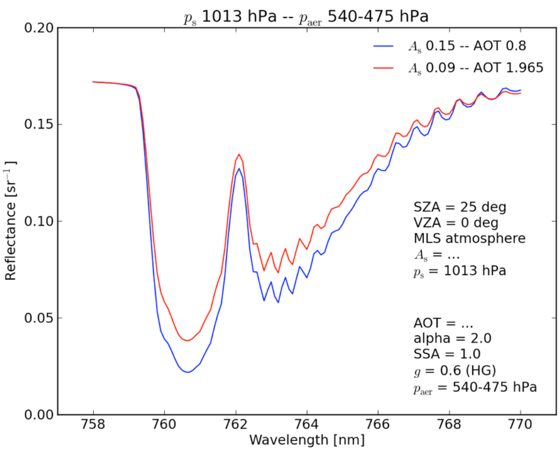

Figure 2. Reflectance spectra for two different combinations of aerosol optical thickness and surface albedo that yield the same continuum reflectance. The aerosol layer was at the same height. From the shape of absorption, the two cases can be distinguished.

Since the O_2 A band contains limited profile information at TROPOMI's spectral resolution (e.g. [3]), we assume for the operational algorithm that the aerosol are uniformly distributed in a single layer with some small, fixed pressure thickness. The retrieved mid pressure essentially represents an optical average of the actual aerosol profile. This parameterization is most suited for aerosol profiles that are dominated by a single optically thick aerosol layer.

An aerosol layer is modeled as a layer of particles with an associated extinction optical thickness. Scattering and absorption are described by the single scattering albedo (SSA) and the phase function $P(\theta)$. The basic algorithm will assume a single aerosol type in the forward model for retrieval: The aerosol is assumed to have a single scattering albedo of 0.95 and a phase function that is described by a Henyey-Greenstein (HG) function with asymmetry parameter of 0.7. The rationale behind this choice is discussed in Section 5.

Attention is given to the oxygen absorption cross section, because sensitivity studies have shown that aerosol retrieval, much more than cloud retrieval, is sensitive to inaccurate cross section data. Improvement of line parameters and inclusion of line-mixing and collision-induced absorption at the O_2 A band is currently being investigated. In this respect, we also mention that we plan to use concurrent ECMWF pressure-temperature profiles, which is particularly important for the O_2 A band due to the temperature dependence of the cross section.

Chlorophyll in terrestrial vegetation is known to exhibit fluorescence around the O_2 A band. It has been argued that retrieval of parameters from the O_2 A band will be biased if fluorescence is not properly taken into account (e.g. [5]). Including surface emissions in the forward model is currently under investigation.

A final important issue concerns cirrus contamination. We have learned from sensitivity studies that clouds that are optically so thin that they may not be detected by a cloud mask can still cause substantial biases in retrieved aerosol height. Those clouds are typically cirrus clouds at high altitude, even more so because of their homogeneity (see Section 4.4). We are investigating how to account for undetected cirrus in our forward model.

4.3. Radiative transfer calculations

The basic fit window extends from 758 nm (continuum) to 770 nm. Radiances are calculated with the layer-based orders of scattering (LABOS) method. This is a variant of the doubling-adding method in which the adding of the different layers is replaced by the orders of scattering method. Since the O_2 A band is a strong line absorption band, line-by-line calculations are required. Moreover, these calculations have to be performed on-line, because our scattering model excludes the use of lookup tables as these will be too large to handle. Optimization of the algorithm for computational speed will be future work.

4.4. Cloud masking

If the scene is partially clouded, retrieval of aerosol height is problematic. Aerosol height will therefore be retrieved for cloud-free pixels only. Hence, it is important to accurately screen pixels for the presence of clouds.
A TROPOMI cloud mask will be developed that consists of a number of threshold tests. The most important one concerns a test for homogeneity. It is anticipated to read out one wavelength (spectral bin) per spectral band at a much higher spatial sampling ('small pixels') to assess the homogeneity of the scene.
At a later stage, a synergy with Suomi-NPP / VIIRS is foreseen. VIIRS is a multispectral imager that measures in the thermal infrared and is therefore well suited for cloud detection. Sentinel-5 Precursor will fly in formation with Suomi-NPP. A cloud masked for TROPOMI based on VIIRS is expected.

5. AEROSOL MODEL

An important question to answer is to what extent we actually need to know the aerosol type to have a reliable retrieval of aerosol height. We emphasize that the primary purpose of the algorithm is to provide height and not so much to provide, for example, aerosol optical thickness (although it will be a fit parameter). We will now discuss the results from a study that investigated the sensitivity of retrieval to inaccurate knowledge of the single scattering albedo and the phase function.
A sophisticated software package called DISAMAR is being developed at KNMI to simulate retrievals and analyze accuracy (bias) and precision (standard deviation) of retrieved parameters in case of model errors, instrument errors etc. To this end, measured reflectances are replaced by simulated reflectances. We then have two forward models: one for simulation and one for retrieval.

5.1. Error in the single scattering albedo

Measured reflectance spectra were simulated for particular aerosol scenarios. The single scattering albedo either was 0.90 or 1.0. In retrieval, however, we assumed a single scattering albedo of 0.95. The same HG phase function was used in simulation and retrieval (*g* of 0.7). The surface was a dark sea surface (albedo of 0.025). Other settings, including the measurement error, had standard or anticipated values. We consider an uncertainty of 0.05 in the single scattering albedo to represent the typical a priori uncertainty. (Larger uncertainties have been tested as well, which gave the same result).
Fig. 3A shows the bias in retrieved height as a result of a model error in the single scattering albedo. Biases are depicted as a function of AOT for two different heights of the aerosol layer. Fig. 3B shows the precision of retrieved height. The TROPOMI target science requirement for the accuracy and precision of retrieved height is 50 hPa.
From Fig. 3 small biases if the single scattering albedo assumed in retrieval does not correspond to the actual SSA of the aerosol in the scene. Retrieved AOT and surface albedo, however, are biased more pronounced (not shown). If only this model error in the SSA is

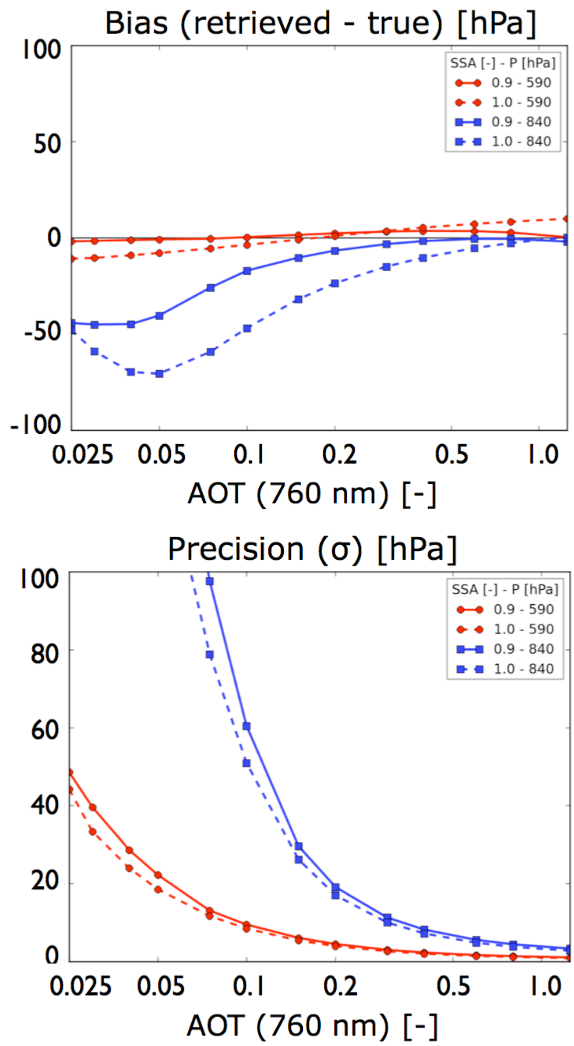

Figure 3. Bias in retrieved aerosol pressure (A) and precision of retrieved pressure (B) as a function of optical thickness in the O_2 A band for an aerosol layer at two different heights and for two different single scattering albedos. The SSA assumed in retrieval was 0.95.

present, both accuracy and precision are below the target requirement of 50 hPa already for AOTs above ~0.1.

5.2. Error in the phase function

A similar sensitivity analysis has been carried out for model errors in the phase function. We have simulated reflectance spectra with phase functions based on the generic aerosol models that are used within the framework of ESA's Climate Change Initiative project (www.esa-aerosol-cci.org/). In the forward model for retrieval we used HG functions with a corresponding asymmetry parameter. We present results here for a Dust particle. Optical properties are based on Mie calculations.
Fig. 4 shows the accuracy of retrieved height for the Dust aerosol as a function of optical thickness if a simplified HG phase function is used in retrieval. In case of a model error in the phase function, already for AOTs at 550 nm above ~0.1-0.2, accuracy and precision (not shown) are below 50 hPa.

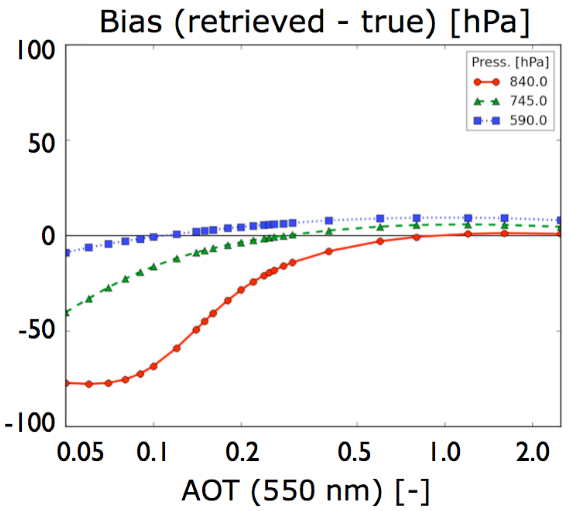

Figure 4. Bias in retrieved aerosol pressure as a function of optical thickness for a Dust layer at three different heights. The phase function for retrieval was a HG function.

5.3. Aerosol model for retrieval

We have found that our retrieval algorithm is robust against inaccurate knowledge of the single scattering albedo and the phase function. Based on the present results, we estimate that a single aerosol model is sufficient for an accurate and precise retrieval of aerosol height. This simplifies the algorithm because we don't need a priori information on the aerosol type or pre-select from a set of aerosol models. Furthermore, we have found that we can use a Henyey-Greenstein phase function. This is advantageous because radiative transfer calculations are faster compared to, for example, phase functions from Mie calculations (less streams needed).
In developing the operational algorithm we therefore proceed with a single aerosol model and a Henyey-Greenstein phase function. As the standard aerosol model we take a particle with a single scattering albedo of 0.95 and an asymmetry parameter of 0.7 at the O_2 A band. These values are intermediate to the SSAs and *g* parameters in this wavelength range for all main aerosol types as found in long-term AERONET observations by [6].

6. CONCLUSION AND OUTLOOK

The TROPOMI Aerosol Layer Height product will be a new and unique product providing global observations of aerosol height. We have discussed key aspects of the operational algorithm. Based on a sensitivity study, we have found our retrieval algorithm is robust against inaccurate knowledge of the single scattering albedo and the phase function. A single aerosol model is probably sufficient for an accurate and precise retrieval of aerosol height. The same retrieval technique can be used for the Sentinel-4 and Sentinel-5 missions. Further development of the algorithm is ongoing at KNMI. Future work during the pre-launch phase includes testing the algorithm on MetOp-A / GOME-2 data.

7. REFERENCES

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