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Discussing the effect of sampling error on the estimation of ozone variability and trend in UT/LS

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Summary. — One of the main focuses of the investigation of climate change is the ozone layer in the upper troposphere/lower stratosphere (UT/LS) and its relationship to temperature. Multiple studies have calculated trends at the regional and global scale in the UT/LS, using a variety of measurement methods including data from satellites and the ground. Nonetheless, the predicted trends could be greatly impacted by the coverage and quality of the measurements over time and space. Using a dataset that combines the ozonesoundings provided by SHADOZ, NDACC, and WOUDC, this work examines the effects of sampling error in the Northern Hemisphere mid-latitudes (NH, 30°N-60°N), and for different vertical layers in the UT/LS on the estimation of the ozone inter-annual variability and trends in the periods pre-2000 (1978–1999) and post-2000 (2000–2022). The vertical ozone concentration profiles are grouped into three categories, according to the temporal gaps of the historical time series, and assessed in terms of their usage for climate studies.

1. – Introduction

Studying temperature, water vapour, and ozone trends is essential to understanding climatic variability and change. Sea surface temperature (SST) variations and other external factors, such as greenhouse gases (GHGs) and ozone-depleting substances (ODS), are linked to temperature variations in the UT/LS [1]. Numerous investigations have been carried out to assess the patterns for distinct climate variables on both the global and regional scales. Furthermore, using data from the Global Positioning System Radio Occultation (GNSS-RO) and simulations using the Whole Atmosphere Community Climate Model (WACCM) of the National Centre for Atmospheric Research, it was discovered that there was an increase in tropopause temperature between 2001 and 2011 that was linked to a weaker tropopause inversion layer because of the weakened upwelling in the Tropics. Such modifications to the UT/LS's thermal structure may have important implications for climate, such as a possible rise in water vapour in the lower stratosphere [2]. More recently, balloon-borne radiation measurements proved that the stratosphere is warming after years of cooling [3]. It is unclear if a slowing or shift in the temperature sign in the UT/LS will last in the long run. This study estimates ozone trends using balloon-borne measurements from three existing datasets: the Southern Hemisphere Additional Zonesondes (SHADOZ, `https://tropo.gsfc.nasa.gov/shadoz/`), the Network for the Detection of Atmospheric Composition Change (NDACC, `https://www.ndaccdemo.org/`) and the World Ozone and Ultraviolet Radiation Data Centre (WOUDC, `https://woudc.org/`). These networks were developed, respectively, by NASA, NOAA, with the assistance of numerous institutions, and WMO. These datasets are combined to improve sampling and provide enhanced data coverage across different latitudes to estimate ozone concentration anomalies and trends.

The paper is organised as follows: sect. **2** describes the dataset used for the study; sect. **3** outlines the description of the regression methods used to estimate trends and shows the results of the analysis; sect. **4** presents the conclusions.

2. – Unified ozonesonde dataset

In this work, the dataset used was built from the merging of three existing ozonesounding datasets, provided by SHADOZ, NDACC, and WOUDC, for the period 1978–2022.

The SHADOZ network provides ozone profiles, as well as pressure, temperature and relative humidity profiles, measured at 17 sites since 1998. The SHADOZ network was designed to reduce data heterogeneity in ozone probe profiles between different measurement sites in tropical and subtropical areas, and the network data have recently been reprocessed to homogenize the database further. In the unified dataset, SHADOZ V6.0 for measurements and SHADOZ V1.0 for uncertainty were considered, also providing uncertainties for 14 of the 17 sites, with the former all having operated for more than a decade. SHADOZ is the only one of the three datasets to provide a detailed estimate of observational uncertainty for each data record [4].

The NDACC network, composed of more than 90 globally distributed, ground-based, remote-sensing research stations with more than 160 currently active instruments, provides ozone vertical profile and column data products from different measurement techniques but, for this study, only ozonesounding profile data were processed, which were provided by only 33 stations [5]. NDACC does not routinely provide uncertainties for the ozonesoundings measurements, but only for a subset of measurements an estimation of the total uncertainties is provided but not with the same level of detail as SHADOZ.

The WOUDC network, with over 150 stations, is the most comprehensive initiative for collecting ozonesounding measurements which, although quality controlled for their consistency in data and metadata are less characterized in terms of traceability and uncertainties, are not provided such as by SHADOZ and NDACC [6].

2˙1. *Handling of the duplicated profiles and station classification.* – The primary challenge in consolidating the data from the three datasets into a single database was handling duplicate profiles, which arose from the existence of two or more profiles for the same station and day that belonged to separate datasets. To address this issue, profiles were chosen according to their quality, coverage, and measurement uncertainty characterisation using the selection criteria listed below:

- In case of a single profile for a day (no duplicates), this profile will be saved in the database.

- In case of duplicates, the profile selection is driven by the dataset maturity and by the availability of measurement uncertainties (provided mainly by SHADOZ and for some locations also by NDACC, WOUDC, on the other hand, does not provide uncertainty estimates) on the ozone concentration profiles.

- Discarded profiles are eventually used to densify the vertical sampling if they provide measurements at different pressure levels not available in the selected profiles.

Depending on their activity and the number of ozone soundings they provide each month, the 155 Stations have different amounts and quality of data. Studying data coverage is critical for a more accurate analysis of anomalies and trends to calculate estimates with plausible uncertainties. For this reason, constraints were defined to identify the highest-quality stations on which to carry out the analysis. As a result, the stations of the unified dataset were grouped according to their monthly coverage. This was done by determining that a month was covered if there was at least one ozone profile in that month. Three separate clusters were created out of the available stations:

1) Long coverage (LC): 26 stations (with a data time series of at least 20 years).

2) Medium coverage (MC): 23 stations (with a data time series between 10 and 20 years).

3) Short coverage (SC): 106 stations (with data time series less than 10 years).

The first two clusters are the only ones capable of providing sufficient data coverage (at least one decade) for estimating anomalies and trends. Furthermore, a third cluster (Long and Medium coverage cluster, LMC), obtained from the combination of LC and MC, was considered to compare the relative effect of data completeness *versus* spatial data coverage. Figure 1 displays the 49 stations that are categorised as LC or MC, and on which the following analysis is performed.

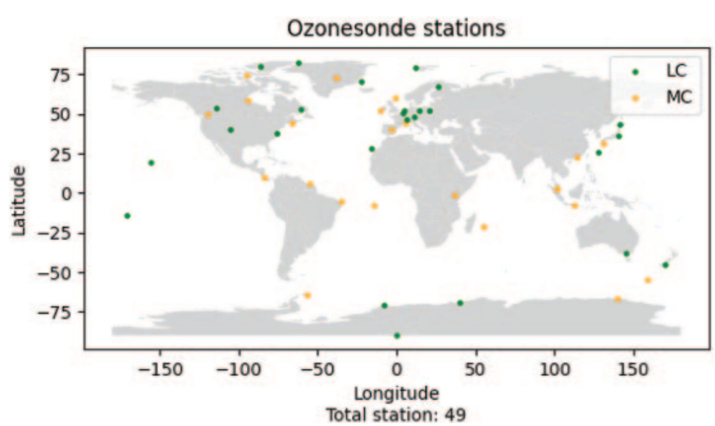

Fig. 1. – Map of global ozonesounding stations, for long coverage (LC, stations with a data time series of at least 20 years) and medium coverage (MC, stations with a data time series between 10 and 20 years) clusters, available in the unified database.

3. – Methodology and results

3˙1. *Regression methods*. – To estimate the average monthly anomalies, Theil-Sen regression (TS) was used which involves the calculation of the slopes between every possible pair of points in the time series, taking the median value as an estimate of the trend. It can be significantly more accurate than simple linear regression for skewed and heteroscedastic data and shows similar performance to non-robust least squares even for normally distributed data in terms of statistical power [7-10]. This method is very similar to classic least squares [11]. To statistically evaluate whether there is a significant trend of the variable of interest over time, the Mann-Kendal (MK) test is also used [12, 13].

3˙2. *Calculating trends*. – The average monthly anomalies from the LC and LMC cluster for the Northern Hemisphere mid-latitudes (NH, 30° N-60° N) at three vertical ranges (200–100 hPa, 100–50 hPa, and 50–1 hPa) were used to calculate the ozone decadal trends. The linear regression methods previously described have been applied. The following formula is used to compute percentage monthly anomalies using data from all stations for each vertical range:

$$anomaly_{\%m_{x_{1978-2022}}} = \frac{m_{x(y)} - mean(m_{x_{1978-2022}})}{mean(m_{x_{1978-2022}})} \cdot 100, \qquad (1a)$$

where $m_{x(y)}$ is the average of the ozone values of month x of the year y, $mean(m_{x_{1978-2022}})$ is the average of the ozone values for month x calculated from the average of the same month for all years of the time series (from 1978 to 2022).

3˙3. *Cluster comparing*. – To assess the effect of spatial sampling error on the trend estimate and, consequently, on our understanding of the variability of ozone across time, we compare the LC and LMC clusters. The estimates of the ozone concentration trends were computed, and the MK test was used to determine whether the estimated trends were significant to assess the benefits of using LMC over the LC cluster. The MK test results for the two distinct periods, pre-2000 (1978–1999) and post-2000 (2022–2022), are displayed in table I. The values for each cluster are included, expressed as a percentage per decade (%/dec).

Given that trends are significant across all of the vertical ranges, it is reasonable to compare the clusters. The trend differences for the vertical ranges of 50–1 hPa and 100–50 hPa are less than 1.4% when the pre-2000 era is taken into consideration, while the

TABLE I. – *Percentage per decade (%/dec) of the trend estimates obtained with the Theil-Sen (TS) regressors for the Northern Hemisphere mid-latitudes sector at the three vertical ranges for pre-2000 and post-2000 periods. Legend: Positive value (increasing trend); Negative value (decreasing trend); NT (No Trend).*

Cluster	Period	50-1 hPa	100-50 hPa	200-100 hPa
LC	pre-2000	–6.45	–8.23	–9.42
	post-2000	–0.71	4.45	10.37
LMC	pre-2000	–5.09	–9.09	–11.54
	post-2000	–0.77	3.2	5.21

difference for the range of 200–100 hPa almost exceeds 2% because there is less data available for this range. For post-2000, the differences for the 50–1 hPa and 100–50 hPa ranges are less than 0.1% and 1.2%, respectively. Whereas, the difference for the 200–100 hPa range exceeds 5% for the same reason as for the pre-2000 era. Sampling error is the major cause of trend variations between the clusters. Small differences between LC and LMC indicate consistency across clusters, which allows for trend characterization using fewer stations in the NH. Additionally, at all vertical ranges, the estimations for the LC cluster (table I) for the pre-2000 and post-2000 periods demonstrate agreement with the trends shown in [14] and [15]. Figure 2 shows the trend estimation for the LC cluster for the pre-2000 and post-2000 periods (left and right panels, respectively).

4. – Conclusion

The primary goal of this work is to create a new unified ozonesounding dataset by combining the profiles supplied by SHADOZ [4], NDACC [5] and WOUDC [6]. Specifically, this work aims to estimate the ozone trends in the UT/LS for the Northern Hemisphere mid-latitudes sector. The study will examine the impact of sampling frequency. Only profiles that exhibit adequate plausibility, coherency, and consistency of the ozone partial pressure data have been chosen for this study. The stations in the unified ozonesounding dataset are first divided into two clusters —a Long Coverage cluster (LC) and a Medium Coverage cluster (MC)— based on the evaluation of temporal coverage and completeness to examine ozone trends. A combination of the Long and Medium Coverage clusters (LMC) has been contemplated as a third cluster. This comparison is made using the trends estimated for the various clusters. The trend estimates were carried out using the Theil-Sen linear regression method [7-10]. The significance of the trends was verified using the Mann-Kendall test [12, 13]. The comparison revealed that the LC cluster offers significant trends that are often close to those of LMC, suggesting that trend characterization with fewer stations in the NH may be achieved while maintaining high observation quality in the entire UT/LS region.

The future work will be extended to analyse synergically the trends of ozone in the UT/LS. Trends from in situ soundings will be also compared with satellite and reanalysis

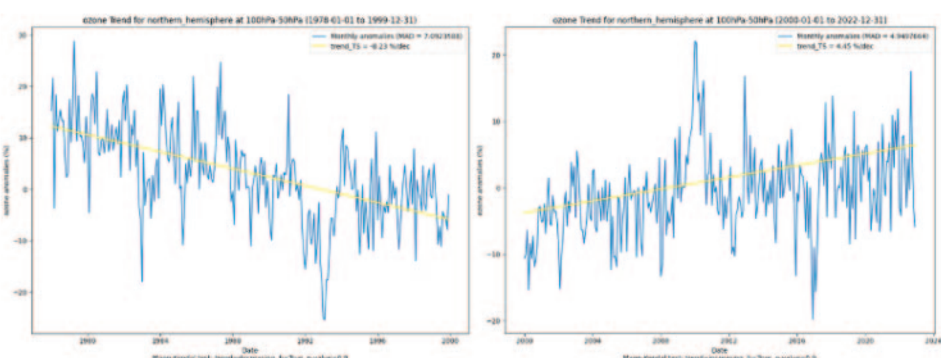

Fig. 2. – Trends estimations for the NH latitudinal sector at 100–50 hPa vertical range for the pre-2000 (left panel) and post-2000 (right panel) periods, estimated with Theil-Sen regression (TS). The resulting percentage per decade (%/dec) for TS and the MAD calculated on the average anomalies are shown in the figure legend. Finally, at the bottom centre is the result of the MK test.

data. A key issue to investigate before further comparisons with other datasets will be to assess the effect of inhomogeneities due to changes over time in the measurement sensors and algorithms, which can influence the trend estimates. Moreover, the effect of serial measurement correlation will be added to the trend estimates, comparing the existing solution provided in the literature.

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