A Global Climatology of Tropopause Folds in CAMS and MERRA-2 Reanalyses

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Abstract Tropopause folds are the main mechanism underlying stratosphere-to-troposphere transport and influence tropospheric composition and weather systems by triggering convection. Here, we present the global climatology of tropopause folds in Copernicus Atmosphere Monitoring Service (CAMS) and Modern-Era Retrospective analysis for Research and Applications, version 2 (MERRA-2) reanalyses for the period from 2003 to 2018. We applied a 3-D labeling algorithm in CAMS and MERRA-2 reanalysis data to detect tropopause folding events. In constructing their climatologies, we show that the bulk of the folds are vertically shallow and are mainly found at the subtropical zones in the vicinity of the jet streams, while deeper folds also occur over the storm tracks, consistent with previous studies. The spatiotemporal characteristics of fold climatology are captured in a similar manner in CAMS and MERRA-2, with MERRA-2 capturing slightly higher frequencies during all seasons. In quantitative terms, there is a good agreement between CAMS and MERRA-2 fold frequencies with spatiotemporal $R^2$ values of $\sim 0.9$ for DJF, MAM, and JJA, and 0.75 for SON. The two reanalysis products are in close agreement regarding the intra- and interannual variability in fold frequency, with temporal correlation scores higher than 0.7 over the subtropical bands where the majority of folds are found. The agreement between the two reanalyses is lower in the Southern Hemisphere compared to the Northern Hemisphere. Thus, the global climatology of tropopause folds in both CAMS and MERRA-2 reanalyses are similar to those of previous studies.

1. Introduction

Tropopause folds are considered to be the key processes underlying stratosphere-to-troposphere transport (STT) events (Stohl et al., 2003) and have been described to influence tropospheric composition (RoeLOFS & Lelieveld, 1997) and occasionally local air quality (Akritidis et al., 2010; Langford et al., 2009; Lin et al., 2012, 2015). Through dynamic coupling with lower tropospheric levels, tropopause folds also influence weather, and they are linked with rapid cyclogenesis (Uccellini, 1990) and convective storms (Antonescu et al., 2013). A tropopause fold emerges as a portion of the lowermost stratosphere that is being transported downward into the troposphere (Cooper et al., 2002, 2004; Holton et al., 1995; Knowland, Ott, et al., 2017; Stohl et al., 2003). In this way, dry stratospheric air penetrates the troposphere, a process known as stratospheric intrusion (Danielsen & Mohnen, 1977). Therefore, tropopause folds are regions characterized by high potential vorticity (PV) values, high ozone concentrations, low water vapor mixing ratio, and high static stability compared to typical tropospheric values. Tropopause folds are usually shallow in the vertical extent, with their spatiotemporal distribution mainly governed by the location, intensity, and seasonality of the jet streams (Stohl et al., 2003). With respect to their climatological characteristics, during boreal winter the frequency of tropopause folding events in the Northern Hemisphere (NH) exhibits a maximum in the subtropics (Škerlak et al., 2015; Sprenger et al., 2003), while deep folds are observed further north over the North Atlantic storm track (Elbern et al., 1998; Sprenger et al., 2003). During boreal summer, the occurrence of tropopause folds is highest in the Southern Hemisphere (SH) subtropics, although there is a hotspot of fold activity over the eastern Mediterranean and Middle East, which results from the complex interaction between the South Asian Monsoon and the subtropical jet stream (Tyrlis et al., 2014; Y. Wu et al., 2018).
The environmental significance of tropopause folds can be largely explained by two phenomena: (a) they are the main STT mechanism influencing tropospheric ozone budget, and (b) they are linked with surface weather systems, potentially leading to severe weather events. Tropospheric ozone is critical for the composition of the troposphere, climate, and air quality, as it regulates the oxidation capacity of the troposphere (Lelieveld et al., 2016); in terms of climate change, it is the third most important anthropogenic greenhouse gas (Myhre et al., 2013), and near the Earth’s surface excessive ozone exposure is harmful to human health and the ecosystems (Monks et al., 2015). Although the main source of ozone in the troposphere is photochemical production, the downward transport of ozone from the stratosphere is also a significant contributor (Archibald et al., 2021; Stohl et al., 2003), especially for regions where the meteorological conditions favor subsidence and the formation of tropopause folds, such as during the summertime in the eastern Mediterranean and Middle East (Akritidis et al., 2016; Zanis et al., 2014), Afghanistan (Ojha et al., 2017; Tyrli et al., 2014), and during springtime in the western United States (Langford et al., 2009; Lin et al., 2012, 2015). Tropopause folds are largely responsible for mediating the STT of ozone, making them a key factor influencing tropospheric ozone levels and variability. When deep folds reach into the lower troposphere, ozone concentrations may be significantly increased in both high (Cristofanelli et al., 2010; Lefohn et al., 2011, 2014) and low (Akritidis et al., 2010; Gerasopoulos et al., 2006) altitude sites, which occasionally results in violations of air quality regulations (Kaldunski et al., 2017; Knowland, Ott, et al., 2017; Langford et al., 2009, 2015; Yates et al., 2013; Zhang et al., 2014). In a global study applying a Lagrangian methodology on ERA-Interim reanalysis, it was shown that near-surface ozone concentrations along the west coast of North America and around the Tibetan Plateau are likely to be markedly influenced by deep folds; particularly pronounced positive trends in the net downward mass flux were revealed for the period 1979–2011 over North America (Škerlak et al., 2014). Recently, Akritidis et al. (2019) stressed the role of tropopause folding in STT processes under a changing climate, suggesting that tropopause folds will be associated with both future increases and interannual variability in ozone STT.

Since folding events are characterized by positive PV anomalies, they affect tropospheric dynamics and may influence surface weather systems. The stratospheric reservoir that descends into the troposphere can impose positive PV advection and therefore induce or enhance the cyclonic circulation in the lower troposphere (Hoskins et al., 1985; Uccellini, 1990; Wernli et al., 2002). Furthermore, tropopause folds are known to promote or suppress convective storms, affecting the location, intensity, and morphology of the convection (Antonescu et al., 2013; Cooper et al., 2005; Homeyer et al., 2011; Waugh & Funatsu, 2003). In addition, tropopause folds can give rise to extreme surface winds through downward transport of momentum (Browning & Reynolds, 1994; Škerlak et al., 2015).

Despite the great importance of tropopause folds for tropospheric ozone and weather, the number of climatological studies on folds is rather limited. Ozonesonde (Beekmann et al., 1997; Van Haver et al., 1996) and radar (Antonescu et al., 2013) data were employed to detect foldings of the tropopause and to construct the climatology of the folds, but the analysis was restricted to specific sites. The first attempts to create global tropopause fold climatologies used meteorological analysis data and identified folds as regions of PV and Q-vector divergence maxima (Ebel et al., 1996; Elbern et al., 1998), while other studies were based on Lagrangian trajectories (James et al., 2003; Stohl, 2001). With increasing resolution in global atmospheric models, a new technique for fold detection was developed by Sprenger et al. (2003); this method is based on structural features and was used by the authors to construct a one-year global climatology of tropopause folding events. More recently, Škerlak et al. (2015) built on the ideas behind the 3-D labeling algorithm of Sprenger et al. (2003); the authors applied this algorithm to the ERA-Interim reanalysis data set for the time period 1979–2012 and were able to construct a more robust global climatology of folds. As well as climatologies of tropopause folds, there are also studies describing the climatologies of STT ozone flux based on reanalysis products (Jaeglé et al., 2017; Škerlak et al., 2014).

In recent years, several atmospheric composition reanalysis data sets were produced through the synergistic use of global atmospheric chemistry models, observations (ground-based, satellite, and aircraft), and assimilation techniques. The two most recent state-of-the-art atmospheric composition products are a) the Copernicus Atmosphere Monitoring Service (CAMS) reanalysis (CAMSRA; Inness et al., 2019) produced by the CAMS (http://atmosphere.copernicus.eu), which is operated by the European Center for Medium-Range Weather Forecasts (ECMWF, https://www.ecmwf.int/) on behalf of the European Commission, and b) the
Modern-Era Retrospective analysis for Research and Applications, version 2 (MERRA-2) reanalysis (Gelaro et al., 2017) provided by the NASA Global Modeling and Assimilation Office (GMAO, https://gmao.gsfc.nasa.gov/). As state-of-the-art reanalysis data sets that provide both meteorological and atmospheric composition fields, CAMSRA and MERRA-2 might constitute a framework in which to study STT processes and their implications for tropospheric ozone and air quality. Several studies investigated STT processes using atmospheric composition reanalysis products, such as the Monitoring Atmospheric Composition and Climate (MACC) reanalysis (Knowland, Doherty, et al., 2017; Knowland et al., 2015) and the MERRA-2 reanalysis (Ott et al., 2016; Ryoo et al., 2017) over the last years. Nevertheless, to date, there is no report in the literature documenting a global climatology of tropopause fold occurrence in an atmospheric composition reanalysis product.

Here we present a 16-year (2003–2018) global climatology of tropopause folding events in CAMSRA and MERRA-2 reanalysis products. We used the latest version of the 3-D labeling and fold detection algorithm by Škerlak et al. (2015), with the aim of assessing the level of agreement both between the two reanalysis products as well as with previous studies. Section 2 provides information about the CAMSRA and MERRA-2 reanalysis data and describes the 3-D labeling and fold detection algorithm. Section 3 presents the fold climatology in the two reanalysis products and the comparison between them, and finally, Section 4 summarizes the key conclusions.

2. Data and Methods

2.1. CAMS Reanalysis

CAMSRA (Inness et al., 2019) is the latest reanalysis product of atmospheric composition produced by ECMWF, including 3-dimensional fields of meteorology, chemical species, and aerosols for the time period from 2003 onwards; CAMSRA is a follow-up of earlier reanalysis products: the MACC reanalysis (Inness et al., 2013) and the CAMS interim reanalysis (Flemming et al., 2017). CAMSRA is based on the ECMWF’s Integrated Forecast System (IFS) CY42R1 release and the 4D-Var data assimilation system with two 12-h (09:00–21:00 UTC and 21:00–09:00 UTC) assimilation windows. It is based on the minimization of a penalty function that takes the deviations of the model’s background fields from the observations to provide the optimal forecast during the assimilation window by adapting accordingly the initial conditions. The IFS incorporates meteorological observations, including satellite, in situ, PILOT (wind report from pilot balloon), radiosonde, dropsonde, and aircraft measurements. In addition, satellite retrievals of total column CO, tropospheric column NO$_2$, aerosol optical depth, and total column, partial column and profile ozone retrievals are also assimilated in the IFS. More information on the satellite/instruments and the obtained satellite retrievals assimilated into CAMSRA are provided in Table 2 of Inness et al. (2019). The chemical mechanism used in the IFS is an extended version of the Carbon Bond 2005 (CB05) chemical mechanism (Flemming et al., 2015). The CAMSRA data have a spatial resolution of approximately 80 km ($0.7^\circ \times 0.7^\circ$ grid) with 60 hybrid sigma-pressure (model) levels up to 0.1 hPa, and a temporal resolution of 3 h.

2.2. MERRA-2 Reanalysis

MERRA-2 is the latest atmospheric reanalysis product (Gelaro et al., 2017) provided by the NASA GMAO, covering the time period from 1980 onwards. It represents an update of the modeling and data assimilation system of the original MERRA data set (Rienecker et al., 2011). MERRA-2 was produced using the Goddard Earth Observing System, Version 5 (GEOS-5) atmospheric model (Molod et al., 2015) and the Gridpoint Statistical Interpolation (GSI) assimilation system (Kleist et al., 2009). Specifically, GSI applies a 3D-VAR algorithm (W. Wu et al., 2002) with 6 h windows, producing the analyses through a process of incremental analysis update (Bloom et al., 1996). GEOS-5 integrates a radiatively coupled version of the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model (Chin et al., 2002) to simulate aerosol components. Along with meteorological observations (see Table 1 of Gelaro et al. (2017) for further details), the model also assimilates ozone partial and total column, stratospheric ozone profiles, and aerosol optical depth at 550 nm. More information on the observational system used in MERRA-2 for ozone and aerosol optical depth assimilation are provided in Table 1 of Wargan et al. (2017) and Table 2 of Randles et al. (2017),
respectively. The horizontal resolution is 0.5° × 0.625° latitude by longitude, with 72 hybrid sigma-pressure model layers up to 0.01 hPa.

2.3. Detection of Tropopause Folds

We adopted the latest version of the 3-D labeling algorithm of Škerlak et al. (2015) to identify tropopause folds in CAMSRA and MERRA-2 data, similarly to Akritidis et al. (2016, 2019). The initial inputs for the algorithm are the 3-D fields of PV, potential temperature, and specific humidity and the 2-D fields of surface pressure. Subsequently, the algorithm constructs the 3-D fields of pressure and determines the pressure level of the dynamical tropopause (Holton et al., 1995; Sprenger et al., 2003; Stohl et al., 2003) using the lower of the isosurfaces of PV at 2 PVU and potential temperature at 380 K. A vertical profile is then taken for each grid point and a fold is assigned when multiple crossings of the tropopause are identified. Yet, there are specific situations where air with PV > 2 PVU is either not connected to the stratosphere (stratospheric cut-offs) or is not of stratospheric origin (diabatic PV anomalies or surface-bound PV anomalies), which should not be considered as stratospheric. To this end, the algorithm performs a 3-D labeling (from 1 to 5) of air masses as follows: tropospheric = 1, stratospheric = 2, stratospheric cut-off or diabatically produced PV anomaly = 3, tropospheric cut-off = 4 and surface-bound PV anomaly = 5. A more detailed description of the criteria used for the 3-D labeling can be found in Škerlak et al. (2015). Therefore, a fold is detected when a 2 → 1 → 2 → 1 or 3 transition is found on a vertical profile from the upper to the lower model level, and the algorithm produces as outputs a binary variable (0:no fold, 1:fold) for every grid point and time step. In addition, the upper (pu), middle (pm), and lower (pl) pressure levels of the tropopause crossings are identified along with the difference Δp = pm - pu which reveals the vertical extent of the fold. According to the Δp values, the detected folding events are divided into the three following categories:

- shallow folds, 50 ≤ Δp < 200 hPa
- medium folds, 200 ≤ Δp < 350 hPa
- deep folds, Δp ≥ 350 hPa

As PV and potential temperature are not available in model levels for the CAMSRA product, the "pot_vort_hybrid" NCL (NCAR Command Language) function (https://www.ncl.ucar.edu/Document/Functions/Contributed/pot_vort_hybrid.shtml) is applied to calculate them, using as input the 3-D fields of pressure, u-v wind components, and temperature for every time step. For consistency, PV and potential temperature in MERRA-2 are obtained with the same method as in CAMSRA. The 3-D labeling algorithm is implemented in CAMSRA and MERRA-2 data for the period from 2003 to 2018 with a time interval of 3 h.

3. Results and Discussion

3.1. Climatology of Tropopause Folds Frequency

We first examined the global spatial distribution of shallow, medium, and deep tropopause fold frequency (%) in CAMSRA and MERRA-2 for DJF (December, January, and February), MAM (March, April, and May), JJA (June, July, and August), and SON (September, October, and November). Figure 2 presents the mean seasonal shallow tropopause fold frequency along with the horizontal wind speed (≥20 m/s) at 250 hPa for CAMSRA (left panel) and MERRA-2 (right panel). During DJF and MAM, and based on the seasonal behavior of the subtropical jet stream, the vast majority of shallow folds in both CAMSRA (Figure 2a and 2c) and MERRA-2 (Figure 2b and 2d) are found in the NH mainly in the vicinity of high wind speed regions. In both reanalyses, the highest shallow fold frequencies during DJF and MAM are seen over eastern Asia and further west over Northern India, respectively, with regional values exceeding 15%. During JJA, and as
the subtropical jet stream strengthens in the SH, a band of high fold frequencies up to 15% is found over the southern Indian Ocean and Australia, while in the NH a hotspot of shallow fold activity is identified over the eastern Mediterranean and the Middle East as a result of the complex interaction between the subtropical jet stream and the south Asian Monsoon (Tyrlis et al., 2014). Overall, the geographical distribution of shallow fold frequency in the two reanalysis products is similar, reproducing the spatiotemporal features globally. Nevertheless, shallow folds occur somewhat more frequently in MERRA-2 compared to CAMSRA during all seasons.

Figure 1. Longitude-pressure cross section of CAMSRA (a) and MERRA-2 (b) PV (PVU) at 38.25°N and 38°N, respectively, at 00:00 UTC on October 9, 2003. Gray contours represent the potential temperature (K), the thick black line denotes the dynamical tropopause (2 PVU), and the dashed black line depicts the detected fold. CAMSRA, Copernicus Atmosphere Monitoring Service (CAMS) reanalysis; MERRA-2, Modern-Era Retrospective analysis for Research and Applications, version 2.
The mean seasonal frequency of medium folds for CAMSRA and MERRA-2 is presented in Figure 3, revealing that medium folds are rarer than shallow ones as they occur with frequencies of approximately one order of magnitude lower. More specifically, medium folds mainly co-occur with shallow folds in the proximity of high wind speed regions and over the eastern Mediterranean and the Middle East, yet with lower frequencies that are up to 1%. In addition, medium folds are also found along the storm tracks in both the NH and SH, namely the North Atlantic (mainly appearing during DJF and SON), the North Pacific (during DJF, MAM, and SON), and the Southern Ocean (during MAM, JJA, and SON). Although there is a qualitative agreement between the frequencies of medium folds captured by CAMSRA and MERRA-2, in quantitative terms MERRA-2 exhibits up to ~0.5% higher frequencies over almost all aforementioned regions, which on average corresponds to approximately one extra medium fold event per month.

Figure 2. Mean seasonal shallow tropopause fold frequency (%) for CAMSRA and MERRA-2 for DJF (a and b), MAM (c and d), JJA (e and f), and SON (g and h) for the period from 2003 to 2018. Blue contours denote horizontal wind speed (≥20 m/s) at 250 hPa. CAMSRA, Copernicus Atmosphere Monitoring Service (CAMS) reanalysis; DJF, December, January, and February; JJA, June, July, and August; MAM, March, April, and May; MERRA-2, Modern-Era Retrospective analysis for Research and Applications, version 2; SON, September, October, and November.
Figure 4 presents the spatial distribution of the frequency of deep fold occurrence in CAMSRA and MERRA-2. Deep folds are even rarer compared to the shallow and medium ones, with frequencies of up to $\sim 0.2\%$. In contrast to shallow and medium folds, the majority of deep folds in the NH appear over the storm tracks in the western North Atlantic and the North Pacific, mainly during DJF and to a lesser extent during MAM and SON. Similarly, deep folds are identified in the SH along the storm tracks mainly during JJA and less often during MAM and SON, while the highest frequencies are seen west of Australia during JJA with regional values exceeding $\sim 0.2\%$. MERRA-2 captures higher deep fold frequencies compared to CAMSRA, except for the region off the east coast of Antarctica during JJA where CAMSRA identifies higher number of folds.

Figure 3. Mean seasonal medium tropopause fold frequency (%) for CAMSRA and MERRA-2 for DJF (a and b), MAM (c and d), JJA (e and f), and SON (g and h) for the period from 2003 to 2018. Blue contours denote horizontal wind speed ($\geq 20$ m/s) at 250 hPa. CAMSRA, Copernicus Atmosphere Monitoring Service (CAMS) reanalysis; DJF, December, January, and February; JJA, June, July, and August; MAM, March, April, and May; MERRA-2, Modern-Era Retrospective analysis for Research and Applications, version 2; SON, September, October, and November.
The spatial distribution of shallow tropopause fold frequency in CAMSRA and MERRA-2 is found to be both qualitatively and quantitatively in very good agreement over all seasons with the findings of Škerlak et al. (2015) based on the ERA-Interim tropopause fold climatological study. For the medium folds, CAMSRA climatology is in line with the results depicted in the work by Škerlak et al. (2015), while MERRA-2 recapitulates the respective spatiotemporal patterns, yet mainly exhibits higher frequencies. Finally, both CAMSRA and MERRA-2 reproduce the regions and season of occurrence for deep folds reported in Škerlak et al. (2015) but with higher frequencies. Overall, the best match is seen with CAMSRA, yet it should be noted that both ERA-Interim and CAMSRA were produced with different versions of the same forecast system (IFS). ERA-Interim used an older IFS model cycle (CY31R2) than CAMSRA (CY42R1), but the horizontal and vertical resolutions of the datasets are the same. Moreover, the climatology in Škerlak et al. (2015) was

Figure 4. Mean seasonal deep tropopause fold frequency (%) for CAMSRA and MERRA-2 for DJF (a and b), MAM (c and d), JJA (e and f), and SON (g and h) for the period from 2003 to 2018. Blue contours denote horizontal wind speed (≥20 m/s) at 250 hPa. CAMSRA, Copernicus Atmosphere Monitoring Service (CAMS) reanalysis; DJF, December, January, and February; JJA, June, July, and August; MAM, March, April, and May; MERRA-2, Modern-Era Retrospective analysis for Research and Applications, version 2; SON, September, October, and November.
constructed for the period 1979–2012, while the CAMSRA and MERRA-2 climatologies refer to the period 2003–2018.

The mean annual cycle of zonal mean tropopause fold (folds with \( \Delta p \geq 50 \) hPa namely shallow, medium, and deep) frequency is presented in Figure 5 for CAMSRA (Figure 5a) and MERRA-2 (Figure 5b). In the NH, both reanalyses capture the highest fold frequencies during the period between January and April and within the latitudinal band of 20°–40°N where the subtropical jet stream occurs, with frequencies in MERRA-2 1% higher compared to those in CAMSRA. From June to August and as the NH subtropical jet stream weakens and shifts further north, the highest zonal mean fold frequencies are seen at ∼40°N, which is due to the high summertime fold frequencies over the eastern Mediterranean and Middle East. In the SH,
and following the strengthening of the subtropical jet stream during the austral winter, folds occur more often during the period from May to October at ∼30°S, a feature that is more pronounced in MERRA-2.

3.2. Level of Agreement Between CAMSRA and MERRA-2 Tropopause Fold Climatologies

We quantitatively assessed the agreement in spatiotemporal variability in tropopause fold climatologies in CAMSRA and MERRA-2. Due to the different horizontal resolutions in CAMSRA and MERRA-2, the MERRA-2 fold frequencies were bilinearly interpolated to the coarser CAMSRA grid. Figures 6a–6d present the scatter plots of tropopause fold (folds with Δp ≥ 50 hPa) frequency for all grid points (512 × 256) and for each season (16 seasonal means for each season and grid point) in CAMSRA and MERRA-2. Furthermore, Figure 6e shows the scatter plot of tropopause fold frequency for all grid points (512 × 256) and months (12 × 16 = 192 monthly means for each grid point). Also shown is the distribution of fold frequencies in the two reanalysis products in every case. The explained variance in Figures 6a–6d depicts the spatial and the interannual covariance between CAMSRA and MERRA-2 tropopause fold frequency for each hemisphere and season. In addition, the explained variance in Figure 6e includes the intra-annual covariance (from month to month within a year) between CAMSRA and MERRA-2 tropopause fold frequency.

As depicted for DJF (Figure 6a), there is a very good agreement between CAMSRA and MERRA-2 fold frequencies on a global scale (blue and orange points) with $R^2$ (proportion of MERRA-2 variance explained by CAMSRA) and mean absolute difference (MAD) values of 0.88% and 0.63%, respectively; the match is better in the NH (blues points) ($R^2 = 0.91$) than in the SH (orange points) ($R^2 = 0.78$). A similar behavior on a global scale is seen for MAM (Figure 6b), with $R^2 = 0.88$ and MAD = 0.59% and a better agreement in the NH ($R^2 = 0.92$) with regards to the SH ($R^2 = 0.75$). During JJA (Figure 6c), and as the fold activity shifts also in the SH, CAMSRA and MERRA-2 match each other closely, with $R^2 = 0.88$ and MAD = 0.58%; the closest agreement is found in the NH ($R^2 = 0.93$ compared to $R^2 = 0.85$ in the SH). The weakest agreement among all seasons is identified for SON (Figure 6d) with $R^2 = 0.75$ and MAD = 0.67%, but again with a better match in the NH ($R^2 = 0.82$ compared to $R^2 = 0.7$ in the SH). Overall, and when considering all monthly values over the examined period (Figure 6d), the above pattern remains the same with $R^2 = 0.8$ and MAD = 0.72%, while in the NH and SH the respective $R^2$ values are 0.86 and 0.69. Considering the embedded figures of fold frequency distributions, there is a clear preponderance of folds in the NH for the whole year, DJF, and MAM, which is reproduced by both reanalyses. During JJA, there are more instances of fold frequencies below ~10% in the SH, while there are more above ~15% in the NH, a feature in both CAMSRA and MERRA-2. For SON, the distribution of fold frequencies in the two hemispheres is more similar than in the other seasons. Overall, the distributions reveal a good agreement between MERRA-2 and CAMSRA, with MERRA-2 exhibiting slightly higher fold frequencies, an aspect which is also mentioned above in Section 3.1. Moreover, there is a better agreement between CAMSRA and MERRA-2 in the NH than in the SH for each season and when considering all months, with a higher $R^2$ and a lower MAD (except DJF). This may be related with the fact that more observations are available for assimilation in the NH compared to the SH.

In order to compare tropopause fold climatology in the two reanalysis products in more detail, we explored the interannual variability and calculated the Pearson correlation coefficients between the CAMSRA and MERRA-2 fold frequency for every grid point from both seasonal (16) and monthly (12 × 16 = 192) values of the period 2003–2018. Figure 7 presents the spatial distribution of these correlations, with all colors except black depicting significant correlation coefficients at the 95% significance level (following t-statistic) and the gray color denoting undefined values (cases where at least one of the series consists of zero frequencies).

Significant positive correlations predominate over all seasons across the globe, and values exceed 0.7 over the subtropical zones where the main fold activity is identified; over the regions with lower fold activity, for example, the storm tracks, meanwhile, the correlation is lower but still significant and higher than 0.5 (Figures 7a–7d). This indicates that, overall, there is a good agreement between the year-to-year variability for the seasonal fold frequency between CAMSRA and MERRA-2. In addition to Figures 7a–7d, Figure 7e shows both inter- and intra-annual covariance between MERRA-2 and CAMSRA fold frequency for each grid point. The correlation coefficients of monthly fold frequency between CAMSRA and MERRA-2 show significant correlations higher than 0.8 over the subtropical regions; these values decrease with latitude and are higher over the NH with values exceeding 0.5 over the mid-latitudes (Figure 7e). These results suggest
Figure 6. Scatter plot of CAMSRA and MERRA-2 DJF (a), MAM (b), JJA (c), SON (d), and monthly (e) tropopause fold (Δp ≥ 50 hPa) frequencies (%) for all the grid points. The blue and orange colors denote grid points from the NH and SH, respectively. The blue, orange, and black solid lines represent the regression line of the CAMSRA and MERRA-2 fold frequencies for the NH, the SH, and the whole globe, respectively, while the corresponding equation, p-value, $R^2$, and MAD are also shown. The black dashed line is the 1:1 line. The embedded figures depict the histogram lines of tropopause fold (Δp ≥ 50 hPa) frequencies for CAMSRA and MERRA-2 in the NH (blue and light blue) and SH (red and orange). CAMSRA, Copernicus Atmosphere Monitoring Service (CAMS) reanalysis; DJF, December, January, and February; JJA, June, July, and August; MAM, March, April, and May; MERRA-2, Modern-Era Retrospective analysis for Research and Applications, version 2; SON, September, October, and November.
that, in both reanalysis products, the combined intra- and interannual variability of fold frequency is reproduced in a similar way, at least for the regions where the majority of tropopause fold events occur.

Any discrepancies between the two climatologies are due to the different modeling and assimilation techniques applied for the production of CAMSRA and MERRA-2 reanalyses, as well as the differences between them in horizontal and vertical resolution. For example, for the western United States region which is a hotspot of medium and deep folds (see Figures 3 and 4) that are known to affect tropospheric ozone and air quality during MAM (Knowland, Ott, et al., 2017; Lin et al., 2012, 2015), MERRA-2 captures more folds compared to CAMSRA. Nevertheless, when we consider fold events (Δp ≥ 200 hPa) over a specific grid point of this region that are detected in MERRA-2 and not in CAMSRA, a quite similar increase (decrease) of ozone (specific humidity) is found in the troposphere and near the folds for both reanalysis products.
indicating that the STT processes are also reproduced by CAMSRA (see Figures S1–S3 in supporting information). Presumably, the coarser vertical and horizontal resolution in CAMSRA compared to MERRA-2 is responsible for the non-detection of these folds in CAMSRA by the applied algorithm.

4. Conclusions

We presented the climatology of tropopause folds in CAMS and MERRA-2 state-of-the-art reanalysis products for the time period 2003–2018 using a 3-D labeling algorithm for the detection of folding events. In particular, we examined the spatiotemporal characteristics of tropopause fold occurrence around the globe in both reanalyses and assessed the degree of agreement between the two products and with previous climatological studies. The most notable findings of the current study are summarized as follows:

- The bulk of tropopause folds are vertically shallow (50 ≤ Δp < 200 hPa) and occur mainly in the vicinity of the NH/SH subtropical jet streams, while deeper folds, which are rarer, also develop over the storm track regions. During DJF and MAM, the majority of folds are seen in the NH, while during JJA and SON, most folds are observed in the SH. These features are seen in both CAMS and MERRA-2 analyses, which is in line with previous climatological studies such as the ERA-Interim-based approach of Škerlak et al. (2015).
- The two reanalysis climatologies perform similarly well in capturing the global spatial distribution of tropopause fold frequency throughout the seasons, with MERRA-2 capturing an overall slightly higher frequency of occurrence. In quantitative terms, the comparison between CAMSRA and MERRA-2 indicates a good agreement for DJF, MAM, and JJA (R² = 0.88 and MAD = 0.6%), while during SON the agreement is slightly weaker but remains strong (R² = 0.75 and MAD = 0.67%).
- A lower agreement between CAMSRA and MERRA-2 is found for the SH compared to the NH, with R² values decreasing in all seasons. This probably reflects the lower amount of observational data available for assimilation in the SH.
- Finally, the interannual variability in seasonal fold frequency is similar between the two reanalyses, with significantly positive correlations; over the subtropical bands where the majority of folds occur, these coefficients have values higher than ~0.7.

In summary, this study indicates that both CAMS and MERRA-2 reanalysis products reproduce the key characteristics of tropopause fold occurrence reported by previous studies. Despite quantitative discrepancies, overall the two climatologies are highly similar. Tropopause folds are a key process that determine the influence of STT on tropospheric composition. Therefore, recording them and reporting their reliability in CAMS and MERRA-2 atmospheric composition reanalysis products is expected to be critical for future research studies.

Data Availability Statement

The CAMS Reanalysis data (Inness et al., 2019) were obtained from ECMWF’s web repository at https://apps.ecmwf.int/data-catalogues/cams-reanalysis/?class=mc&expver=eac4 through the corresponding WebAPI and can be also accessed at the CAMS Atmosphere Data Store (ADS) https://ads.atmosphere.copernicus.eu/cdsapp#!/dataset/cams-global-reanalysis-eac4?tab=form. The MERRA-2 data (Gelaro et al., 2017) were obtained from the NASA Earthdata website (GMAO, 2015) and can be accessed at https://disc.gsfc.nasa.gov/datasets/M2I3NVASM_5.12.4/summary. This study contains modified Copernicus Atmosphere Monitoring Service Information (2020); neither the European Commission nor ECMWF is responsible for any use that may be made of the information it contains.

References

Akritidis, D., Pozzer, A., & Zanis, P. (2019). On the impact of future climate change on tropopause folds and tropospheric ozone. Atmospheric Chemistry and Physics, 19(22), 14387–14401. https://doi.org/10.5194/acp-19-14387-2019
Akritidis, D., Pozzer, A., Zanis, P., Tyrlis, E., Škerlak, B., Sprenger, M., & Lelieveld, J. (2016). On the role of tropopause folds in summertime tropospheric ozone over the eastern Mediterranean and the Middle East. Atmospheric Chemistry and Physics, 16, 14025–14039. https://doi.org/10.5194/acp-16-14025-2016
Akritidis, D., Zanis, P., Pyhara, T., Mavragas, A., & Karacostas, T. (2010). A deep stratospheric intrusion event down to the earth's surface of the megacity of Athens. Meteorology and Atmospheric Physics, 109(1–2), 9–18. https:// doi.org/10.1007/s00703-010-0096-6
Antonescu, B., Vaughan, G., & Schultz, D. M. (2013). A Five-year radar-based climatology of tropopause folds and deep convection over Wales, United Kingdom. *Monthly Weather Review, 141*(5), 1693–1707. https://doi.org/10.1175/MWR-D-12-00246.1

Archibald, A., Neu, J., Eshlebory, Y., Cooper, O., Young, P., Akiyoshi, H., et al. (2021). Tropospheric ozone assessment report: A critical review of changes in the tropospheric ozone burden and budget from 1850 to 2100. *Elementa: Science of the Anthropocene*. https://doi.org/10.1525/elementa.2020.034

Beekmann, M., Ancellet, G., Blonsky, S., De Muer, D., Ebel, A., Elbern, H., et al. (1997). Regional and global tropopause fold occurrence and related ozone flux across the tropopause. *Journal of Atmospheric Chemistry, 28*, 29–44. https://doi.org/10.1023/A:1005897131463

Bloom, S. C., Takacs, L. L., da Silva, A. M., & Ledvina, D. (1996). Data assimilation using incremental analysis updates. *Monthly Weather Review, 124*(6), 1256–1271. https://doi.org/10.1175/1520-0493(1996)124<1256:DAUAIA>2.0.CO;2

Browning, K. A., & Reynolds, R. (1994). Diagnostic study of a narrow cold-frontal rainband and severe winds associated with a stratospheric intrusion. *Quarterly Journal of the Royal Meteorological Society, 120*(516), 235–257. https://doi.org/10.1002/qj.4971051602

Chin, M., Ginoux, P., Kinne, S., Torres, O., Holben, B. N., Duncan, B. N., et al. (2002). Tropospheric aerosol optical thickness from the GO-CART model and comparisons with satellite and Sun photometer measurements. *Journal of the Atmospheric Sciences, 59*(3), 461–483. https://doi.org/10.1029/2001JD000901

Cooper, O., Forster, C., Parrish, D., Dunlea, E., Hübler, G., Fehsenfeld, F., et al. (2004). On the life cycle of a stratospheric intrusion and its dispersion into polluted warm conveyor belts. *Journal of Geophysical Research, 109*(D23). https://doi.org/10.1029/2003JD004006

Cooper, O., Moody, J. L., Parrish, D. D., Trainer, M., Ryerson, T. B., Holloway, J. S., et al. (2002). Trace gas composition of midlatitude cyclones over the western North Atlantic Ocean: A conceptual model. *Journal of Geophysical Research, 107*(D7). https://doi.org/10.1029/2001JD000901

Cooper, O., Stohl, A., Hübler, G., Hsie, E., Parrish, D., Tuck, A., et al. (2005). Direct transport of midlatitude stratospheric ozone into the lower troposphere and marine boundary layer of the tropical Pacific Ocean. *Journal of Geophysical Research, 110*(D23). https://doi.org/10.1029/2005JD005783

Danielsen, E. F., & Mohnen, V. A. (1977). Project dustorm report: Ozone transport, in situ measurements, and meteorological analyses of tropopause folding. *Journal of Geophysical Research, 82*(37), 5867–5877. https://doi.org/10.1029/jc082i37p05867

Elbern, H., Elberth, J., Hendricks, J., & Meyer, R. (1996). Stratosphere-troposphere exchange and its impact on the structure of the lower stratosphere. *Journal of Geodynamics and Geoelectricity, 48*(1), 135–144. https://doi.org/10.5636/jgg.48.135

Hendricks, J., Elbern, H., and Meyer, R. (1998). A climatology of tropopause fold by global analyses. *Theoretical and Applied Climatology, 59*, 181–200. https://doi.org/10.1007/s007040050023

Flemming, J., Benedetti, A., Inness, A., Engelen, R. J., Jones, L., Huijnen, V., et al. (2017). The CAMS interim reanalysis of carbon monoxide, ozone and aerosol for 2003–2015. *Atmospheric Chemistry and Physics, 17*(3), 1945–1983. https://doi.org/10.5194/acp-17-1945-2017

Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., et al. (2015). Tropospheric chemistry in the integrated forecasting system of ECMWF. *Geoscientific Model Development, 8*(4), 975–1003. https://doi.org/10.5194/gmd-8-975-2015

Gelaro, R., McCarty, W., Suárez, M. J., Todling, R., Molod, A., Takacs, L., et al. (2017). The Modern-era retrospective analysis for research and applications, version 2 (MERRA-2). *Journal of Climate, 30*(4), 5419–5454. https://doi.org/10.1175/JCLI-D-16-0758.1

Jordà, J., Soler, J., Moya, A., & del Rosal, J. (2006). Multyear composite view of ozone enhancements and stratosphere-troposphere transport in dry intrusions of Northern Hemisphere extratropical cyclones. *Journal of Geophysical Research: Atmospheres, 111*(D23). https://doi.org/10.1029/2005JD006724

Knowland, E., Doherty, R., & Marsh, A. (2003). Multyear composite view of ozone enhancements and stratosphere-troposphere transport in dry intrusions of Northern Hemisphere extratropical cyclones. *Journal of Geophysical Research: Atmospheres, 111*(D7). https://doi.org/10.1029/2005JD006756

Kleist, D., Forster, C., Parrish, D., Treadon, R., Wu, W., & Lord, S. (2009). Introduction of the GSI into the NCEP global data assimilation system. *Weather and Forecasting, 24*(6), 1691–1705. https://doi.org/10.1175/2009WAF222201.1

Knowland, E., Doherty, R., Hedges, K., & Ott, L. (2017). The influence of mid-latitude cyclones on European background surface ozone. *Atmospheric Chemistry and Physics, 17*(20), 12421–12447. https://doi.org/10.5194/acp-17-12421-2017

Knowland, E., Ott, L., Duncan, B., & Wargan, K. (2017). Stratospheric intrusion-influenced ozone air quality exceedances investigated in the NASA MERRA-2 reanalysis. *Journal of Geophysical Research Letters, 44*(20), 10–491. https://doi.org/10.1002/2017GL074532

Langford, A. O., Akiyoshi, H., Eubank, C. S., & Williams, E. J. (2009). Stratospheric contribution to high surface ozone in Colorado during springtime. *Journal of Geophysical Research, 114*(D3). https://doi.org/10.1029/2009GL038367
Langford, A. O., Senff, C. J., Alvarez, R. I., Briaud, J., Cooper, O. R., Holloway, J. S., et al. (2015). An overview of the 2013 Las Vegas ozone study (LVOS): Impact of stratospheric intrusions and long-range transport on surface air quality. *Atmospheric Environment*, 109, 305–322. https://doi.org/10.1016/j.atmosenv.2014.08.040

Lefohn, A. S., Emery, C., Shadwick, D., Wernli, H., Jung, J., & Oltmans, S. J. (2014). Estimates of background surface ozone concentrations in the United States based on model-derived source apportionment. *Atmospheric Environment*, 84, 275–288. https://doi.org/10.1016/j.atmosenv.2013.11.033

Lefohn, A. S., Wernli, H., Shadwick, D., Limbach, S., Oltmans, S. I., & Shapiro, M. (2011). The importance of stratospheric-tropospheric transport in affecting surface ozone concentrations in the western and northern tier of the United States. *Atmospheric Environment*, 45(28), 4845–4857. https://doi.org/10.1016/j.atmosenv.2011.06.014

Lelieveld, J., Gromov, S., Pozzer, A., & Taraborrelli, D. (2016). Global tropospheric hydroxyl distribution, budget and reactivity. *Atmospheric Chemistry and Physics*, 16(19), 12477–12493. https://doi.org/10.5194/acp-16-12477-2016. Retrieved from https://www.atmos-chem-phys.net/16/12477/2016/

Lin, M., Fiore, A. M., Cooper, O. R., Horowitz, L. W., Langford, A. O., Levy, H. I., et al. (2012). Springtime high surface ozone events over the western United States: Quantifying the role of stratospheric intrusions. *Journal of Geophysical Research*, 117(D21). https://doi.org/10.1029/2012jd018151

Lin, M., Fiore, A. M., Horowitz, L. W., Langford, A. O., Oltmans, S. J., Tarasick, D., & Rieder, H. E. (2015). Climate variability modulates western US ozone air quality in spring via deep stratospheric intrusions. *Nature Communications*, 6. https://doi.org/10.1038/ncomms8010

Molend, A., Takacs, L., Suarez, M., & Bacmeister, J. (2015). Development of the GEOS-5 atmospheric general circulation model: Evolution from MERRA to MERRA2. *Geoscientific Model Development*, 8(5), 1339–1356. https://doi.org/10.5194/gmd-8-1339-2015

Monks, P. S., Archibald, A. T., Colette, A., Cooper, O., Coyle, M., Derwent, R., et al. (2015). Tropospheric ozone and its precursors from the urban to the global scale from air quality to short-lived climate forcer. *Geoscientific Model Development*, 8, 1233–1281. https://doi.org/10.5194/gmd-8-1233-2015

Ott, L. E., Duncan, B. N., Thompson, A. M., Diskin, G., Fasnacht, Z., Langford, A. O., et al. (2016). Frequency and impact of summertime stratospheric intrusions over Maryland during DISCOVER-AQ (2011): New evidence from NASA’s GEOS-5 simulations. *Geophysical Research: Atmospheres*, 121(7), 3687–3706. https://doi.org/10.1002/2015JD024052

Randles, C. A., da Silva, A. M., Buchard, V., Colarco, P. R., Darmenov, A., Govindaraju, R., et al. (2017). The MERRA-2 aerosol reanalysis, 1980 onward. Part I: System description and data assimilation evaluation. *Journal of Climate*, 30(17), 6823–6850. https://doi.org/10.1175/JCLI-D-16-0609.1

Rienecker, M. M., Suarez, M. J., Gelaro, R., Todling, R., Bacmeister, J., Liu, E., et al. (2011). MERRA: NASA’s modern-era retrospective analysis for research and applications. *Journal of Climate*, 24(14), 3624–3648. https://doi.org/10.1175/JCLI-D-11-00015.1

Roelofs, G.-J., & Lelieveld, J. (1997). Model study of the influence of cross-tropopause O3 transports on tropospheric O3 levels. *Tellus B: Chemical and Physical Meteorology*, 49(1), 38–55. https://doi.org/10.1034/j.1600-0889.49.issue1.3.x

Roelofs, G.-J., & Lelieveld, J. (1998). Processes contributing to the rapid development of extratropical cyclones. In C. W. Newton & E. O. Holopainen (Eds.), *Extratropical cyclones: The erik palmeen memorial volume* (pp. 81–105). American Meteorological Society. https://doi.org/10.1007/978-1-944970-33-8_6

Roelofs, G.-J., & Lelieveld, J. (2000). Processes contributing to the rapid development of extratropical cyclones. In C. W. Newton & E. O. Holopainen (Eds.), *Extratropical cyclones: The erik palmeen memorial volume* (pp. 81–105). American Meteorological Society. https://doi.org/10.1007/978-1-944970-33-8_6

Van Haver, P., De Muer, D., Beekmann, M., & Manier, C. (1996). Climatologie of tropopause folds at midlatitudes. *Geophysical Research Letters*, 23(9), 1033–1036. https://doi.org/10.1029/96GL00956

Wargan, K., Labow, G., Frith, S., Pawson, S., Livesey, N., & Partyka, G. (2017). Evaluation of the ozone fields in NASA’s MERRA-2 reanalysis. *Journal of Climate*, 30(8), 2961–2988. https://doi.org/10.1175/JCLI-D-16-0699.1

Waugh, D. W., & Funatsu, B. M. (2003). Intrusions into the tropical upper troposphere: Three-dimensional structure and accompanying ozone and OLR distributions. *Journal of the Atmospheric Sciences*, 60(4). https://doi.org/10.1175/1520-0469(2003)060<0837:ilittuv>2.0.co;2

Wernli, H., Dirren, S., Liniger, M. A., & Zillig, M. (2002). Dynamical aspects of the life cycle of the winter storm ‘Lothar’ (24–26 December 1999). *Quarterly Journal of the Royal Meteorological Society*, 128(580), 405–429. https://doi.org/10.1002/qj.493

Wu, W., Purser, R., & Parrish, D. (2002). Three-dimensional variational analysis with spatially inhomogeneous covariances. *Monthly Weather Review*, 130, 2905–2916. https://doi.org/10.1175/1520-0493(2002)130<2905:dvahow>2.0.co;2

Wu, Y., Chen, G., Taylor, L., & Zhang, P. (2018). On the linkage between the Asian summer monsoon and tropopause folds. *Journal of Geophysical Research: Atmospheres*, 123(4), 2037–2049. https://doi.org/10.1002/2017JD027970
Yates, E. L., Iraci, L. T., Roby, M. C., Pierce, R. B., Johnson, M. S., Reddy, P. J., et al. (2013). Airborne observations and modeling of springtime stratosphere-to-troposphere transport over California. *Atmospheric Chemistry and Physics, 13*(24), 12481–12494. https://doi.org/10.5194/acp-13-12481-2013

Zanis, P., Hadjinicolaou, P., Pozzer, A., Tyrlis, E., Dafka, S., Mihalopoulos, N., & Lelieveld, J. (2014). Summertime free-tropospheric ozone pool over the eastern Mediterranean/Middle East. *Atmospheric Chemistry and Physics, 14*(1), 115–132. https://doi.org/10.5194/acp-14-115-2014

Zhang, L., Jacob, D. J., Yue, X., Downey, N. V., Wood, D. A., & Blewitt, D. (2014). Sources contributing to background surface ozone in the US intermountain west. *Atmospheric Chemistry and Physics, 14*(11), 5295–5309. https://doi.org/10.5194/acp-14-5295-2014