Separation of stratospheric and tropospheric NO_2 sub-columns in Corpernicus Sentinel-4 observations

Isabell Krisch[1,*] & Ben Veihelmann[1]

[1] European Space Agency (ESA/ESTEC), Mission Science Division, Noordwijk, The Netherlands
* now at: Institut für Energie- und Klimaforschung, IEK-7, Forschungszentrum Jülich GmbH, Jülich, Germany

Background

Nitrogen Dioxide (NO_2) is an important atmospheric pollutant originating mainly from combustion processes, but also from microbiological activity in soils and lightning. It acts as a precursor for tropospheric ozone production, and leads to ozone depletion in the stratosphere. Satellite measurements of tropospheric NO_2 are needed for air quality protocol monitoring, emission estimation, near real time services, etc.

Tropospheric NO_2 is a key parameter measured by a number of current and future space borne UV-visible sounding instruments. The vertical resolution of such measurements is not sufficient for separating the NO_2 amount at low altitudes relevant to air-quality, from the total column amount as obtained by individual observations. For Low Earth Orbiting (LEO) instrumentation, several concepts exist for the separation of stratospheric and tropospheric sub-columns relying on observations over unpolluted areas.

Several geostationary sensors, including Sentinel-4, dedicated to air quality are currently being developed by various space agencies (ESA, NASA, and KARI). The concepts for the separation of stratospheric and tropospheric sub-columns established for LEO instrumentation appear not applicable to geostationary observations due to the lack of persistently unpolluted regions in the geographic area covered by such instruments. New concepts need to be explored for this purpose.

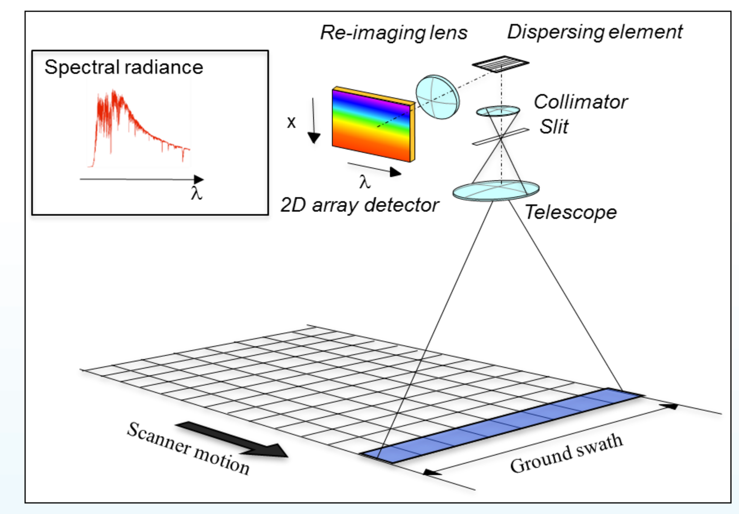


Figure 1: *The Sentinel-4 UVN instrument is a hyperspectral spectrometer operating with designated spectral bands in the solar reflectance spectrum. The earth radiance goes through a telescope and a spectrometer on a 2D array detector where the spectral radiances are measured.*

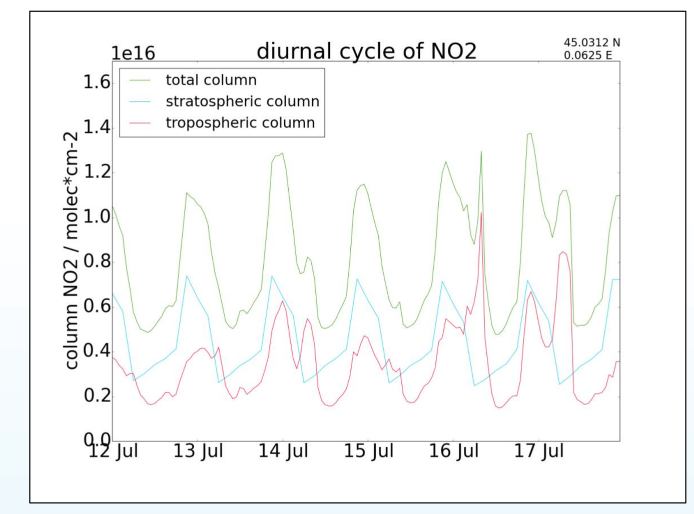


Figure 2: *Diurnal cycle of NO_2 in stratosphere (blue), troposphere (red) and total column (green) for a week in July 2003. Data comes from a vertical combination of the chemical transport models Lotos Euros (up to 3.5 km) and TM5 (above Lotos Euros).*

Concept A – Slant Illumination Geometry

For high solar zenith angles (SZA) the NO_2 total column retrievals gets less sensitive in the troposphere (compare figure 3). This together with the fact that the stratospheric column behaves linearly over the day is used to separate stratospheric and tropospheric subcolumns over the day.

Therefore two reference points – one in the morning and one in the evening – are chosen with SZA between 75°-80°. At this reference points the tropospheric column is taken from a climatology and with the help of the averaging kernel and the NO_2 profile shape (also taken from the climatology) the stratospheric column (STC) is calculated. Between the two stratospheric columns at the two reference points we interpolate over the course of the day. Afterwards we calculate again with the help of the averaging kernel a factor b with which the tropospheric climatology data has to be multiplied to get the measured total columns. The tropospheric columns (TRC) shown in Figure 4 top are calculated by vertical integration over the tropospheric climatology data multiplied by the factor b, where all layers contribute to the column with equal weights. An alternative representation of the results is shown in Figure 4 bottom. Here the vertical sensitivity profile (averaging kernel) of the satellite measurement is taken as a weighting factor before the vertical integration.

For the summer case (Figure 4, left side) the results are quite accurate, because the a-priori tropospheric profile shapes and the tropospheric subcolumns at t1 and t2 from the climatology are close to reality. For the case in winter (Figure 4, right side) with low NO_2 values, the climatology profile shapes and the tropospheric NO_2 amount at t_1 and t_2 differ especially in the boundary layer strongly from the reality, the concept does not work properly. To solve this problem one has to improve the a-priori information. Therefore one can consider to take forecast data from an assimilation system instead of climatological data. A-priori data is considered adequate if there is an agreement with the true profiles within 50%.

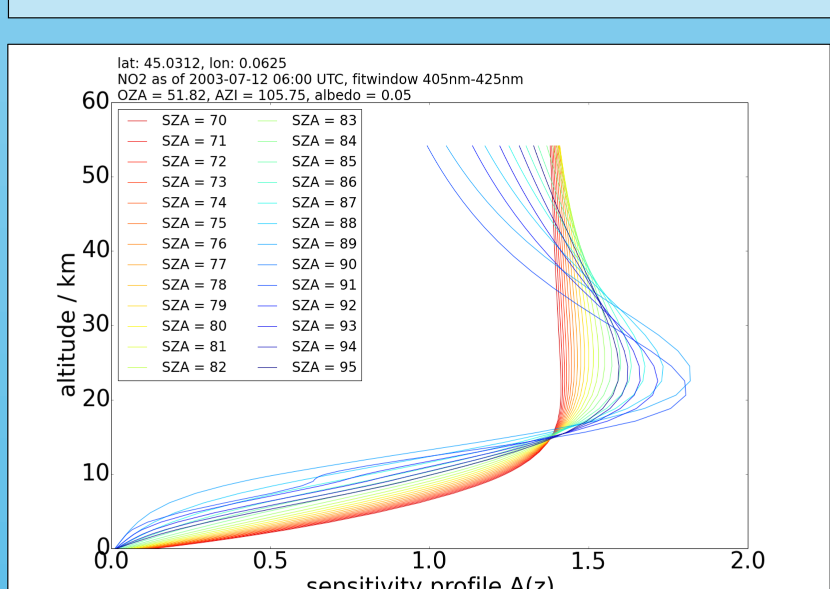


Figure 3: *Sensitivity profile of NO_2 retrieval for different solar zenith angles. The sensitivity of the retrieval to NO_2 in the boundary layer drops strongly at SZA above 85 degree.*

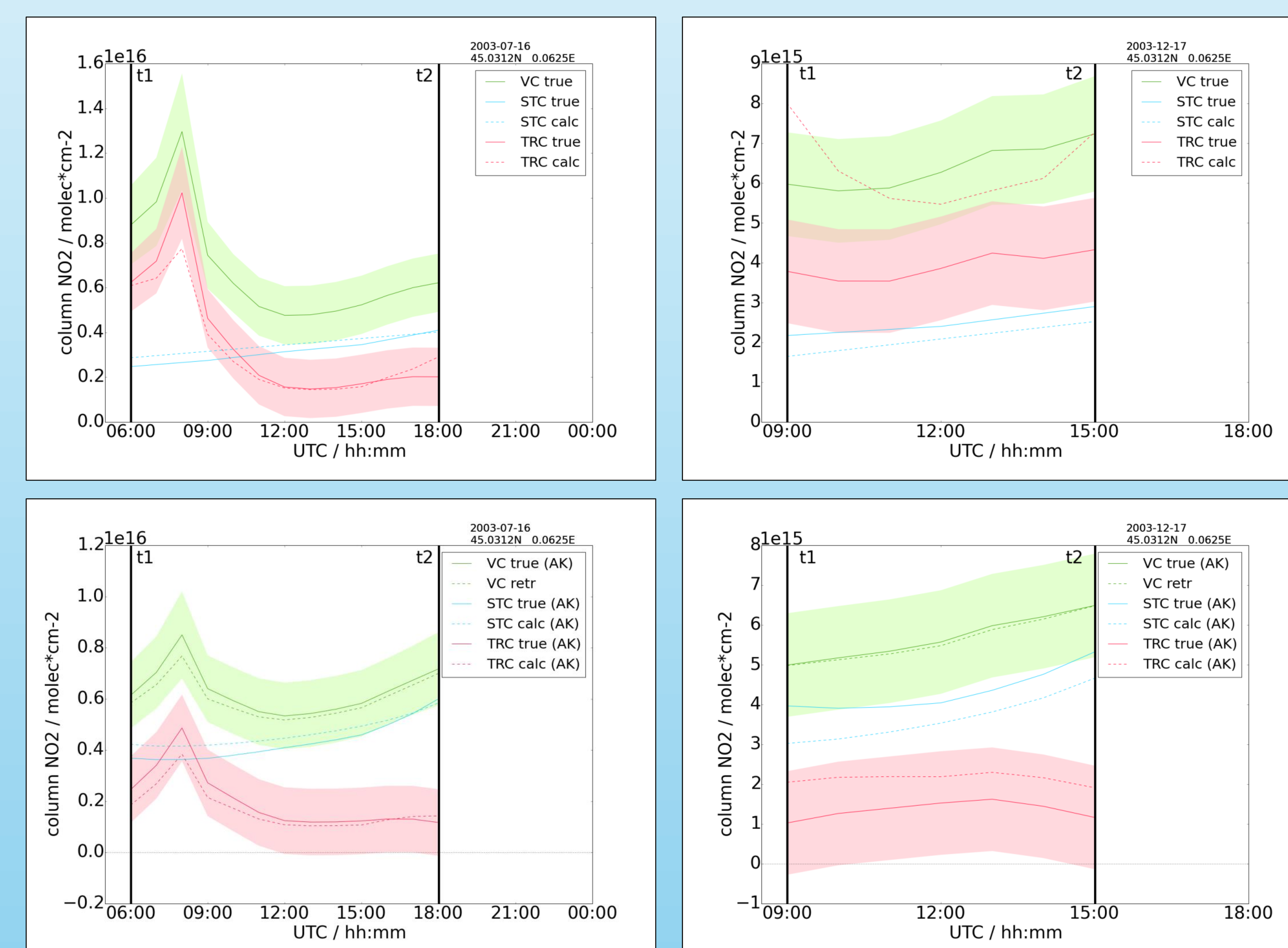


Figure 4: *Test of concept A on two test days in summer (left) and winter (right). This concept uses the averaging kernel from the retrieval and a NO_2 profile from a climatology to calculate the stratospheric columns in early morning and late evening hours. Here we want to use the insensitivity of the retrieval to NO_2 in the troposphere at high solar zenith angles. Over the course of the day we interpolate the stratospheric values between the morning and evening value due to the linear behaviour of NO_2 in the stratospheric diurnal cycle. In the top row the columns are integrated with all layers contributing with equal weights whereas in the bottom row the different layers are weighted with the averaging kernel before integration. Continuous lines are always the true values (in our case coming from the climate model) and the dashed lines belong to retrieved or further calculated values. According to the Sentinel-4 requirements the retrieved/calculated values should lie within the shaded areas. In green the total vertical column is depicted, in blue the stratospheric and in red the tropospheric subcolumns.*

Concept B – Wavelength Method (see also Richter and Burrows [2000])

Reference: Richter, A., & Burrows, J. (2000). A Multi Wavelength Approach to the Retrieval of Tropospheric NO2 from GOME Measurements. *ERS-Envisat Symposium Gothenburg.*

Total columns retrieved from different wavelength windows have a slightly different height sensitivity. This arises from the wavelength dependency of the penetration depth of photons and has many reasons. For example the scattering probability of photons at lower wavelengths is higher due to the higher Rayleigh cross section. Ozone absorption and surface albedo also lead to a lower penetration depth in the UV than in the visible.

$$SC = \vec{x}\cdot\overrightarrow{AMF} = \vec{x}_{trop}\cdot\overrightarrow{AMF}_{trop} + \vec{x}_{strat}\cdot\overrightarrow{AMF}_{strat} \quad (1)$$

If one subtracts now two slant columns from different fitwindows (in our case 340-360 nm and 480-500 nm) assuming that the airmass factors in the stratosphere are for both retrievals the same, one gets:

$$SC^{\lambda_2} - SC^{\lambda_1} = \vec{x}_{trop}\cdot\left(\overrightarrow{AMF}^{\lambda_2}_{trop} - \overrightarrow{AMF}^{\lambda_1}_{trop}\right) \quad (2)$$

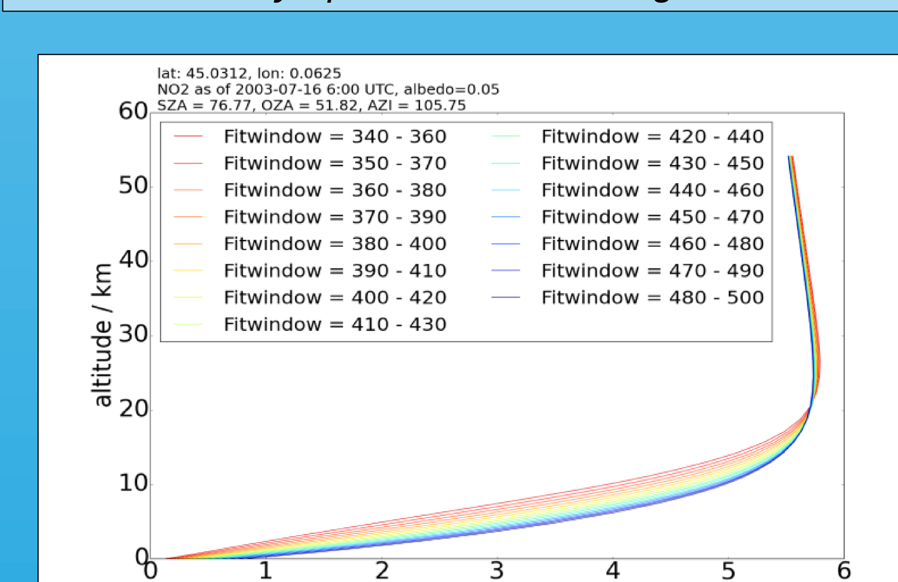
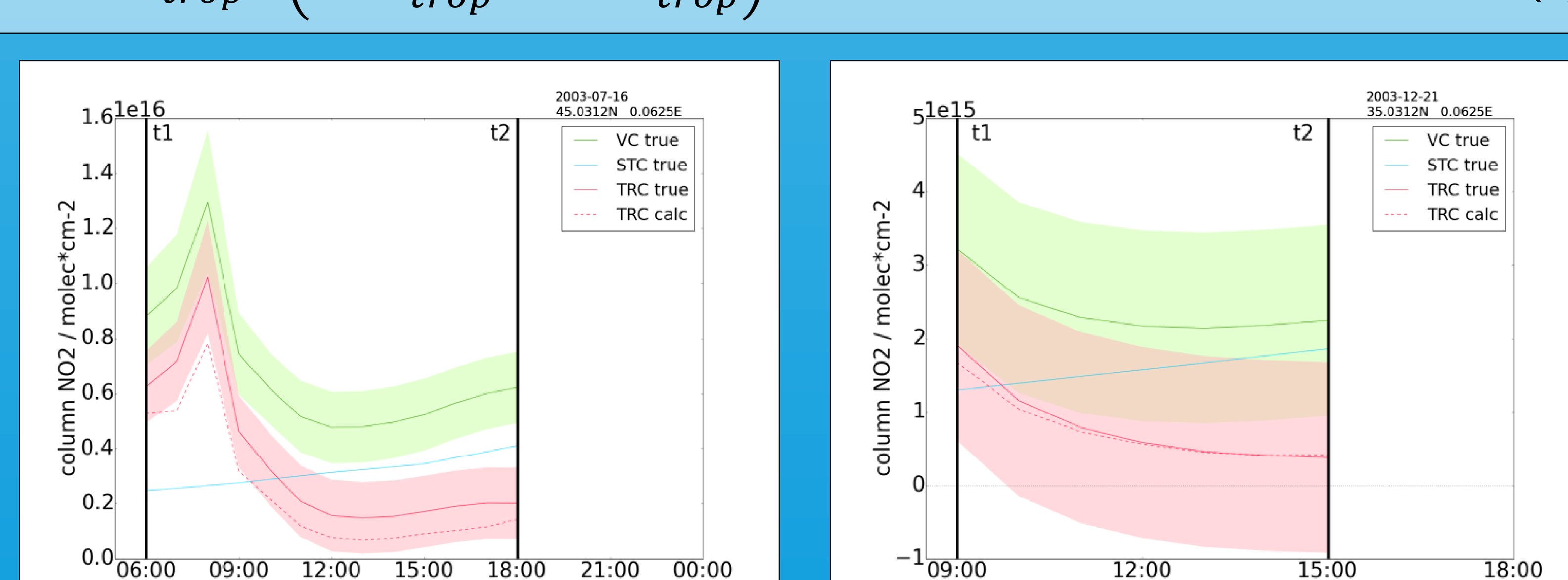


Figure 5: *Airmass factor profiles for different fit windows (colours). The airmass factor is the ratio between measured slant (sub)column and true vertical (sub)column. The airmass factor profile can therefore be seen as a sensitivity profile of the retrieval.*

Figure 6: *Test of the wavelength method on two test days in summer (left) and winter (right). In green the total vertical column is depicted, in blue the stratospheric and in red the tropospheric subcolumn. The wavelength concept for the calculation of the tropospheric NO_2 subcolumn is based on the different airmass factor profiles for different fitwindows. With the help of equation (2) and a tropospheric profile shape from a climatology the dashed red tropospheric columns are calculated.*



For Further Information contact:
European Space Agency-ESTEC (EOP-SM), Mission Science Division,
Keplerlaan 1, 2201 AZ Noordwijk, The Netherlands