

Algorithm Theoretical Basis Document (ATBD) - Tropopause Height Retrieval Along OMPS NASA Orbit Track (v1.0)

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1 Introduction

This document describes the variables contained in the NetCDF4 daily files and their use for the analysis of stratospheric aerosols and tropopause height retrievals. The goal is to provide a tropopause definition suitable for investigations of the aerosol content of the stratosphere, that is which can be used in practice to perform vertical integration of the extinction provided by OMPS-LP to estimate an Aerosol Optical Depth (AOD). The data is derived from OMPS NASA v2.1 and ERA5.

2 Context

The most commonly used definition of the tropopause is the WMO tropopause but it does not correspond to a material separation of the troposphere and the stratosphere. A specific inconvenient is that the subtropics exhibit a double tropopause structure and there is no way to establish a proper continuity between the tropical high tropopause and the extra-tropical low tropopause. Such separation is better provided by quantities which are materially conserved, at least over a short time, and therefore define impermeable surfaces within this approximation.

Several variables meet this criterion. The potential temperature is often used in the stratosphere as a vertical coordinate because the high vertical stability inhibits vertical motion and changes due to heating/cooling are much slower than those induced by horizontal motion on isentropic surfaces. In practice the 380 K is often used as the bottom boundary of the stratospheric overworld. In the tropical region, this surface is also commonly used as the definition of the stratospheric entry gate of the upwelling flow from the troposphere. This surface is usually located above the WMO tropopause and much smoother.

The stratosphere is also characterized by large absolute values of the Ertel potential vorticity (PV) which is an exact material invariant of the inviscid and adiabatic motion. In the GFD literature, the tropopause is often defined as a PV surface. However PV cannot be used in the tropics because the Coriolis parameter vanishes and changes sign at the equator. Ozone is a gas which is mostly found in the stratosphere and it is mostly a passive scalar in the lowest layers of the stratosphere. Therefore the tropopause can also be defined as an ozone surface, except perhaps at very high latitude.

Here we provide a tropopause defined from the 380 K surface in the tropics and the 3.5 PVU PV surface in the extra-tropics (Hoerling et al., 1991). It exploits the good conservation properties of the PV in the ERA5 (Hoffmann et al., 2019).

3 Definition of the Tropopause

The ERA5 is used at a temporal resolution of 3 h and space-filtered on a $1^\circ \times 1^\circ$ grid in latitude and longitude. It was found in previous studies that calculating the tropopause at higher spatial resolution leads to numerous spurious features in regions of deep convection at all latitudes. The full vertical resolution on model levels is used and the PV is calculated directly from the native vorticity and temperature variable. Winds are only involved in corrective terms. The tropopause is calculated on the full grid and then interpolated in time and space to the OMPS-LP orbit.

The basic definition of the tropopause in this product is the altitude of the $\theta = 380$ K surface in the tropics and the PV surface ± 3.5 PVU according to the hemisphere in the extratropics. As the OMPS-LP track is always ascending at low latitudes, the transition is calculated in the northern hemisphere as the last location where the 380 K surface is less than 500 m above the 3.5 PVU surface and at latitude $< 35^\circ\text{N}$. Similarly it is calculated in the southern hemisphere as the first location where the 380 K surface is less than 500 m above the 3.5 PVU surface and at latitude $> 35^\circ\text{S}$.

In most circumstances, the PV tropopause is very close to the WMO tropopause in the extra tropics. As the PV surface is calculated from the top, it happens that tropospheric intrusions in the stratosphere with low PV are wrongly identified as the tropopause. This is tested by comparing the PV tropopause with the WMO tropopause. If the PV tropopause is higher by more than 1.5 km, it is replaced by the WMO tropopause. Another filter removes all single point positive peaks of more than 500 m with respect to both adjacent points in the tropopause replacing its value by the average of the adjacent points.

A remaining problem is the presence of tropopause folds in the extra-tropics corresponding to stratospheric intrusions in the troposphere which are the main return pathway of stratospheric air. As these deformations are mostly irreversible, it is not worth to count this air as stratospheric. They are also often contaminated by clouds. The solution offered in this product is to smooth the tropopause from the above using an osculating parabola using Legendre transform (Legras et al., 2005) with parameter $p = 1000 \text{ second}^2 \text{ km}^{-1}$. This smoothing also slightly shift polarward the large slope of the tropical transition.

The product contains both the unsmoothed and the smoothed versions of the tropopause and contains also the WMO tropopause as a complement.

4 Recommendation for SAOD Calculations

One of the aims of highly accurate tropopause height calculations is to provide a SAOD (Stratospheric AOD) calculation that is as representative as possible of aerosol injection from major stratospheric events (megafires, volcanic eruptions of extreme intensity) whose frequency has increased over the last few years.

With this in mind, we recommend applying some of the quality filters included in the NASA OMPS files to the raw extinction data. One is used to filter OMPS-LP data disturbed by the South Atlantic Anomaly (SAA) of charged particles (Jaross et al., 2014).

We also found that clouds may be present in the dataset at the bottom of the stratosphere, especially at high latitude. Some of these structures are eliminated by OMPS NASA cloud filters, but others persist and bias SAOD results. To minimize the impact of these structures close to the tropopause, we have implemented a detection algorithm based on the extinction. Results take the form of an offset containing the value of the height to add to the tropopause altitude. We calculate an SAOD curve by varying the lower limit kilometer by kilometer from the tropopause, then its first and second derivatives. At each kilometer from the tropopause, if the first derivative exceeds the threshold of 0.12 km^{-1} (close to maximum extinction detection)

or if the second derivative is equal to or greater than the threshold of 0.003 km^{-2} (statistical study), then the offset, initially set to 0, is raised by 1 km (OMPS-LP vertical resolution). Maximum value is 2 km except beyond 70° - where the offset can reach 7 km above the tropopause without exceeding 15 km in altitude, added to the tropopause height. If the algorithm does not fit this criterion in the first kilometer above the tropopause, it restarts from 1 km above the tropopause and if it does not succeed again, the offset is left at 0 except at high latitudes where two more trials are attempted from 2 and 3 km above the tropopause - in the case of any detached structures slightly above the tropopause. There is large differences between considered latitudes due to the scattering angle, data close to the south pole being much more contaminated and producing large offsets.

5 Global Attributes

The following metadata provides information about the dataset:

- **Title:** Tropopause height retrieval along OMPS NASA v2.1 orbit track for considered day (v1.0)
- **Authors:** Clair Duchamp, Bernard Legras
- **Institution:** Laboratoire de Météorologie Dynamique (LMD-IPSL)
- **History:** Generated from OMPS NASA v2.1 and ERA5 data
- **Date:** Date of the considered day
- **Creation:** March, 2025
- **Version:** 1.0
- **Generator:** `combinatExt_netCDF4_NASA.ipynb`

6 Dataset Dimensions

The dataset contains the following dimensions:

- **time (varying number of values):** Represents different measurement times along the satellite orbit. Expressed in seconds from the beginning of the day (UT).
- **altitude (41 values):** Represents different altitude levels from the ground. Expressed in kilometers (km).

7 Variable Overview

The dataset consists of the following variables:

Name	Long Name	Units	Dimensions
time	Time	second	time
altitude	Altitude	km	altitude
extinction_no_filt	Raw retrieved extinction coefficient at 869 nm	km ⁻¹	time, altitude
extinction_filt	Filtered retrieved extinction coefficient at 869 nm (recommended for SAOD calculations)	km ⁻¹	time, altitude
km_above_tropopause	Kilometers above tropopause (for SAOD calculations)	km	time
SAOD	Stratospheric Aerosol Optical Depth (SAOD)		time
latitude	Latitude	°N	time
longitude	Longitude	°E	time
orbit	Orbit number		time
event	Event number		time
tropopause_height_zT	Tropopause height with zT method from ERA5	km	time
tropopause_height_zT_smoothed	Smoothed tropopause height with zT method from ERA5	km	time
tropopause_height_wmo	Tropopause height with WMO method from ERA5	km	time
SAA	South Atlantic Anomaly (SAA)		time
cloud_type	Cloud type		time
cloud_height	Cloud height	km	time
retrieval_flag	Retrieval flag		time
T_curtain	Temperature curtain	K	time, altitude
PT_curtain	Potential Temperature curtain	K	time, altitude
PV_curtain	Potential Vorticity curtain	PVU	time, altitude
O3_curtain	Ozone mixing ratio curtain	kg.kg ⁻¹	time, altitude

8 Variable Descriptions

The following descriptions provide additional details about each variable:

- **time**: Seconds from the beginning of the day (UT).
- **altitude**: Altitude from the ground.
- **extinction_no_filt**: Raw retrieved aerosol extinction coefficient at 869 nm, center slit.
- **extinction_filt**: Filtered retrieved extinction coefficient at 869 nm, center slit. Filters used are: SAA, cloud_type, cloud_height, retrieval_flag.
- **km_above_tropopause**: Offset containing the value of the height to add to the tropopause altitude because of the presence of residual clouds at the bottom of the stratosphere determined from a

sensitivity analysis of the SAOD. We calculate an SAOD curve by varying the lower limit kilometer by kilometer from the tropopause, then its first and second derivatives. At each kilometer from the tropopause, if the first derivative exceeds the threshold of 0.12 km^{-1} (close to maximum extinction detection) or if the second derivative is equal to or greater than the threshold of 0.003 km^{-2} (statistical study), then the offset, initially set to 0, is raised by 1 km (OMPS-LP vertical resolution). Maximum value is 2 km except beyond 70° - where the offset can reach 7 km above the tropopause without exceeding 15 km altitude, added to the tropopause height. If the algorithm does not fit this criterion in the first kilometer above the tropopause, it restarts from 1 km above the tropopause and if it does not succeed again, the offset is left at 0 except at high latitudes where two more trials are attempted from 2 and 3 km above the tropopause - in the case of any detached structures slightly above the tropopause. The value is masked when the entire corresponding extinction profile from `extinction_filt` is filtered.

- SAOD: Integration of `extinction_filt` over altitude from `tropopause_height_zT_smoothed + km_above_tropopause` to 30 km.

- `latitude`: Latitude.

- `longitude`: Longitude.

- `orbit`: ID number of the orbit to which this measurement belongs.

- `event`: Sequential number of measurement within an orbit.

- `tropopause_height_zT`: Combination of the 380 K surface and the ± 3.5 PVU surface in the extratropics. The boundaries of the tropical region on each orbit are defined as the first location where the 380 K and the -3.5 PVU surfaces are closer than 500 m at latitude $> 35^\circ\text{S}$ from the south and the last location where the 380 K and the 3.5 PVU surface are closer than 500 m at latitude $< 35^\circ\text{N}$ in the north.

- `tropopause_height_zT_smoothed`: Smoothed version of `tropopause_height_zT`. Tropopause folds are smoothed by using an osculating parabola from the above using Legendre transform (Legras et al., 2005) with $p = 1000 \text{ second}^2 \text{ km}^{-1}$.

- `tropopause_height_wmo`: Tropopause height according to the WMO highest definition.

- `SAA`: 0 = estimated SAA effects at satellite location are $< 5\%$ of nominal maximum value, based on OMPS-LP climatology. 1 = estimated SAA effects are 5-40% of nominal maximum value. 2 = estimated SAA effects are 40-75% of nominal maximum value. 3 = estimated SAA effects are $> 75\%$ of nominal maximum value. For SAOD calculations, the user is recommended to filter non-zero values with `SAA` ≥ 1 .

- `cloud_type`: Cloud type flag: 0 = no cloud. 1 = cloud. 2 = enhanced aerosol. 3 = PSC. For SAOD calculations, the user is recommended to filter clouds (1) until cloud top height (`cloud_height`) and PSCs (3) for the whole profile.

- `cloud_height`: Observed cloud height for each event.

- `retrieval_flag`: Retrieval processing status flag; non-zero value = failure. For SAOD calculations, the user is recommended to filter data with `retrieval_flag` $\neq 0$.

- `T_curtain`: Temperature curtain along the satellite central track from ERA5 interpolated to OMPS NASA altitudes.

- `PT_curtain`: Potential Temperature curtain along the satellite central track from ERA5 interpolated to OMPS NASA altitudes.

- `PV_curtain`: Potential Vorticity curtain along the satellite central track from ERA5 interpolated to OMPS NASA altitudes.

- `03_curtain`: O₃ curtain along the satellite central track from ERA5 interpolated to OMPS NASA altitudes.

9 Data Usage

The dataset is intended for the study of stratospheric aerosols using tropopause height retrievals. Users are advised to apply appropriate filters based on quality flags and cloud conditions for SAOD calculations, the filtered extinction coefficient (`extinction_filt`) is recommended. Variables from these files can be applied to the other OMPS-LP products available by interpolating the data to the respective grids of each product (usually a few tenths of a degree difference). The complete dataset covers the period from February 7, 2012 (start of OMPS NASA data) to December 31, 2024. All dates are covered except where there are no corresponding OMPS NASA files.

References

- Hoerling, M. P., Schaack, T. K., & Lenzen, A. J. (1991). Global Objective Tropopause Analysis. *Monthly Weather Review*, 119(8), 1816–1831. [https://doi.org/10.1175/1520-0493\(1991\)119\(1816:GOTA\)2.0.CO;2](https://doi.org/10.1175/1520-0493(1991)119(1816:GOTA)2.0.CO;2)
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- Legras, B., Pissot, I., Berthet, G., & Lefèvre, F. (2005). Variability of the Lagrangian turbulent diffusion in the lower stratosphere. *Atmospheric Chemistry and Physics*, 5(6), 1605–1622. <https://doi.org/10.5194/acp-5-1605-2005>