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Abstract

One of the primary targets of the TROPOspheric Monitoring Instrument (TROPOMI), which was launched on 13 October 2017 on-board the Copernicus Sentinel-5 Precursor satellite, is to provide measurements of the total column concentrations of carbon monoxide (CO) in the atmosphere with daily global coverage and a high spatial resolution up to $5.5 \times 7 \text{ km}^2$. SRON, the Netherlands Institute for Space Research, developed the Shortwave Infrared CO retrieval (SICOR) algorithm that infers CO columns simultaneously with effective cloud parameters from TROPOMI's $2.3 \mu\text{m}$ measurements and is deployed by the European Space Agency (ESA) for the near real-time and offline processing of TROPOMI data. Already early in the mission, the TROPOMI CO data set was validated with reference measurements of the Total Carbon Column Observing

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Network (TCCON), the Infrared Working Group of the Network for the Detection of Atmospheric Composition Change (NDACC-IRWG), and the Measurements Of Pollution in the Atmosphere (MOPITT) and inter-compared with the calculation of the European Centre for Medium-Range Weather Forecasts (ECMWF) assimilation system (ECMWF-IFS). The overall conclusion is that the TROPOMI CO data set is well within the mission requirements of 10% precision and 15% accuracy, and so the product was released by ESA for public access via the Copernicus Open Access Hub (<http://www.tropomi.eu/data-products/carbon-monoxide>). The TROPOMI CO data set proves useful to track the transport of air pollution on regional and global scales. The high signal to noise ratio of the measurements additionally allows to monitor pollution hot spots like cities, main traffic roads, and plumes from industrial activities, e.g., steel plants and biomass burning events using data from individual satellite overpasses.

1 Introduction

Carbon monoxide (CO) is an atmospheric trace gas that is mainly emitted to the atmosphere by incomplete combustion processes, e.g., emissions from vehicles, biomass burning, and industrial activity. It is a poisonous reactive gas considered an anthropogenic atmospheric pollutant. CO is removed from the atmosphere by chemical reaction with hydroxyl radicals (OH). Its atmospheric residence time varies between weeks to months [1, 2]. An increase in atmospheric CO concentration would imply a higher loss of OH through chemical reaction. This in turn results in less availability of OH for the depletion of other trace gases such as methane (CH₄). That way CO indirectly affects the atmospheric concentration of an important greenhouse gas and is considered an indirect greenhouse gas because of its important contribution in determining the chemical composition and radiative properties of the atmosphere [3]. Due to its relatively low background concentration, CO is well established as a tracer for air pollution and its transport within the atmosphere (e.g., [4–6]).

The TROPospheric Monitoring Instrument (TROPOMI) is a grating spectrometer that was launched on 13 October 2017 as the single payload on the European Space Agency's Copernicus Sentinel-5 Precursor (S-5P) satellite. One of the primary goals of the mission is to provide total column measurements of the carbon monoxide (CO) with daily global coverage and a high spatial resolution of $7 \times 7 \text{ km}^2$ [7]. The bias (accuracy) requirement for the column-averaged dry air mole fraction of CO is 15%, and the random error (precision) requirement is $<10\%$. Since the 6th of August 2019, the spatial sampling of the CO product at satellite nadir geometry has been improved to $5.5 \times 7 \text{ km}^2$ due to a shorter readout time of the detector. Figure 1 shows the retrieved CO columns of TROPOMI on the 17th of August 2018. Elevated CO values over Canada, Siberia, Africa, and the Amazon are caused by biomass burning, while enhancements, e.g., over China and India, reflect local anthropogenic pollution. The TROPOMI measurements indicate that the pollution from the fires in

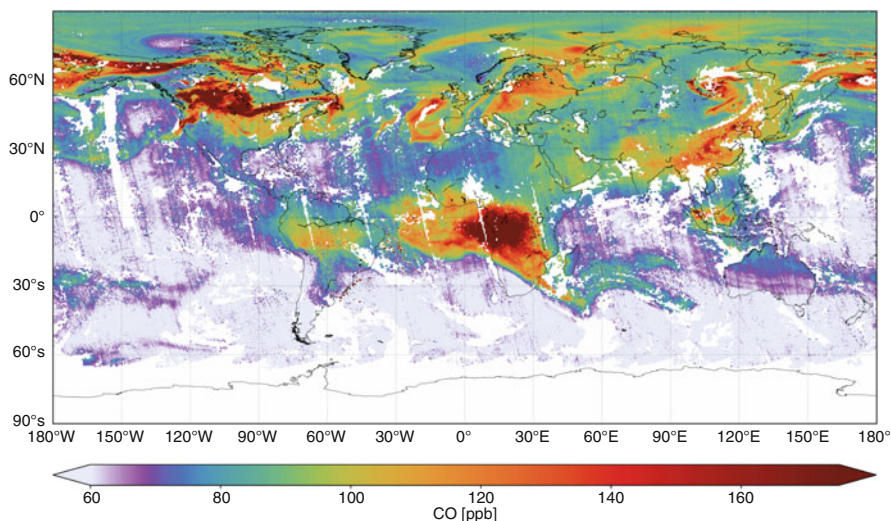


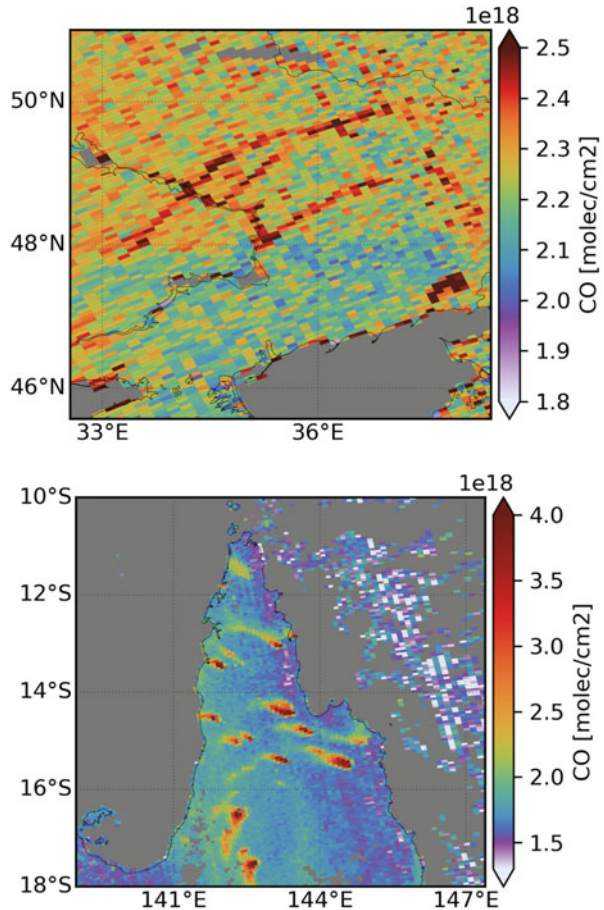
Fig. 1 TROPOMI CO retrievals for the 17th of August 2018. CO total column mixing ratios (ppb) are shown for all orbits of the day

Canada and Siberia is transported and disposed in the whole Northern Hemisphere within only a few days.

The TROPOMI CO is operationally retrieved from the shortwave-infrared channel measurements at $2.3 \mu\text{m}$ deploying the shortwave infrared CO retrieval (SICOR) algorithm developed by SRON. A first validation of the TROPOMI CO data set against reference ground-based measurements, space-based measurements, and intercomparison with model presented at the S-5P first products release workshop (<https://nikal.eventsair.com/QuickEventWebsitePortal/sentinel-5p-first-product-release-workshop/sentinel-5p>) showed that the CO data is compliant with the mission requirements, and therefore it was released for public usage [8–13].

CO retrieval from individual ground pixels observed by TROPOMI contains valuable information allowing to monitor pollution from hotspots like emissions from mid-sized cities, industrial areas, and biomass burning events [8]. For example, Fig. 2 shows well-isolated CO pollution plumes from biomass burning events in the North of Australia and three steel plants in Ukraine. The well-shaped CO enhancements can be used to estimate CO emissions of burning events or industrial activities and by that improve emission inventories or enable pollution monitoring. For example, missing sources in the EDGAR v4.2 emission inventory could be identified by comparing simulations of the Weather Research and Forecasting (WRF) model with TROPOMI CO measurements over Armenia [14]. Furthermore, fitting the simulated CO fields of WRF to TROPOMI observations provided CO emission estimates for cities like Tehran [14]. For Mexico City, it was shown that TROPOMI can even resolve the emission in different suburbs of the city and can sense a weekly cycle in the emissions in agreement with inventories [15].

Fig. 2 CO total column concentration (molec/cm^2) is shown retrieved from the measurements of single orbit overpasses over Ukraine (top panel) on the 29th of April 2020 and the Northern part of Australia on the 8th of December 2019 (lower panel)



2 Retrieval Approach

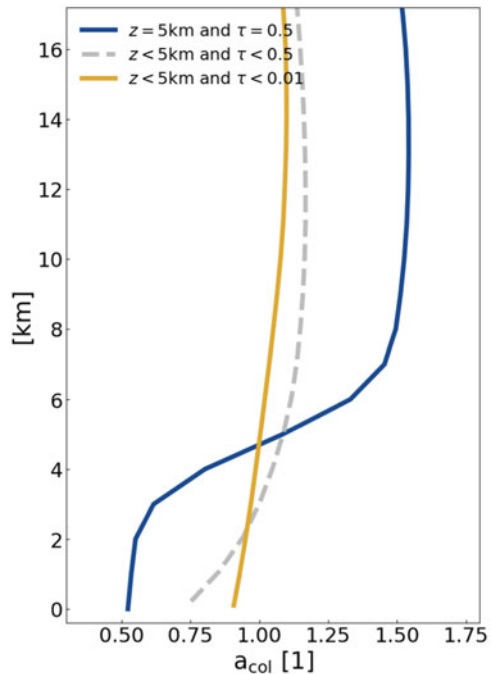
The SICOR algorithm accounts for scattering in the atmosphere by retrieving effective cloud parameters (altitude z , optical thickness τ) together with the total column concentrations of CO and of the interfering gases H₂O (water vapor), HDO (heavy water), and CH₄ (methane). The inversion process of the trace gas columns is built upon the profile scaling approach that scales a vertical reference concentration profile for each trace gas to fit the spectral measurement [16]. Here, the reference profile is taken from a spatiotemporally resolved atmospheric transport simulations of the TM5 model [17]. Currently, the radiative transfer simulation uses the HITRAN 2008 spectroscopic database [18] with updates for water vapor, [19] but in the future, this will be updated to SEOM-IAS (<https://doi.org/10.5281/zenodo>).

1009122; [20]) to further improve the bias with TCCON [14]. Detailed settings of the algorithm like the definition of the retrieval window, the a priori profiles and other auxiliary data are reported by [21]. In addition to the retrieved total CO column and precision, the TROPOMI CO data set provides total column averaging kernels a_{col} that relates the true vertical CO profile ρ_{true} to the retrieved total column concentration c_{ret} following the equation

$$c_{\text{ret}} = a_{\text{col}}\rho_{\text{true}} + \epsilon \quad (1)$$

with the uncertainty ϵ . Figure 3 shows that the CO retrieval under clear-sky conditions (yellow) or clear-sky equivalent (gray) provides a good vertical sensitivity throughout the atmosphere (the total column averaging kernel is near to one for all altitudes). However, under cloudy condition (blue), the CO retrieval sensitivity is reduced below the cloud (values lower than 1), and the total column of CO is retrieved based on the information of the partial column above the cloud (values higher than 1). Hence, clouds in the observation geometry of the satellite are significantly changing the sensitivity of the retrieval which can lead to differences between the retrieved TROPOMI CO columns and reference measurements that can exceed up to 30% [16]. This is a so-called null-space error which can be completely avoided when accounting for the total column averaging kernel when comparing, e.g., with model calculations or air-borne profiles. The validation with TCCON

Fig. 3 Total column averaging kernels of the TROPOMI CO retrieval on the 10th of November 2017. The global average is shown for three different categories of cloudiness strict cloud clearing (yellow), clear-sky equivalent (gray), and high optical thick clouds (blue). Here, z is the cloud altitude and τ the cloud optical thickness retrieved from the SWIR measurements of TROPOMI



stations showed that this error is small for clear-sky and moderate cloudy scenes for unpolluted atmospheric conditions [8]. This corresponds to quality assurance value $QA > 0.5$, which is also provided with the S-5P data product. The CO retrievals from individual orbits of TROPOMI show an artificial striping in the flight direction. The origin of this error is not yet known but is most probably related to a deficient instrument calibration. An approach for an effective posteriori correction of the feature has been developed and will be implemented in the operational processing of ESA in future [14].

3 Validation

Validation is an intrinsic part for the quantification of errors in the satellite data and provides a subsequent measure of the success of a satellite mission. The S-5P Mission Performance Center Validation Data Analysis Facility (MPC-VDAF; <https://mpc-vdaf.tropomi.eu/>) is coordinating the operational validation service for the level-1 and level-2 data products generated by the near real-time and offline processors. The service integrates validation monitoring with the automated validation server (VDAF-AVS; <http://mpc-vdaf-server.tropomi.eu/>), in-depth studies by the S-5P MPC, ad hoc support from the AO projects led by the S-5P Validation Team (S5PVT), and feedback from the Copernicus Atmosphere Monitoring Service (CAMS) at ECMWF. The up-to-date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR; <https://mpc-vdaf.tropomi.eu/>).

The TROPOMI CO data are validated against Fiducial Reference Measurements from the well-established reference ground-based networks of TCCON and NDACC-IRWG [8, 12, 14, 22] and the upcoming complementary Collaborative Carbon Column Observing Network (COCCON) and other low-resolution Fourier transform infrared (FTIR) instruments tested during the ESA funded FRM4GHG campaigns (<https://frm4ghg.aeronomie.be/>) [23, 24]. The latest validation results of about 3 years of TROPOMI CO measurements show a mean bias (systematic error) of $2.36 \pm 3.22\%$ against 28 TCCON stations (without application of empirical scaling factor), $6.44 \pm 3.79\%$ against 20 NDACC stations, and $3.70 \pm 1.58\%$ against 5 COCCON stations with a correlation coefficient above 0.9 for most stations in the three networks. The few exceptions are due to limited data sets available for the validation. The validation results performed with multiple stations covering a wide range of latitudinal bands, atmospheric conditions, and surface conditions are within the mission requirements for bias of 15%. The standard deviation of the relative bias, which is a measure of the precision (random error), is well below the mission requirement for a random error of $<10\%$ for all sites (5.2% for TCCON, 5.6% for NDACC, and 4.4% for COCCON). Since processor version 01.03.02 (starting 3rd of July 2019), the same configuration settings are used for the near real-time and offline data processing streams; therefore, the data products are of the same quality.

Recently, 1.5 years of TROPOMI CO measurements were compared with the CO retrievals of the Measurement of Pollution in the Troposphere (MOPITT) satellite mission achieving a good agreement with a mean bias of $-3.73 \pm 11.51\%$,

$-2.24 \pm 12.38\%$, and $-3.22 \pm 11.13\%$ compared to the MOPITT TIR (thermal infrared), NIR (near infrared), and TIR + NIR (multispectral products). A similar good agreement could be achieved comparing the TROPOMI CO data with airborne measurements of the Atmospheric Tomography mission (ATom) (bias of 3.25% and standard deviation of 11.46%) [25].

The European Center for Medium-Range Weather Forecasts (ECMWF) plans to assimilate TROPOMI CO data with their Integrated Forecasting System (IFS) in the future. A first comparison of TROPOMI CO and the calculation of the ECMWFIFS model showed good agreement (a mean bias of $3.2 \pm 5.5\%$ with a correlation coefficient of 0.97). Furthermore, the TROPOMI CO data reflects the transport of CO polluted air north alongside the Himalaya to China with daily coverage and in good agreement with the ECMWF-IFS model [26].

The validation results of the TROPOMI CO data against reference ground-based FTIR data sets, airborne, and satellite data sets and intercomparison with model calculations show that the TROPOMI systematic and random error fulfils the mission requirements and is of good quality.

4 Data Usage

The TROPOMI CO data are available as the near real-time and offline timeliness data products and can be downloaded from the Copernicus Open Access Hub (<https://scihub.copernicus.eu>). The near real-time data are delivered within 3 h after sensing, and the offline data are available a few days after sensing. The CO retrievals of the offline data are provided as NetCDF files for each orbit, while the near real-time NetCDF files contain chunks of an orbit due to the different timeliness. The essential details for data usage are given in the Algorithm Theoretical Baseline Document (ATBD), Product User Manual (PUM), and the Product Readme File (PRF) that can be downloaded from <http://www.tropomi.eu/data-products/carbon-monoxide>. It is advised to at least filter the data using the quality assurance values provided in the NetCDF files by using QA value >0.5 ; this will filter out faulty retrievals and select retrievals under clear-sky and moderate cloudy conditions. The detailed definition of the QA values is given in the PRF. With the aim to provide the scientific community with a version of the CO retrieval that already includes features planned to be integrated into the official TROPOMI CO data product in the future, a scientific beta version of the TROPOMI CO retrieval is developed and available from <ftp://ftp.sron.nl/open-access-data-2/TROPOMI/tropomi/coi/>.

5 Conclusion

The TROPOMI instrument onboard the Copernicus Sentinel-5 Precursor satellite provides measurements of CO in the atmosphere with daily global coverage and a spatial resolution up to $5.5\sim 7$ km². The measurements are compliant with the mission requirements (accuracy $<15\%$ and precision $<10\%$). The TROPOMI CO

dataset allows to monitor transport of air pollution on regional and global scales as well as hot spots like cities, main traffic roads, and individual plumes from industrial activities. The dataset is publicly available and provided via the Copernicus Open Access Hub. The Sentinel-P Precursor mission is the first of ESA's upcoming Sentinel 5 satellites that together will provide a long-term record of measurements for the coming 30 years.

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