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TROPOMI NO₂ slant column retrieval: uncertainties and comparisons with other satellite based NO₂ data

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The NO₂ slant column (SCD) retrieval for TROPOMI is based on improvements^{5,6} of the DOAS approach operationally used for the NO₂ SCD retrievals of OMI (the OMNO2A processor). Below some first TROPOMI NO₂ SCD retrieval results are compared to results using QDOAS 7 as well as to NO $_2$ SCDs from OMI (from QA4ECV 8 processing). Also shown are NO $_2$ SCD error estimates in comparison with results using an independent statistical uncertainty estimate based on spatial variability $^9.$







TROPOMI NO₂ SCD processor

– DOAS equation is solved in intensity fit formulation in wavelength window [405:465] nm – Included are: NO₂, O₃, O₂-O₂, H₂O-vapour, H₂O-liquid, Ring effect (all sampled @ 0.01 nm and pre-convolved with the ISRF)

 $-\chi^2$ minimisation using an Optimal Estimation (OE) routine with a-priori errors set very large, so that these do not limit the solution; a prewhitening of the data is performed to improve numerical stability

- Reflectance: $R(\lambda) = \pi/\mu_0 \cdot I(\lambda)/E_0(\lambda)$

Comparing TROPOMI and OMI

Slant column retrieval results for the Pacific Ocean orbit on 20 Feb. 2018 of TROPOMI are compared to those for the (almost) overlapping OMI orbit and to those of a similar OMI orbit from 20 Feb. 2005. The NO₂ slant column (SCD) and vertical column (VCD = SCD / AMFgeo) [*left*] and the SCD error [*right*] of TROPOMI show much less across-track variation than OMI's, and the SCD error of TROPOMI is some 30% lower than OMI's.

Data of scanlines with nadir latitude in the range $\left[-20^\circ\,;+20^\circ\right]$ is averaged along-track; orbits are over the Pacific Ocean. OMI data is processed within the QA4ECV framework $^8.$

SCD uncertainty & error estimate

A statistical estimate using the spatial variability over a remote Pacific Ocean sector can be used to compare SCD uncertainties of different retrieval methods⁹. Statistical uncertainty of TROPOMI [*left*] is clearly much lower than OMI's, and TROPOMI data processed with QDOAS⁷ gives results very similar to the TROPOMI processor. Like for other instruments⁹, the SCD error estimates for TROPOMI [*right*] are on average larger than the statistical uncertainties. Data of scanlines with nadir latitude in the range [-60° :+ 60°] is used, without cloud filtering; orbits are over the Pacific Ocean.

Effect of irradiance choice

The NO₂ slant column (SCD) and vertical column (VCD = SCD / AMF_{geo}) for radiance orbit 00661 of 28 Nov. 2017 using the irradiance of the same day (orbit 00657) are compared to results using the irradiance of 20 Feb. 2018 (orbit 01878) [*left*] and results for radiance orbit 01852 of 20 Feb. 2018 using the corresponding irradiance [*right*]. Clearly it is best to use the irradiance measured nearest in time to the radiance for the NO₂ retrieval.

Data of scanlines with nadir latitude in the range $[-20^\circ;+20^\circ]$ is averaged along-track; orbits are over the Pacific Ocean.

NO₂ slant column error of TROPOMI and OMI





Intensity Fit DOAS using Optimal Extimation ("IFDOE")

 Wavelength calibration of irradiance and radiance is performed prior to the DOAS fit in the full fit window
The irradiance is interpolated to the radiance wavelength grid with a high-sampling interpolation which uses a high-resolution solar spectrum (pre-convolved with the ISRF)

- Cross sections are interpolated to the reflectance grid with a cubic spline

– If more than 1% of the wavelength pixels in the fit window are flagged as "saturated", the ground pixel is discarded

– SCD error estimates are scaled with the normalised χ^2 , where χ^2 is normalised by (N-D), with N the number of wavelength pixels (≈ 305) and D the degrees of freedom, which is almost equal to the number of fit parameters (12)

– Model reflectance at 440 nm is used to derive the cloud fraction and from that the cloud radiance fraction in the NO₂ window; FRESCO provides the cloud pressure & scene albedo and scene pressure

 $\underline{\text{Note:}} \ 10 \, \mu \text{mol}/\text{m}^2 = 6 \times 10^{14} \, \text{molec}/\text{cm}^2$

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⁷ Danckaert et al., 2017: http://uv-vis.aeronomie.be/software/QDOAS/

⁸ Boersma et al., 2018: http://www.qa4ecv.eu/

⁹ Zara et al., AMT, in review, 2018.

dation Team (S5PVT) or Level 1/Level 2 Product Working Group activities. Results are based on preliminary (not fully calibrated/validated) Sentinel-5 Precursor data that will still change. **Acknowledgement** Sentinel-5 Precursor is a European Space Agency (ESA) mission on behalf of the European Commission (EC). The TROPOMI payload is a joint development by ESA and the Netherlands Space Office (NSO). The Sentinel-5 Precursor ground-segment development has been funded by ESA and with national contributions from The Netherlands, Germany, and Belgium.

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⁵ Van Geffen et al., AMT **8**, 1686–1699, 2015.

 $^{^6}$ Van Geffen et al., TROPOMI NO $_2$ ATBD v2.0, in preparation, 2018.