Algorithm Theoretical Basis Document (ATBD) - Tropopause Height Retrieval Along OMPS NASA Orbit Track (v2.0)

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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 three OMPS-LP products to estimate an Aerosol Optical Depth (AOD). The data is derived from OMPS NASA v2.5, OMPS USASK v2.1, OMPS IUP v2.1 and ERA5 data.

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 extratropical 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 a composite from the 3.5 PVU PV surface in the extratropics (Hoerling et al., 1991), the WMO tropopause and the ozone tropopause. 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 an then interpolated in time and space to the OMPS-LP orbit.

We use several definitions of the tropopause in this product to temperate the spurious effects which are associated with each definition.

In the tropic we use the altitude of the $\theta = 380$ K surface which is usually easily determined as the potential temperature varies monotonically with altitude in the tropopause range. In practice, the last model level counted from the top where $\theta > 380$ K is determined and the proper level is determined by interpolation between this level and the next one below. The WMO tropopause determination follows the WMO definition (World Meteorological Organization, 1957).

The PV tropopause is determined as the PV = ± 3.5 PVU surface (Hoerling et al., 1991). First the highest level where the PV is less that the threshold and this is also true for the 7 levels below is identified on each column. This is intended to avoid the patches of low PV detached from the tropical troposphere which often float in the subtropical lower stratosphere. The depth of 7 levels corresponds approximately to 2000 m at tropopause level. The proper level is then determined from interpolation with the next model level above.

The ozone tropopause is determined according to Bethan et al. (1996) as the last level counted from above where the ozone mixing ratio is larger than 80 ppbv with the levels above larger than 110 ppbv and a vertical gradient larger then 60 ppbv/km. No vertical interpolation is performed and hence this estimate is discretized by the model levels.

The altitude used in these estimates is a geopotential calculated by integrating the dry hydrostatic equation using the ERA5 temperature profile and the archived geopotential at 62 hPa which is the lowest pure pressure model level in the ERA5. We refrained from integrating starting from the surface because of the effect of moisture on density (which can be neglected in the lower stratosphere) and because the archived surface geopotential at the same resolution as air parameters contains noise that generates spurious upper air oscillations.

In most circumstances, the WMO, PV and ozone tropopause are very close. We define two composite products in the extratropics. The first one, labeled as $z\mathrm{T}$, is based on the PV tropopause and uses only the WMO tropopause when the PV tropopause is above this latter by more than 1.5 km. The second product, labeled as $z\mathrm{T}_2$, is determined from a majority rule as the average between the two closest products among the PV, ozone and WMO tropopause, the third one being discarded. A further filter is applied to both $z\mathrm{T}$ and $z\mathrm{T}_2$ by replacing any isolated peak of more than 500 m on a single pixel by the average of its two adjacent pixels.

The transition between the tropics and the extratropics on each orbit is defined as follows for both products. 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 $z\mathrm{T}$ or $z\mathrm{T}_2$ level and at latitude $< 35^\circ$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 $z\mathrm{T}$ or $z\mathrm{T}_2$ level and at latitude $> 35^\circ$S. The criterion $\max(z\mathrm{T}, z\mathrm{T}_2)$ shows the best performance and is recommended for SAOD calculations.

A remaining problem is the presence of tropopause folds in the extratropics 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 $p = 1000$ second^2 km^{-1}. This smoothing also slightly shifts 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 raw 380K, WMO, PV and ozone tropopause as a complement for the benefit of users who would like to derive his own criterion.

4 Recommandation 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. This work is conducted in the context of a comparison of the three OMPS-LP products: NASA v2.5 (Taha et al., 2025), USASK v2.1 (Bourassa et al., 2023) and IUP v2.1 (Rozanov et al., 2024).

We begin by explaining how the OMPS data is processed to ensure a robust comparison of the SAOD between the three products. First, we linearly interpolate the USASK and UB extinction data onto the NASA grid, and then apply the following filters to the extinction data, which we harmonize across each dataset to ensure a robust comparison :

- NASA: normal and polar stratospheric clouds, extinction coefficients > 0.1 km^{-1}, retrieval residuals $> 50\%$ (Duchamp et al., 2026; Taha et al., 2025)
- USASK: first and last 5 profiles from each orbit
- IUP: levels for which all standard deviations of the extinction coefficient are 0 for a given orbit, extinction coefficients > 0.1 km^{-1} (Rozanov et al., 2024)

Then, 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 filters mentioned above, 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 derivatives. At each kilometer from the tropopause, if the second derivative is equal to or greater than the threshold of 0.0097 km^{-2} (99.7 percentile calculated from OMPS NASA), then the offset, initially set to 0, is raised by 1 km (OMPS-LP vertical resolution). Maximum value is 2 km except beyond 70°S - 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 southern 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. This algorithm is performed for each product, and the maximum value obtained — added to the selected and smoothed tropopause height — is retained as the lower limit for the SAOD calculation for all products (the upper limit is set at 30 km). Finally, it should be noted that the SAOD calculation by profile is performed only if fewer than 50% of the pixels are filtered out in the corresponding altitude range.

5 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).
- **altitude_red (34 values):** Reduced grid of **altitude**. Expressed in kilometers (km).

6 Variable Overview

The dataset consists of the following variables:

Name	Long Name	Units	Dimensions
`time`	Time	second	time
`altitude`	Altitude (OMPS NASA, ERA5)	km	altitude
`altitude_USASK`	Altitude USASK	km	altitude_red
`altitude_IUP`	Altitude IUP	km	altitude_red
`extinction_filt_NASA`	Filtered NASA extinction coefficient at 869 nm	km^{-1}	time, altitude
`extinction_filt_USASK`	Filtered USASK extinction coefficient at 869 nm	km^{-1}	time, altitude_red
`extinction_filt_IUP`	Filtered IUP extinction coefficient at 869 nm	km^{-1}	time, altitude_red
`km_above_tropopause`	Kilometers above tropopause (for SAOD calculations)	km	time
`SAOD_NASA`	NASA SAOD at 869 nm		time
`SAOD_USASK`	USASK SAOD at 869 nm		time
`SAOD_IUP`	IUP SAOD at 869 nm		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_zT2`	Tropopause height with $z\mathrm{T}_2$ method from ERA5	km	time
`tropopause_height_zT_max`	Tropopause height using max between zT and $z\mathrm{T}_2$ methods ($z\mathrm{T}_{max}$)	km	time
`tropopause_height_zT_max_smoothed`	Smoothed $z\mathrm{T}_{max}$ tropopause height (recommended for SAOD calculations)	km	time
`tropopause_height_wmo`	Tropopause height with WMO method from ERA5	km	time
`tropopause_height_380K`	Tropopause height with 380K method from ERA5	km	time
`tropopause_height_PV`	Tropopause height with PV method from ERA5	km	time
`tropopause_height_O3`	Tropopause height with O_3 method from ERA5	km	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

7 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.

- `altitude_USASK`: USASK altitude grid.

- `altitude_IUP`: IUP altitude grid.

- `extinction_filt_NASA`: Filtered retrieved NASA extinction coefficient at 869 nm, center slit. NASA filtering procedure is used.

- `extinction_filt_USASK`: Filtered retrieved and interpolated USASK extinction coefficient at 869 nm. Data are interpolated on NASA horizontal grid and NASA filtering procedure is used.

- `extinction_filt_IUP`: Filtered retrieved and interpolated IUP extinction coefficient at 869 nm. Data are interpolated on NASA horizontal grid and NASA filtering procedure is used.

- `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 derivatives. At each kilometer from the tropopause, if the second derivative is equal to or greater than the threshold of 0.0097 km^{-2} (99.7 percentile calculated from OMPS NASA), then the offset, initially set to 0, is raised by 1 km (OMPS-LP vertical resolution). Maximum value is 2 km except beyond 70°S - 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 southern 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 is filtered.

- `SAOD_NASA`: Integration of `extinction_filt_NASA` over altitude from `tropopause_height_zT_max_smoothed` + `km_above_tropopause` to 30 km. The value is masked when at least 50% of the `extinction_filt_NASA` values in the selected interval are masked.

- `SAOD_USASK`: Integration of `extinction_filt_USASK` over altitude from `tropopause_height_zT_max_smoothed` + `km_above_tropopause` to 30 km. The value is masked when at least 50% of the `extinction_filt_USASK` values in the selected interval are masked.

- `SAOD_IUP`: Integration of `extinction_filt_IUP` over altitude from `tropopause_height_zT_max_smoothed` + `km_above_tropopause` to 30 km. The value is masked when at least 50% of the `extinction_filt_IUP` values in the selected interval are masked.

- `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 in the tropics and the ±3.5 PVU surface in the extratropics. The boundaries of the tropical region on each orbit are defined as the first location counted from the south where the 380 K and the -3.5 PVU surfaces are closer than 500 m at latitude > 35°S and the last location where the 380 K and the 3.5 PVU surface are closer than 500 m at latitude < 35°N in the north.

- tropopause_height_zT2: The $z\mathrm{T}_2$ estimator is calculated as $z\mathrm{T}$ in the tropical region, that is using the 380 K surface. Outside the tropical region it is computed as the mean of the two closest values among WMO, PV and O_3 tropopause, discarding the third.

- tropopause_height_zT_max: $z\mathrm{T}_{max}$ tropopause height is determined by taking the maximum value between the $z\mathrm{T}$ and $z\mathrm{T}_2$ estimation methods.

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

- tropopause_height_wmo: Raw tropopause height according to the WMO highest definition (World Meteorological Organization, 1957).

- tropopause_height_380K: Raw tropopause height according to the 380K method.

- tropopause_height_PV: Raw tropopause height according to the PV method (Hoerling et al., 1991).

- tropopause_height_O3: Raw tropopause height according to the O3 method (Bethan et al., 1996).

- 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.

- O3_curtain: O_3 curtain along the satellite central track from ERA5 interpolated to OMPS NASA altitudes.

8 Data Usage

The dataset is intended for the study of stratospheric aerosols using tropopause height retrievals and for the comparison of the OMPS-LP products using the stratospheric AOD quantity. This dataset contains the results from all the methods used for the final tropopause height calculation, as well as the filtered extinction profiles and the resulting SAOD values for each OMPS-LP product, enabling the reproduction of a rapid and robust comparison. Meteorological data from ERA5 (T, θ, PV, and O_3 mixing ratio) are also provided along the satellite track to support further investigations of stratospheric phenomena. The complete dataset covers the period from February 7, 2012 (start of OMPS data) to December 31, 2025. Extinction data (and thus SAOD data) before 2014 should be used with caution, because instrument settings were in the process of being tweaked and finalized, which may impact their quality. All dates are available except when one of the OMPS-LP or ERA5 files is missing.

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