3DCTRL project

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1. Summary of the aims of the ESA 3DCTRL project

The *Handling of 3D Clouds in Trace Gas Retrievals*, 3DCTRL project is 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, but also 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[1] which basically rejects all cloud-covered scenes, with a cloud radiance fraction > 0.5, i.e. a cloud fraction > 0.2. As a result, during the winter months especially, entire days of crucial space-borne observations are excluded from further analysis and consideration. For this reason, the 3DCTRL project is aiming to demonstrate 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 Sentine-4 and -5, missions.

The major goals of the 3DCTRL project are:

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

The **first goal of 3DCTRL** is to evaluate the performance of currently used operational retrieval algorithms for Sentinel-4, Sentinel-5, and Sentinel-5p. In the recent ESA-funded study *Impact of 3D Cloud Structures on the Atmospheric Trace Gas Products from UV-VIS Sounders* (3DCATS), synthetic and observational data were used to identify and quantify possible cloud-related bias in NO_2 tropospheric vertical column densities (TVCD). Cloud shadow fraction, cloud top height, cloud optical depth, solar zenith and viewing angles, were identified as the metrics being the most important in identifying 3D cloud impacts on NO_2 TVCD retrievals. For a solar zenith angle less than about 40° the synthetic data show that the NO_2 TVCD bias is typically below 10%. For larger solar zenith angles both synthetic and observational data often show NO_2 TVCD bias on the order of tens of %. Specifically, for clearly identified cloud shadow bands in the observational data, the NO_2 TVCD appears low-biased when the cloud shadow fraction > 0.0 compared to when the cloud shadow fraction is zero. For solar zenith angles between 50-60°, about 16% of TROPOMI pixels with high quality value NO_2 TVCD retrievals, were found to be impacted by cloud effects larger than 20%. In the proposed 3DCTRL, the current operational cloud retrieval algorithms, FRESCO, O2-O2 and OCRA/ROCINN, will be applied on the same synthetic dataset, so that their performance can directly be compared.

The **second goal of 3DCTRL** is to explore ways to improve handling of realistic clouds in the retrievals of atmospheric species by designing new retrieval algorithms that take into account 3D cloud scattering. The reason for the aforementioned large bias is that the majority of operational retrieval algorithms are based on the so-called independent pixel approximation (IPA). The IPA for an atmosphere exhibiting partial cloudiness means to compute separately the radiances for completely cloudy and clear skies, and then to express the partially cloudy radiance as a weighted sum of the separate radiances; the weighting factor being provided by cloud fraction. The clouds within each pixel are assumed to be plane-parallel and homogeneous in both horizontal and vertical directions. The main advantage of the IPA is its computational efficiency, since it requires the solution of only two independent one-dimensional radiative transfer problems. The disadvantage is that for cloudy scenes of small horizontal extent, the errors due to the three-dimensional effects may be very significant and fast and more accurate models accounting for the cloud inhomogeneities are crucial and will be developed during this project.

To **reach these goals**, 3DCTRL has the following **three main objectives**:

[1] https://sentinel.esa.int/documents/247904/3541451/Sentinel-5P-Nitrogen-Dioxide-Level-2-Product-Readme-File

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 will be obtained from LES model
b) Explore ways to improve the handling of realistic clouds in trace gas retrievals, specifically for NO_2
c) Testing and evaluation of improved approaches for cloud correction by application on synthetic and real TROPOMI-S5P data

Objective (a) was addressed successfully by generating a set of synthetic observations, following up on the work of Emde et al. 2022. The synthetic dataset includes cloud setups with different complexities, namely a (a) 1D cloud, (b) 2D box cloud and (c) broken clouds from LES simulation which includes cloud properties simulated by the LES model ICON for a region covering Germany and parts of surrounding countries with a spatial resolution of approximately 1x1km². Typical sun-observer geometries for LEO and GEO orbits were chosen. This dataset extended the ESA project 3DCATS dataset to the OCRA/ROCINN requirements, namely for Sentinel-S5P, band 3/4 (310-495nm) and band 6 (O2A-band, 758-772nm). The 3DCTRL project has a dedicated website, https://websites.auth.gr/3dctrl/, with a password-protected Data Pool, http://datapool.corgi.web.auth.gr/DataPool/ hosting this synthetic spectra under the sub-folder D4.1.

Objective (b) was addressed successfully by designing new algorithms for trace gas retrievals from S5P measurements by considering the influence of clouds. Focussing on NO_2 retrieval algorithms for 3D cloudy scenes and extending the results established in Doicu et al. (2021) we were able to both (I) consider a simplified retrieval algorithm and (ii) analyzing the accuracy and efficiency of the retrieval algorithms through a more comprehensive numerical analysis. The simplified retrieval algorithm was applied to both synthetic and real spectra and was assessed in the project VR v2.0, found in the Documentation Section of the 3DCTRL project website, hence converting point (i). The different retrieval algorithms and their accuracy estimates were fully analysed and presented in the project ATBD v2.0 document, found in the Documentation Section of the 3DCTRL project website, hence converting point (ii).

Objective (c) was addressed successfully by evaluating the handling of clouds in the NO_2 retrievals based on both synthetic and real data. The standard NO_2 retrieval including cloud correction approaches were applied to a series of synthetic spectra generated from addressing objective (a). The radiative transfer settings in the NO_2 and cloud retrievals were made as consistent as possible with those used to generate the synthetic data sets, in order to ensure that the differences between retrieved column and truth are due to the clouds, which include the uncertainty due to the simplified cloud correction approach and the 3D cloud effects. The evaluation was be performed for real observations using S5P/TROPOMI and NPP-VIIRS data, and an extensive presentation of all this analysis can be found in the project VR v2.0, in the Documentation Section of the 3DCTRL project website.

2. Scientific and technical priority areas for future projects

The following points might help identify scientific and technical priority areas and provide guidance for future projects in the Research activity.

• The current cloud correction approach, using 1D radiative transfer modelling (RTM), is insufficient for adequately correcting 3D cloud effects in trace gas retrievals. A rapid and robust method to correct these effects in trace gas retrievals is needed. This could involve using a 3D RTM, employing a machine learning approach, or adopting a more advanced cloud model in the operational cloud retrieval algorithm.

• There are consistent differences in the tropospheric columns reported by the ground-based remote sensing instruments, MAX-DOAS, and space-born remote sensing instruments, such as S5P/TROPOMI. These differences appear to be greater in magnitude than the cloud effects this research activity aims to enumerate. In order to be able to proceed in the right direction with different cloud corrections/cloud treatments, the systematic discrepancies between satellite and ground should be minimised. Full 3D RTM simulations of MAX-DOAS and S5P measurements could be used together with standard retrievals to understand these differences. Such investigations should be done for both clear skies and cloudy skies. From the theoretical findings of this in-tandem simulations, suggestions for improved algorithms for both set of instruments may arise.

• LES model results as used here are extremely useful, but also expensive in terms of computer resources required. EarthCARE will soon provide fully 3D input data for a number of real cloud conditions. These may be combined with future S4 measurements to further understand the impact of various cloud situations on NO_2 tropospheric VCD retrievals.

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