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Table 1. List of acronyms pertaining to this project.

AMF	AirMass Factor
ATBD	Algorithm Theoretical Basis Document
CA	Cloud Albedo
CAL	Clouds-As-Layers model
CAMS	Copernicus Atmosphere Monitoring Service
CF	Cloud Fraction
CLASS	Comprehensive Large Array-data Stewardship System
CH	Cloud-centroid Height
CTH	Cloud-Top Height
COT	Cloud Optical Thickness
CRB	Clouds-as-Reflecting-Boundaries model
DLER	Directionally dependent Lambertian-equivalent reflectivity
DOAS	Differential Optical Absorption Spectroscopy
EVDC	ESA Atmospheric Validation Data Centre
FOV	Field Of View
FRESCO	Fast Retrieval Scheme for Clouds from the Oxygen A band
FRM4DOAS	Fiducial Reference Measurements for ground-based DOAS air-quality observations
GEO	Geostationary Orbit
LES	Large Eddy Simulation
LEO	Low Earth Orbit
MAX-DOAS	Multi-Axis Differential Optical Absorption Spectroscopy
OCRA	Optical Cloud Recognition Algorithm
ROCINN	Retrieval Of Cloud Information using Neural Networks
SZA	Solar Zenith Angle
TOA	Top Of the Atmosphere
TROPOMI	TROPOspheric Monitoring Instrument
TVCD	Tropospheric Vertical Column Density
VIIRS	Visible Infrared Imaging Radiometer Suite

1. Handling of 3D Clouds in Trace Gas Retrievals, 3DCTRL goals

The *Handling of 3D Clouds in Trace Gas Retrievals*, 3DCTRL project was dedicated to improving the handling of clouds in trace gas retrievals, specifically the retrieval of tropospheric NO_2 columns. This trace gas is of great interest to the scientific community, but also to the air quality forecast modelling community, as it is the major air quality marker. The current operational S5P/TROPOMI tropospheric NO_2 product developers suggest that a filter be applied to the dataset which basically rejects all cloud-covered scenes, with a cloud radiance fraction > 0.5, i.e. a cloud fraction > 0.2. As a result, especially during the winter months, entire days of crucial space-borne observations are excluded from further analysis and consideration. For this reason, the 3DCTRL project demonstrated that realistic cloud treatments can be introduced into the operational retrieval analysis chains both for current, such as S5P/TROPOMI, as well as future, such as Sentinel-4 and -5, missions.

The major goals of the 3DCTRL project were:

1. to evaluate cloud correction methodologies in Copernicus Sentinel-4, Sentinel-5 and Sentinel-5P trace gas retrieval schemes, and
2. to explore ways to improve handling of realistic clouds in the retrievals of atmospheric species.

To reach these goals, 3DCTRL followed the scientific pathways to:

a) Generate synthetic reference datasets in which true cloud properties including their 3D structure and vertical distribution are known by means of 3D radiative transfer simulations, realistic synthetic data of cloud properties were obtained from LES model
b) Explore ways to improve the handling of realistic clouds in trace gas retrievals, specifically for NO_2
c) Test and evaluate improved approaches for cloud correction by application on synthetic and real TROPOMI-S5P data

In the following sections, we briefly discuss how the goals of 3DCTRL were achieved.

The project has a dedicated website https://websites.auth.gr/3dctrl/, where the main project documents can be found in the open part of the website while in the project internal pages and data pool: http://datapool.corgi.web.auth.gr/ [username: datapool, password: some_random_password] the datasets created during this project are being made available to interested parties. Furthermore, the project has a Twitter account: https://twitter.com/3dctrl_esa.

2. Theoretical analysis of different cloud treatments for trace gas retrievals

A comprehensive theoretical analysis behind the different schemes for treating clouds in the FOV of the satellite pixels was conducted early in the 3DTRL project and was reported fully in the project ATBD v2.0 document, found in the Documentation Section of the 3DCTRL project website.

The main conclusions for the NO_2 retrieval are that the three-dimensional radiative transfer model based on spherical harmonics discrete ordinate method (SHDOM) yields the highest accuracy (the relative error in NO_2 total column retrieval is less than 0.05%, with the error calculated relative to the true value of the NO_2 total column). The atmospheric scene was modelled as a rectangular prism with horizontal dimensions of 15 km by 15 km and vertical dimension of 50 km. However, the extremely high computation time of about 14 hours disqualifies this method for processing a large amount of data. The independent slice approximation with a computation time of 6-8 minutes and relative errors below 5% (as illustrated in Figure 1) is a well-balanced compromise between accuracy and efficiency. The nonlocal independent slice approximation and a zeroth-order stochastic model yield relative errors of about 3-4% (technical terms such as “The nonlocal independent slice approximation” are defined in the Algorithm Theoretical Baseline Document (ATBD)). However, the small accuracy improvement as compared to the independent splice approximation does not justify the high computation times of 25-40 minutes. The tilted independent column approximation with a computational time of 20-30 seconds can lead to large relative errors (of about 20%). Therefore, from the point of view of accuracy, the method is also not recommended.

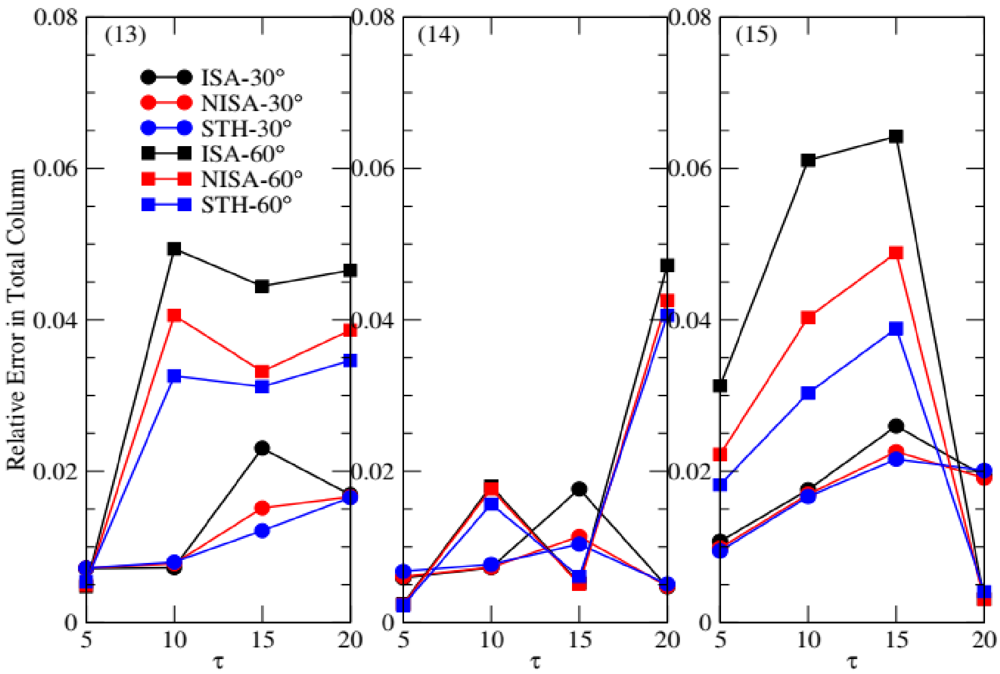

Figure 1. Relative error in total column of NO_2 for cloud optical thickness τα = 5, 10, 15, 20 and solar zenith angle θ_0 = 30°, 60°. The results are computed for the cloud scenes 13, 14, and 15 by using the two-dimensional independent slice approximation (ISA), the nonlocal independent slice approximation (NISA) and the zeroth-order stochastic model (STH).

The main conclusions for the AMF retrieval are that the relative errors of the independent slice approximation are below 4% as shown in Figure 2, while the computation time is around 1-3 minutes; the computation time of the tilted independent column approximation is of about 10-20 seconds, but the relative errors can be extremely large (they can reach values of 30% and even more) and that the 3D-to-2D errors related to the calculation of the air-mass factor with an approximate two-dimensional radiative transfer model (in particular, the independent slice approximation) are below 4%.

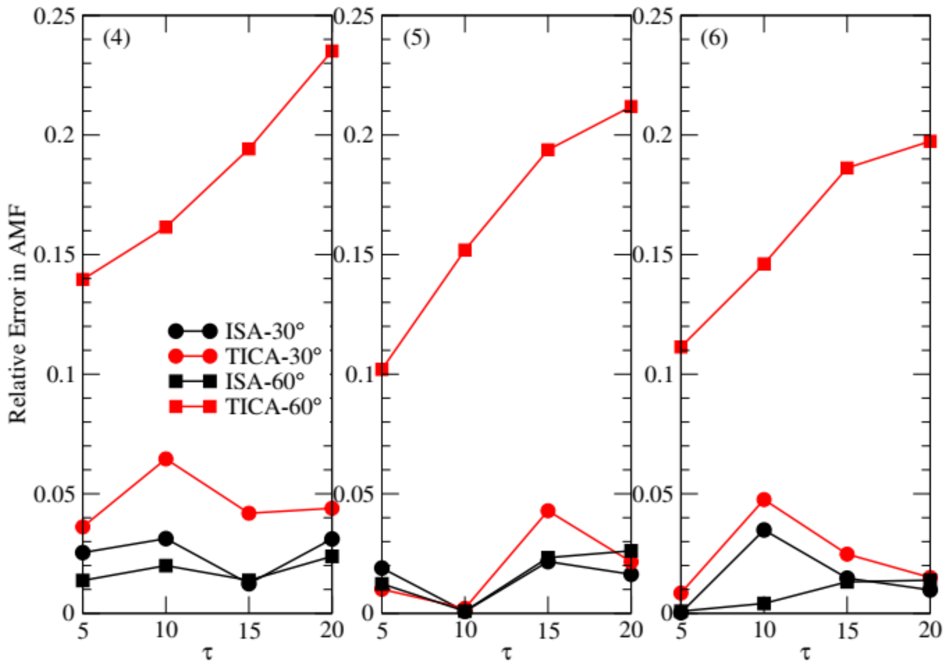

Figure 2. Relative error in air-mass factor for cloud optical thickness $\tau = 5, 10, 15, 20$ and solar zenith angle $\theta_0 = 30^\circ, 60^\circ$. The results are computed for the cloud scenes 1, 2 and 3 described in the ATBD by using the two-dimensional independent slice approximation (ISA) and the one-dimensional tilted independent column approximation (TICA).

The theoretical treatment resulted in the definition of a "surrogate cloud method" which, in short, assumes that regardless of whether the scene is clear or cloudy, a surrogate cloud is introduced in the field of view of the instrument using as primary information the measured TOA reflectance. The surrogate cloud can be introduced by smoothing the cloud fraction field and the width of the radiative smoothing kernel should be in the range 0.2 - 3 km. The influence of cloud smoothing using the same settings of the NO_2 retrieval algorithm can hence be assessed. However, it was expected that the difference in the retrieved NO_2 values due to different settings of the NO_2 retrieval algorithm are larger than those due to cloud fraction smoothing. This method was assessed on the S5P/TROPOMI tropospheric NO_2 columns discussed further below.

3. Investigation on cloud properties using synthetic spectra

3.1 Synthetic spectra generation

In order to investigate the effect of the different cloud treatments on the tropospheric NO_2 retrievals, the synthetic dataset created within the ESA 3DCATS project was extended to include all required spectral bands for the NO_2 retrievals including cloud correction. Hence, the synthetic spectra were extended to the OCRA/ROCINN requirements, namely for Sentinel-S5P, band 3/4 (310-495nm) and band 6 (O2A-band, 758-772nm). Three different cloud setups with different complexities included, for typical sun-observer geometries for both Low Earth, LEO, and Geostationary, GEO, orbits: (a) 1D cloud, (b) 2D box cloud (c) broken (3D) clouds (including cumulus, cirrus, convective clouds, stratus) from LES simulation including Germany and surrounding countries with all typical cloud types contained.

The complete dataset including documentation available in the 3DCTRL project Data Pool, http://data-pool.corgi.web.auth.gr/DataPool/D4.1. Data and quicklooks also available at https://www.meteo.physik.uni-muenchen.de/~emde/doku.php?id=projects:3dctrl:3dctrl_synthetic_dataset

3.2 Evaluation of cloud products using synthetic data

The application of the OCRA/ROCINN cloud algorithms to the synthetic data generated within 3DCTRL was performed in a multitude of ways. Retrievals of cloud properties with synthetic measurements were performed (assuming 1D atmospheres) to use them as inputs in the NO_2 retrievals by the OCRA algorithm providing radiometric cloud fraction (CF); the ROCINN/CRB algorithm, providing cloud-centroid height and cloud albedo (CH, CA) and the ROCINN/CAL algorithm proving cloud-top height and cloud optical thickness (CTH, COT). Then, for the LEO configuration, representing the S5P/TROPOMI instrument, the cloud algorithms were applied to all three different synthetic cloud assumptions, i.e. 1D, Box- and 3D-cloud. For the GEO configuration, representing the future S4/UVN instrument, the 3D-cloud synthetic spectra configuration was employed. Based on these retrievals, it was shown that the OCRA radiometric CF behaves similarly as in previous studies, with a mean difference of about 0.2 with respect to the exact geometric CF; ROCINN compensates the OCRA underestimations in CF with an increase in the retrieved COT and that ROCINN retrievals of cloud-top height (CAL) remain reliable, and its values are higher when compared to the retrieved cloud-centroid height (CRB).

3.3 Evaluation of the impact on NO_2 levels using synthetic data

The impact of clouds on trace gas retrievals via the evaluation of the cloud correction using the synthetic spectra in the retrievals of AMF/NO_2 levels was assessed and, in particular, three cloud algorithms/retrievals were used in the operational trace gas products:

- FRESCO (based on O_2-A band absorption)
  - Cloud fraction (cf), cloud pressure/height and cloud albedo ($ca = 0.8$)
- O_2-O_2 (based on O_2-O_2 absorption at 477nm)
  - Cloud fraction, cloud pressure/height and cloud albedo (=0.8)
- OCRA/ROCINN (based on O_2-A band absorption)
  - OCRA: Cloud fraction (cf)
  - CRB model: cloud albedo (ca) and cloud pressure/height
  - Scaled CRB model: $cf' = cf \cdot ca/0.8$, $ca' = 0.8$
  - CAL model: cloud optical thickness and cloud top/bottom pressure/height with 1km geometrical thickness

The main findings with respect to the NO_2 retrieval with various cloud correction schemes applied to a series of synthetic data are, for the 1D simulation that most of retrieval biases is within 20% except high SZA (>60°) and retrieval using OCRA/ROCINN CRB cloud correction while for the OCRA/ROCINN CRB cloud, if the NO_2 retrieval using a fixed cloud albedo of 0.8 and a corresponding effective cloud fraction, the retrieval biases are significantly reduced. For the 2D simulation, that the in-scattering region, most significant retrieval biases are typically found at cloud edge of the cloudy scene while in the cloud shadow region, largest retrieval biases are found in the cloud shadow. Finally, for the 3D simulation, that all NO_2 retrievals based on all cloud correction approach shows very good agreement and that the most significant bias in NO_2 retrieval is from the cloud shadow effects.

Both evaluation analyses are comprehensively presented in the Validation Report v2.0 found in the Documentation Section of the 3DCTRL project website. The datasets generated to enable this evaluation can be found in the project internal Data Pool, under http://datapool.corgi.web.auth.gr/DataPool/D4.3/ [password protected.]

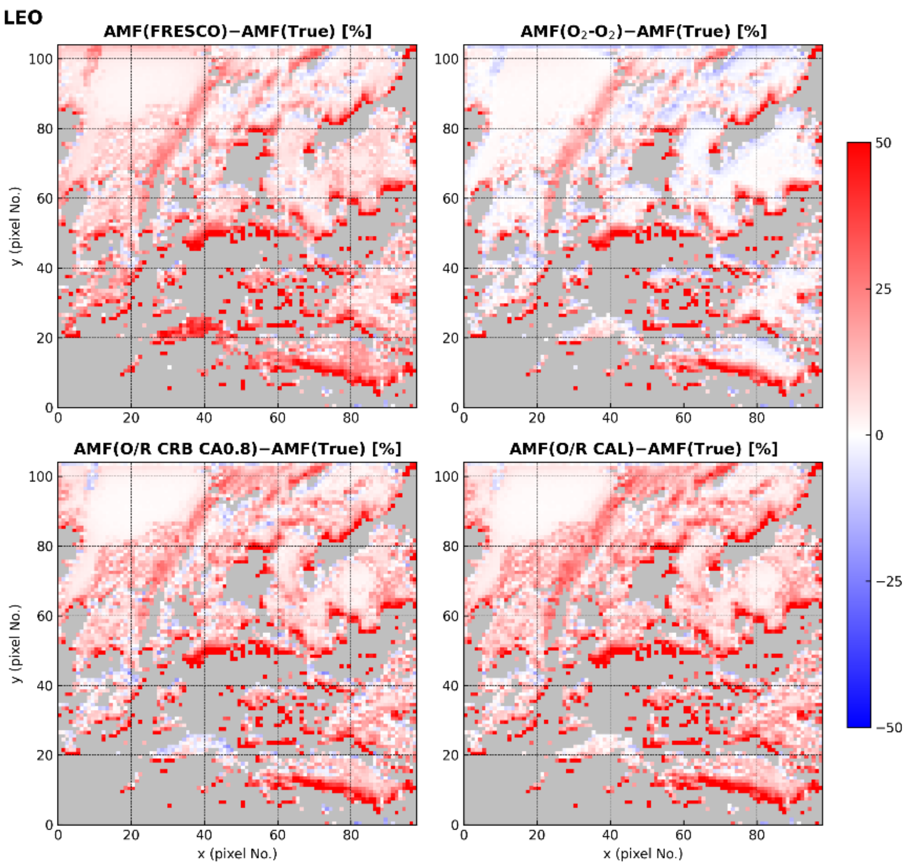

Figure 3. The mean bias of the NO_2 AMF using various cloud correction methods (FRESCO, O_2-O_2, OCRA/ROCINN scaled CRB, OCRA/ROCINN CAL) for all LEO geometries.

4. Investigation on cloud properties using S5P/TROPOMI spectra

4.1 DLR S5P/TROPOMI tropospheric NO_2 research product

An improved scientific S5P/TROPOMI DLR tropospheric NO_2 retrieval algorithm was developed for the needs of the 3DCTRL project which includes fields calculated with the surrogate cloud model, discussed in Section 3.

The final version v3.0 of the DLR S5P/TROPOMI tropospheric NO2 research product can be found in the project internal Data Pool, http://datapool.corgi.web.auth.gr/DataPool/D4.2/TROPOMI_tropospheric_NO2_dataset_v3.0/ [password protected.]

The main improvements of DLR TROPOMI NO_2 retrieval algorithm for 3DCTRL include:

1. **Use of reprocessed TROPOMI data:**
   - TROPOMI L1B v2.1 data (RPRO collection 3, with (ir)radiance degradation correction)
   - OCRA/ROCINN v2.4 cloud parameters (based on reprocessed L1B data)

2. **Latest version of surface albedo dataset (based on reprocessed L1B data):**
   - TROPOMI surface DLER v2.0 (released in Sep 2023)

3. **Improved a priori profiles (higher resolutions, up-to-date chemistry and emissions):**
   - CAMS global forecast a priori NO2 profile (0.4°x0.4°, 137 levels)

4. **Different cloud model datasets for cloud corrections:**
   - OCRA/ROCINN CRB, OCRA/ROCINN CAL, OCRA/ROCINN surrogate CAL

To evaluate the 3D cloud effect on the tropospheric NO_2 retrieval, three different cloud model datasets were used for the cloud corrections:

1. **OCRA/ROCINN CRB (Clouds-as-Reflecting-Boundaries) v2.4**
   - Clouds treated as simple Lambertian reflecting surfaces

2. **OCRA/ROCINN CAL (Clouds-As-Layers) v2.4**
   - Clouds treated as optically uniform layers of light-scattering water droplets -> scattering are described
   - Better represents real situations by reflecting sensitivities both within and below the cloud layers

3. **OCRA/ROCINN surrogate CAL v2.4**
   - Surrogate cloud model is implemented in the OCRA/ROCINN CAL processor to account for 3D cloud effects by reflecting cloud shadow effects
   - Apply smoothing to the OCRA radiometric cloud fraction field (i.e. it uses real three-dimensional radiance field) with a Gaussian kernel

From the initial evaluation of the updated product, it was concluded that distinct variations in tropospheric NO_2 levels are mainly found in heavily polluted areas with significant variability in cloud coverage such as in the cloud boundaries.

4.2 Validation of the DLR tropospheric NO_2 retrievals again MAX-DOAS ground-based instruments

Both validation exercises performed within 3DCTRL and discussed briefly in the sub-sections below are extensively presented in the Validation Report v2.0 found in the Documentation Section of the 3DCTRL project website.

4.2.1 Consolidated validation

The MAX-DOAS observations that were used for validating the DLR S5P/TROPOMI scientific tropospheric NO_2 products were collected through the ESA Atmospheric Validation Data Centre, EVDC. The analysis is focused on days in 2021 and 2022 based on observations from eight European measurement sites, two of which are located in Greece (Thessaloniki and Athens), while the rest of them are distributed in northern Europe, namely in Bremen, Cabauw, De Bilt, Heidelberg, Mainz and Uccle. The MAX-DOAS data sets for the selected sites that are included in EVDC are either generated individually by the instruments' principal investigators or they are commonly processed by the Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations, FRM_4DOAS, based on harmonized tropospheric NO_2 retrieval settings. In order to avoid uncertainties caused by different NO_2 data processing settings, only the MAX-DOAS data that are produced by FRM_4DOAS are used for the validation in this project.

The validation was performed under various pollution levels and cloud coverage conditions. While a clear underestimation by the TROPOMI tropospheric NO_2 columns is found for all stations, mainly due to the relatively larger satellite footprint, CRB, CAL and CAL surrogate cloud treatments lead to similar results by comparison with the MAX-DOAS, especially for less cloudy conditions. For cloud fractions > 20%, even though slightly higher correlation coefficients are found for the CAL retrievals, the performance of CAL and CRB is overall very similar. However, in this case, the MAX-DOAS measurements can also be affected by clouds and thus, further analysis is required for a more detailed TROPOMI validation, by investigating cases where the cloud structure and the NO_2 field around the site are well known.

4.2.2 Case-study analysis

Relatively large solar zenith angles and polluted type NO_2 profiles are conditions for which cloud shadow effects in the NO_2 TVDC are maximized. Thus, for a region roughly covering central Europe, two months (March and April 2021) of VIIRS cloud shadow data was downloaded from CLASS. For these months the solar zenith angle is favorable for making cloud shadows visible from above. For this data set the number of VIIRS pixels with a cloud shadow within a circle of 15 km radius was calculated for the MAX-DOAS stations chosen in this validation exercise. The effect of cloud shadows on TROPOMI NO_2 retrievals have been made for selected cases where cloud shadows are present in the VIIRS data. There are very few cases with "ideal" cloud shadow bands and for one such case there is cloud shadow effect, i.e. the NO_2 TVCD is smaller in the cloud shadow band, in agreement with theory. For other cases including scattered clouds where cloud shadows are present, there is an effect, but the NO_2 TVCD is seen to both increase and decrease. The DLR surrogate cloud model retrieval changes NO_2 column in the presence of clouds compared to the standard CAL retrieval. Overall, the cloud shadow effect was found to be within the uncertainty of the satellite retrievals.

5. Conclusions

Within the *Handling of 3D Clouds in Trace Gas Retrievals*, 3DCTRL project, Synthetic and observational data have been used to assess the effect on clouds TROPOMI NO_2 retrievals and how various cloud correction methods improve the retrievals. The synthetic data set includes 1Dlayer clouds, box clouds and realistic 3D clouds. The observational data sets include TROPOMI, VIIRS and MAX-DOAS observations for the year 2021 and 2022 for selected MAX-DOAS stations in Europe. Both the synthetic and observational data are analyzed by retrieval methods applying several different cloud correction methods. The findings are summarized below:

- **Synthetic data set conclusions.** The standard NO_2 retrieval with various cloud correction schemes was applied to a series of synthetic data. In a 1D layer cloud scene, the results exhibit generally good agreement, with the retrieval biases mostly staying within 20%. However, relatively large biases are observed in cases of high SZAs and when applying the OCRA/ROCINN CRB cloud correction in the NO_2 retrievals. For the latter cases, these biases can be significantly reduced by employing a fixed cloud albedo of 0.8 and a corresponding effective cloud fraction. In 2D box-cloud and 3D LES cloud scenes, the most significant 3D biases arise from cloud shadow effects. All cloud products used in the NO_2 retrieval typically underestimate cloud fraction retrieval for pixels affected by the cloud shadows, resulting in substantial positive biases in the calculation of NO_2 AMF.
- **S5P/TROPOMI Validation against MAX-DOAS observations.** Observations from 8 ground-based MAX-DOAS remote sensing instruments around Europe were used for validating the TROPOMI tropospheric NO_2 VCDs using OCRA/ROCINN CRB, CAL and CAL surrogate cloud models. The validation is performed for selected days in 2021 and 2022, under various pollution levels and cloud coverage conditions. While a clear underestimation by the TROPOMI tropospheric NO_2 columns is found for all stations, mainly due to the relatively larger satellite footprint, CRB, CAL and CAL surrogate cloud treatments lead to similar results by comparison with the MAX-DOAS, especially for less cloudy conditions. For cloud fractions > 20%, even though slightly higher correlation coefficients are found for the CAL retrievals, the performance of CAL and CRB is overall very similar. However, in this case, the MAX-DOAS measurements can also be affected by clouds and thus, further analysis is required for a more detailed TROPOMI validation, by investigating cases where the cloud structure and the NO_2 field around the site are well known.
- **S5P/TROPOMI Validation over selected cloud shadow cases.** The effect of cloud shadows on the TROPOMI NO_2 retrievals has been made for selected cases where cloud shadows are present in the VIIRS data. There are very few cases with "ideal" cloud shadow bands. For one such case there is cloud shadow effect, i.e. that the NO_2 TVCD is smaller in the cloud shadow band, in agreement with theoretical predictions. For other cases including scattered clouds where cloud shadows are present, the NO_2 TVCDs are seen to both increase and decrease. It has mostly been shown that the cloud shadow effect is within the uncertainty of the satellite retrievals. The DLR surrogate cloud model retrieval changes NO_2 column in the presence of clouds compared to the standard CAL retrieval, however the reported changes are within the uncertainty of the two products.

As to **possible future research activities**, these could move in two directions, towards investigations using synthetic spectra and investigations using real space-born measurements. For the former case, these could include to:

- Investigate cloud impact on other trace gas retrievals (e.g. CO_2, CH_4) using synthetic data (in this project, the synthetic data would need to be expanded to other channels).
- Develop methods to correct NO2 retrieval in cloud shadows using cloud shadow data (Trees et al. 2022).
- Use AI for cloud correction in trace gas retrievals (some promising tests in these directions were performed in the ESA project MIT3D).

As to investigations using real measurements, these could focus on:

- Enhancing the computational efficiency of 3Dradiative transfer models. In this regard, one promising direction would be the acceleration of existing 3D radiative transfer code SHDOM through parallelization on multi-core CPUs or GPUs. This approach could significantly reduce computation times, making it possible to enable offline data processing in a reasonable time.
- Involving the tomographic retrieval of cloud properties in conjunction with trace gas information using multi-angle remote sensing measurements. This would require a consistent integration of cloud and trace gas retrievals within a 3D radiative transfer framework, ensuring that both cloud and gas properties are derived in a physically coherent manner.

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