

Ozone Profiles from TROPOMI

Ozone Profile Retrieval from TROPOMI measurements in the UV spectral range

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In Short

- Ozone in the atmosphere is extremely important as it protects humans and environment from the harmful ultraviolet (UV) radiation and is essential for stratospheric dynamics. On the other hand, tropospheric ozone is a harmful pollutant.
- Information on the vertical distribution of ozone in the atmosphere is of great importance because it has varying effects on the atmosphere, humans and environment at different altitudes.
- TROPOMI is a UV-VIS nadir-viewing spectrometer on the satellite S5P launched in 2017.
- The IUP Bremen TOPAS retrieval algorithm determines vertical ozone profiles and a scalar albedo from TROPOMI measurements in the UV spectral range between 270 – 329 nm.
- The quality of our ozone profiles is proven by a validation with stratospheric lidar measurements and ozonesonde profiles.

Ozone in the atmosphere is on the one hand a greenhouse gas and contributes to climate change, and on the other hand in the stratosphere it is an important protection against harmful ultraviolet (UV) radiation. Since the vertical distribution of ozone is not uniform and homogeneous, the study of vertical ozone profiles is of great importance. Although very precise ozone profiles can be measured with in situ measurements and ground-based instruments, these observations are limited in time and spatial resolution. With satellite-based remote sensing it is possible to provide daily and global ozone profiles.

S5P is the latest member of the European family of combined ozone and greenhouse gas monitoring satellites and was launched in 2017 as part of the Copernicus Programme. TROPOMI (TROPOspheric Monitoring Instrument) is a nadir-viewing ultraviolet and visual spectrometer aboard the S5P satellite and was planned to close the gap between the past Envisat and the future Sentinel-5 spacecraft. The instrument provides measurements in the UV (270 – 330 nm), in UVIS (320 – 500 nm), in NIR (675 – 775 nm) and in SWIR (2305 – 2385 nm) [2]. For our ozone profile retrieval the UV1 band from 270 – 300 nm and the UV2 band from 300 – 329 nm is used. The high spatial resolution of TROPOMI is

worth mentioning. One measurement pixel in the middle of the swath covers $28.8 \times 5.6 \text{ km}^2$ (cross- \times along-track) in UV 1 and $3.6 \times 5.6 \text{ km}^2$ in UV2.

As the retrieval of ozone vertical distributions from measurements of back-scattered solar light in the nadir viewing geometry relies on the radiometrically calibrated measurements, the results strongly depend on the quality of the radiometric calibration requiring often an additional (vicarious) calibration correction.

Based on a test data set with measurements from a few weeks in 2018 and 2019, we developed a new IUP Bremen TOPAS (Tikhonov regularized Ozone Profile retrieval with SCIATRAN) algorithm to derive ozone profiles from TROPOMI data and implemented an efficient vicarious calibration correction [1]. In general the TOPAS algorithm comprises 3 steps: First is the radiative transfer model (RTM) calculation with SCIATRAN [3], where a radiance spectrum is simulated using the a priori or previous iteration result information. The second step is a pre-processing to adapt the modelled intensities to effects that can not be handled within the RTM. Finally, in the Tikhonov regularization retrieval step the physical quantities contained in the state vector are determined by iterating a minimized cost function. The resulting state vector consists of the vertical ozone profile between 0 – 60 km and a scalar effective surface albedo

We have validated our ozone profiles by comparing them to collocated globally distributed ozonesonde soundings and to measurements from five stratospheric lidar sites. For the stratosphere we found that the ozone profiles have a vertical resolution of about 9 km and the relative mean difference to the lidar ozone profiles is below $\pm 5\%$ with a standard derivation of 10 – 15%. From the validation with ozonesonde data, similar results were found for the lower stratosphere. In the troposphere, where the vertical resolution decrease, the relative mean difference is about $\pm 10\%$ with a larger standard derivation.

An example for one day (01.10.2018) TROPOMI ozone profile retrieval is given in Fig 1. The profiles are integrated up to sub-columns to adapt them to the vertical resolution. In the surface and tropospheric sub-column (A), large variations of ozone are observed. This reflects the high natural variability in the troposphere due to dynamic processes and local pollution sources. In general the tropical wave one pattern is well reproduced (low ozone in the Pacific, higher ozone in the South Atlantic). In

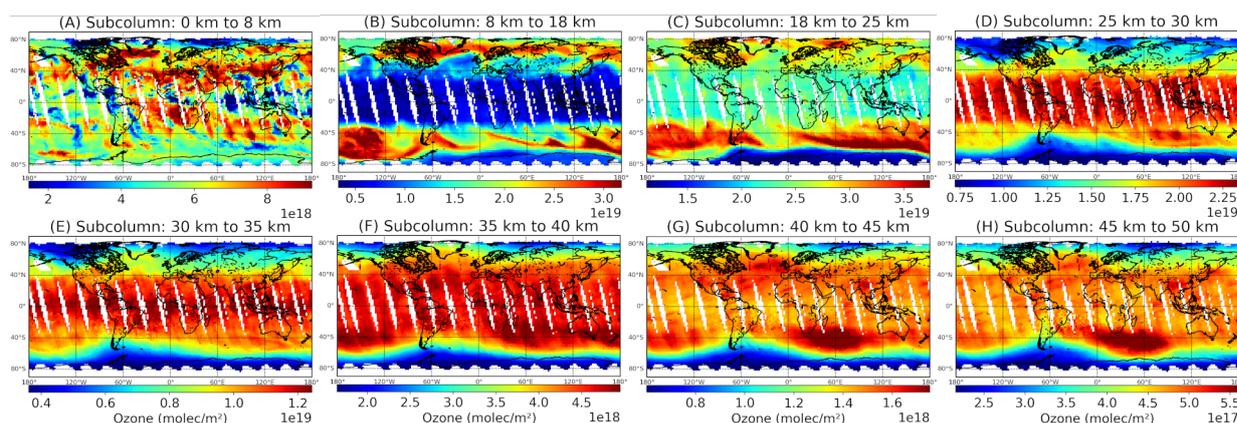


Figure 1: TROPOMI ozone subcolumns from 1 October 2018 derived from integrating ozone profiles in various atmospheric layers between 0 and 50 km. In one day, TROPOMI orbits the Earth 14 times and provides near global coverage. With our TOPAS ozone profile retrieval we can retrieve ozone spatially, temporally, and vertically resolved.

the 8 – 18 km layer, strong latitude gradients and a rather large variability are observed. Most noticeable are large areas with high ozone density at middle and high latitudes, which can be identified as ozone streamers in the lower stratosphere and are related to dynamics in the atmosphere. Between 18 and 25 km, the peak of the ozone number density profile is located and the range of ozone concentration variations is the largest. The largest ozone densities occur in the southern mid-latitudes while the lowest concentrations are seen in the polar vortex. This is a typical situation in the southern hemisphere spring time. The ozone hole seen at polar latitudes is close to its largest extent at this time of the year. From 25-30 km layer upward, the latitude gradient of the ozone number density is reversed with maximum values occurring now in the tropics. At higher latitudes of both hemispheres rather low ozone values are observed.

In the course of this project a subset of the data between July 2021 and December 2022 was processed and validated. The agreement of 5-10% found with the test data from 2018 and 2019 was confirmed by comparing with the data from NASA Aura/MLS instrument measuring the atmospheric emission in the limb viewing geometry. However, a jump in the data related to the change in the calibration of TROPOMI data in June 2022 was noticed, which indicates a need for an adjustment of the used vicarious to process the recent data.

The aim of this project is to provide a validated high quality data set of vertical ozone profiles from TROPOMI measurements. At the end of the project period, TROPOMI data from July 2021 to March 2024 are planned to be available. With these data, more comprehensive comparisons can be made with other ozone profile products and initial evaluations of ozone evolution during this period will be possible.

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<https://www.iup.uni-bremen.de>

More Information

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Funding

University of Bremen, and the federal state Bremen

DFG Subject Area

313-01