

Examining Relationships between Stability and Composition in the Tropopause Transition Layer

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ABSTRACT

The interface separating the upper troposphere from the lower stratosphere is called the tropopause, a complex transition layer contributing to many dynamical aspects of the atmosphere. In this study, observational data is obtained from the ESRL Ozone Data Archive with a multidecadal time-span from 1967-2021 and 1982-2021. Locations in the tropical, polar, and midlatitude regions are examined due to their variation in latitude, climate, and season. After analyzing the tropopause from a composition and stability perspective at each of these areas, the World Meteorological Organization (WMO) lapse-rate definition of $2^{\circ}\text{C km}^{-1}$ is evaluated in comparison. Upon investigation, using a 9 K km^{-1} potential temperature gradient threshold as a stability identifier has proven to be ideal in determining the location of the tropopause in all regions and seasons. The WMO definition and stability threshold are applied to individual profiles and compared to vertical profiles of ozone for evaluation. The stability threshold tends to always mark a tropopause layer directly below the WMO definition in instances where the temperature lapse rate is not met, while the altitude difference between the two vary based on time of year, location and potentially dynamical impacts. Although there are many different definitions that can be used to find the tropopause, the purpose of this study is to investigate the accuracy and consistency of using the stability threshold, especially in situations where the WMO tropopause may not perform well.

1. Introduction

The tropopause is a complex transition layer located between the upper troposphere and lower stratosphere (UTLS) and has been defined in many different ways over the years. The UTLS is otherwise known as a coupling layer, influencing middle-upper latitudinal atmospheric motions (Gettelman et al. 2011), climate, radiation, stratosphere-troposphere exchange (STE) (Pan et al. 2004), and much more. Researchers have been attempting to understand the complexity of the transition layer for decades, but seasonal and latitudinal location can create disparity in tropopause structure and definition. Limitations can also arise due to a lack of data availability, few stations with consistent observations, model resolution and the cost of obtaining such reliable data. As

technology advances and additional studies are being conducted, the tropopause transition layer has slowly become more understood over time.

From a composition perspective, a sharp increase in ozone (O_3) can be seen upon entering the transition layer and concentrations remain high throughout the stable stratosphere, while a decrease in water vapor (H_2O) occurs almost simultaneously with increasing height. This is because H_2O is less prevalent in the stratosphere with mixing ratios near 3-6 ppmv (Tinney and Homeyer 2021; Tilmes et al. 2010). Carbon monoxide (CO) is another identifier, used in tracking of human activity and pollution in the planetary boundary layer (PBL) (Chin et al. 1994). All of these are called trace gases (tracers), or chemical identifiers that can be used to help locate the tropopause and/or STE. It has been shown that using tracer-tracer relationships (plots of coincident tropospheric and stratospheric tracers) can allow for definition of “chemical tropopause” and characterization of the transition layer (Pan et al.

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2004), but in our case, we are looking to identify the tropopause transition layer using stability.

For some background, the tropopause was originally discovered in 1902 by Teisserence de Bort and was defined as a "zone isotherme" (isothermal layer). A short time later, Richard Assmann also announced that he similarly found an "upper inversion" (Hoinka 1997). Although it wasn't called the tropopause until the early 1900s, their research grasped an understanding of the vertical structure of the atmosphere that would branch into many more discoveries, and similarly, definitions.

Once the basis of atmospheric layers was identified by the World Meteorological Organization (WMO), the temperature lapse-rate definition of the tropopause (LRT) soon followed. This is the most conventional and widely used definition for identifying the tropopause transition layer, defined as "*the lowest level at which the lapse rate decreases to $2^{\circ}\text{C km}^{-1}$ or less, provided also the average lapse rate between this level and all higher levels within 2 km does not exceed $2^{\circ}\text{C km}^{-1}$* " (World Meteorological Organization 1957). This is a good threshold to follow and can be applied reliably at any location using both balloon observations and model output, although lapse rates may vary slightly based on seasonal factors, latitudinal location, and current weather patterns.

The so-called dynamical tropopause is one of the most popular alternatives to the WMO definition, which was originally based on the isentropic gradient of potential vorticity (PV; Reed 1955) and is mostly applied in the extratropics due to isentropic surfaces being nearly vertical close to the equator. For tropical locations, the cold point tropopause (CPT) is often used and is a reliable definition in that region, though it is susceptible to bias from temperature fluctuations driven by wave activity. It is important to note that the CPT cannot be used poleward of the subtropical jet due to decoupling between the temperature minimum in a profile and the dominant troposphere-stratosphere composition change. Composition-based tropopause definitions leverage various trace gases, such as—but not limited to— O_3 , H_2O , and CO . Ozonesondes are commonly used in recent decades at select sites around the world and have been used to produce a chemical tropopause definition (Bethan et al. 1996), but such a definition based on O_3 alone can be sensitive to STE and require adjustment when applied to locations at a wide range of latitudes, hence the need for a refined approach (gradients, smoothing, etc) to remove noise and other features. Lastly, a stability-based tropopause definition can be defined as *a fundamental dynamical quantity that measures the vertical temperature stratification of the atmosphere* (Grise et al. 2010). A less stable environment is present in the troposphere, alternating to higher stability in the stratosphere, making it a useful parameter in the UTLS. While most previous UTLS stability studies use the Brunt–Väisälä frequency (Gettelman and Wang 2015;

Duran and Molinari 2019), this study leverages the vertical gradient of potential temperature instead (the dominant term for Brunt–Väisälä frequency).

The motivation of this study is to examine ozonesonde observations, specifically measurements of composition and stability, across the latitudes to identify a consistent stability-based definition of the tropopause. Of the definitions mentioned above (LRT, chemical, PV, etc.), the LRT is the most widely-used simply because it's conventional, allowing for a single temperature profile to produce determination of the tropopause (Bethan et al. 1996) and is therefore used as a baseline comparison of existing definitions in our study. The LRT definition performs well at all latitudes due to similar atmospheric thermal structures Maddox and Mullendore (2018), but can struggle during some seasons. One example is at the South Pole during the winter months, because the atmosphere is so brutally cold there's little to no temperature inversion at the tropopause. The LRT is the most widely-used simply because it's conventional, allowing for a single temperature profile to produce determination of the tropopause (Bethan et al. 1996). Although the LRT definition is highly capable, the purpose of this study is to see how a developed stability threshold, in relation with ozone, can more-accurately define the initial perturbation of the tropopause transition layer. Potential temperature is an inherently dynamic quality that is unaffected by adiabatic processes, allowing it to be more useful in the identification of a dynamic-barrier like the tropopause. This is why a stability-based definitions could relatively be better than the LRT, as it combines both temperature observations and dynamic components of other definitions (such as PV).

Depending on the type of research being conducted concludes which tropopause definition is (or should be) used, because using the wrong parameter-based narrative can lead to erroneous or inconclusive results. This greatly impacts quantitative studies (Pan et al. 2004), and can result in unintentional bias. Each definition has its pros and cons, some useful for specific observations and others based on a broad generalization. The overarching goal of this study is to gain better interpretation, using the above parameters of the tropopause, that can be applied universally in the tropics, extratropics and polar regions.

2. Data and Methods

In order to observe a wide range of environmental structures surrounding the tropopause transition layer, long-term measurements have been obtained from the Earth System Research Laboratories (ESRL) Global Monitoring Laboratory Ozonesonde Data Archive. The ozonesondes used at each location are balloon-borne instruments attached to a radiosonde. During ascent, data is transmitted back to the ground observing station, providing measurements of pressure, humidity, temperature, O_3 and re-

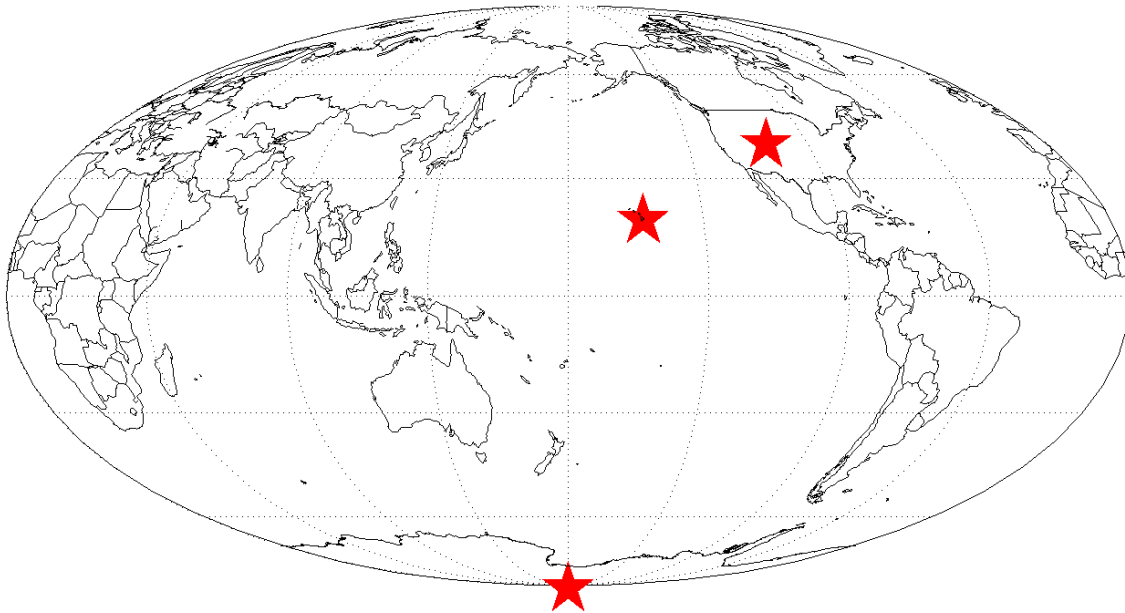


FIG. 1. Red stars in the map above indicate locations (Boulder, CO; Hilo, HI; Amundsen-Scott South Pole Station) of the ozonesonde launch sites used in this study.

lated parameters. We use the 100-m averaged datasets retrieved from the ESRL Global Monitoring Laboratory Ozone Data Archive to relate O_3 and stability parameters against each other. For each of the three locations chosen, data is organized based on season and latitude.

Three different locations, seen in Figure 1, were carefully chosen to provide a diverse latitudinal perspective of the tropopause transition layer. The Boulder, CO (39.992°N, -105.261°W, 1628.00 m above sea level (asl)) station data covers 1967–2021 and represents extratropical air masses, with ozonesonde frequency ranging from once per week to once per month. Hilo, HI (19.7170°N, 155.049°W, 11.00 m asl) was chosen for its tropical position, with ozonesonde frequency of several times per month from 1982–2021. Lastly, the Amundsen-Scott South Pole Station (-90°S, 0.0°E, 2835.00 m asl) was selected to represent polar regions, with ozonesondes available several times monthly from 1967–2021. The lowest 8 km of Hilo and 4 km of Boulder observations are excluded from analysis so each location has similar approximate tropospheric depths. In addition to a dependence on latitude, the tropopause also varies seasonally. We therefore examine each station by season to identify consistencies (or lack thereof) in relationships between stability and composition. There are plenty of observation sites across these regions, but the above sites were chosen specifically for their longevity, frequency, accessibility and data extending into the current year (2021).

The main focus of this work will be upon relating vertical changes in stability and O_3 , then comparing that to

composition change relative to the LRT. Calculations of stability (Equation 1 - the vertical gradient in potential temperature θ) are carried out for each profile to facilitate the analysis discussed above. In order to mitigate large, non-physical variations in stability common to high-resolution profiles such as those used here, 2- σ Gaussian smoothing is applied to θ prior to the following calculation, $\frac{\partial\theta}{\partial z}$, to reduce oscillations. Vertical gradients of θ are calculated using centered differences across 200-m deep layers.

$$(1) \quad \frac{\partial\theta}{\partial z}(z) = \frac{\theta_{[z+100]} - \theta_{[z-100]}}{z_{[z+100]} - z_{[z-100]}}$$

To carry out the initial comparison of O_3 and stability, 2-D histograms (joint frequency distributions) are created. O_3 and $\frac{\partial\theta}{\partial z}$ observations are placed into bins. O_3 , in parts per billion by volume (ppbv), is organized into logarithmic-bins with a bin size of 0.1 dB along the x-axis while $\frac{\partial\theta}{\partial z}$ is placed into 2 K km⁻¹ bins and displayed along the y-axis. If a clear separation between tropospheric and stratospheric air is established, the resulting $\frac{\partial\theta}{\partial z}$ threshold can be used to identify a stability-based tropopause.

Using the stability threshold found in the 2-D histogram analysis, individual plots are chosen from each location where the LRT definition performance is poor. For Boulder, this tends to be most common during the Spring/Fall during double-tropopause events (complex layering of tropospheric and stratospheric air). For Hilo, the LRT appeared to struggle most often during the summer months, something that could be investigated further later on. The

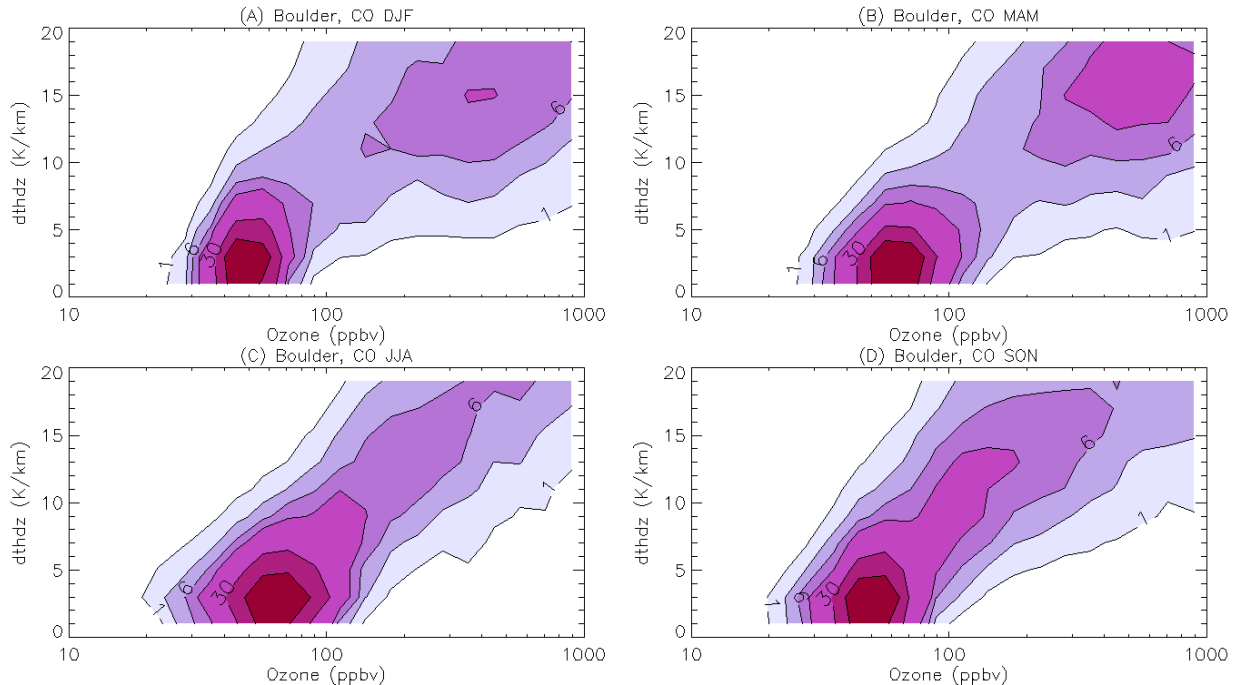


FIG. 2. Seasonal variability of ozone and stability in Boulder, CO. Each panel is meant to be divided by meteorological season, but identified by months to alleviate confusion. Panel (A) is DJF, panel (B) is MAM, panel (C) is JJA, and panel (D) is SON.

LRT is known to fail commonly at the South Pole during their winter months, or the northern-hemispheric summer, tending to greatly overestimate the height of the tropopause transition layer. Using three vertical profiles of temperature, stability, and O_3 , we examine the relative success of the LRT definition and our identified stability threshold, with O_3 being the determining factor of accuracy.

3. Results and Discussion

a. Relationships between O_3 and Stability

Figure 2 shows a 2-D histogram for Boulder, CO comparing O_3 composition and stability. In all four seasons there is an obvious frequency maximum around 40-60 ppbv and $< 5 \text{ K km}^{-1}$ of stability, which is characteristic of tropospheric air with consistently low O_3 and low stability. The spring / summer months feature a slightly higher O_3 budget relative to low stability. Above 9 K km^{-1} stability and $\sim 100 \text{ ppbv}$ of O_3 , we begin to see a strong positive slope between the two, providing a clear separation between the troposphere and stratosphere. Although it is well known the tropopause height varies by season, this 9 K km^{-1} threshold of marking the tropopause appears to be fairly consistent across all seasons, suggesting this as a suitable threshold to broadly delineate the upper troposphere from the lower stratosphere throughout the year.

Figure 3 contains the same histogram, but for Hilo, HI. The tropics appear to have less troposphere-stratosphere contrast than Boulder and more variability in tropospheric ozone, with a more-widely spread frequency maximum below 100 ppbv. The separation between the tropospheric and stratospheric regions are less defined than in Figure 2, and this likely due to upward moving air in the tropics creating a less pronounced O_3 change across the tropopause (Dobson 1956, e.g.). However, 9 K km^{-1} of stability still functions as a good delineation between the two air masses. This too varies slightly by season, as 8 K km^{-1} works best in the warmer months while 10 K km^{-1} does best in the cooler seasons. But, the 9 K km^{-1} threshold is still a good average and marks an obvious separation of troposphere and stratosphere. Upon further inspection, there appears to be higher O_3 concentrations at low stability in the spring (Figure 3b) compared to any other season. This can be attributed to dominating O_3 -rich airflow from Eurasia, on account of powerful mid-latitude westerly flow and the relative location of the Hadley cell in the springtime, leaving Hilo, HI susceptible to the subtropical jet (Lin et al. 2014) to experience higher amounts of O_3 . STE is also a big contributor to O_3 concentrations, especially in events of deep convection and air mass transport (Tinney and Homeyer 2021; Pan et al. 2014). This can also be said for Boulder, CO coinciding with a spring / summer increase in O_3 due to westerly transport and seasonally-

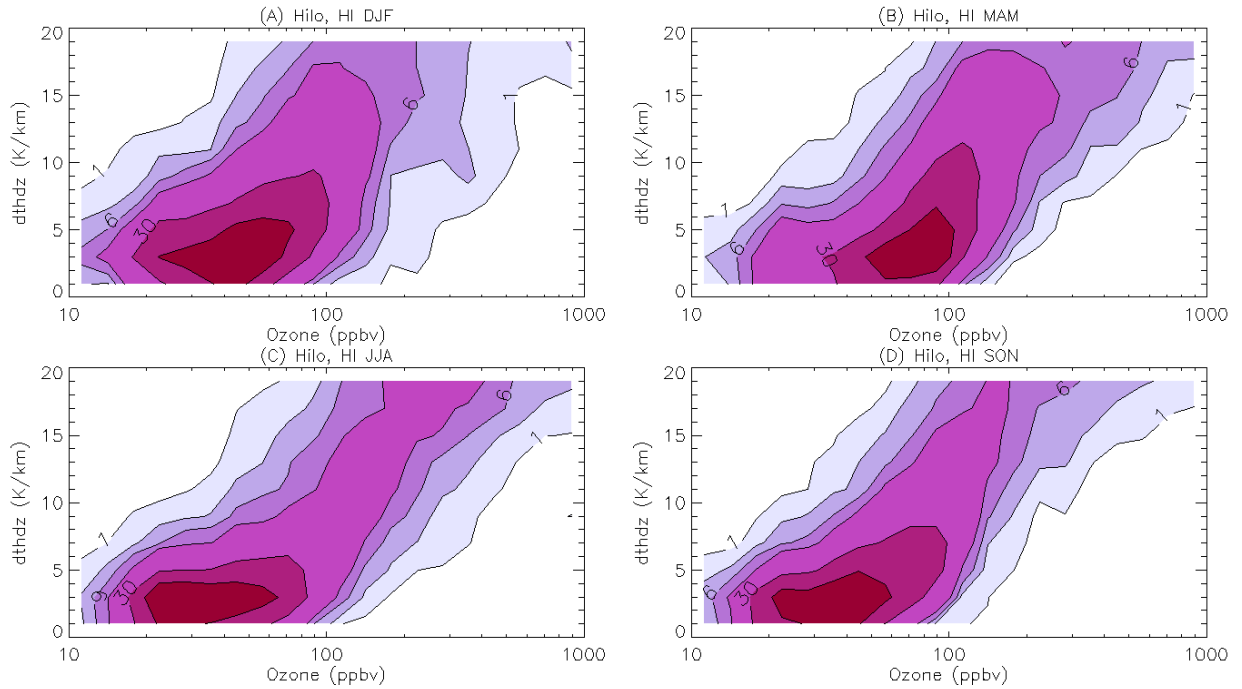


FIG. 3. As in figure 2, but for Hilo, HI.

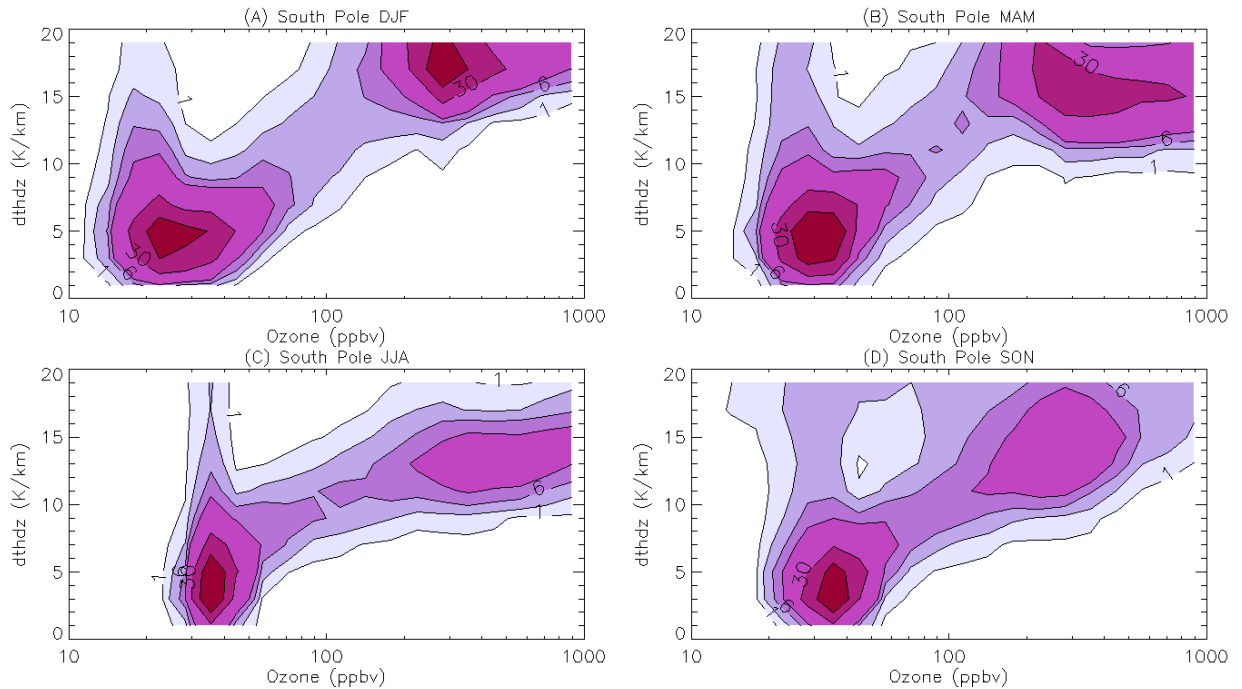


FIG. 4. As in figure 2, but for the Amundsen-Scott South Pole Station.

common tropopause folds in this region (Langford et al. 2009, e.g.).

The South Pole station histogram is shown in Figure 4, and features one of the most distinct comparisons between O_3 and stability. The South Pole contains a tropopause

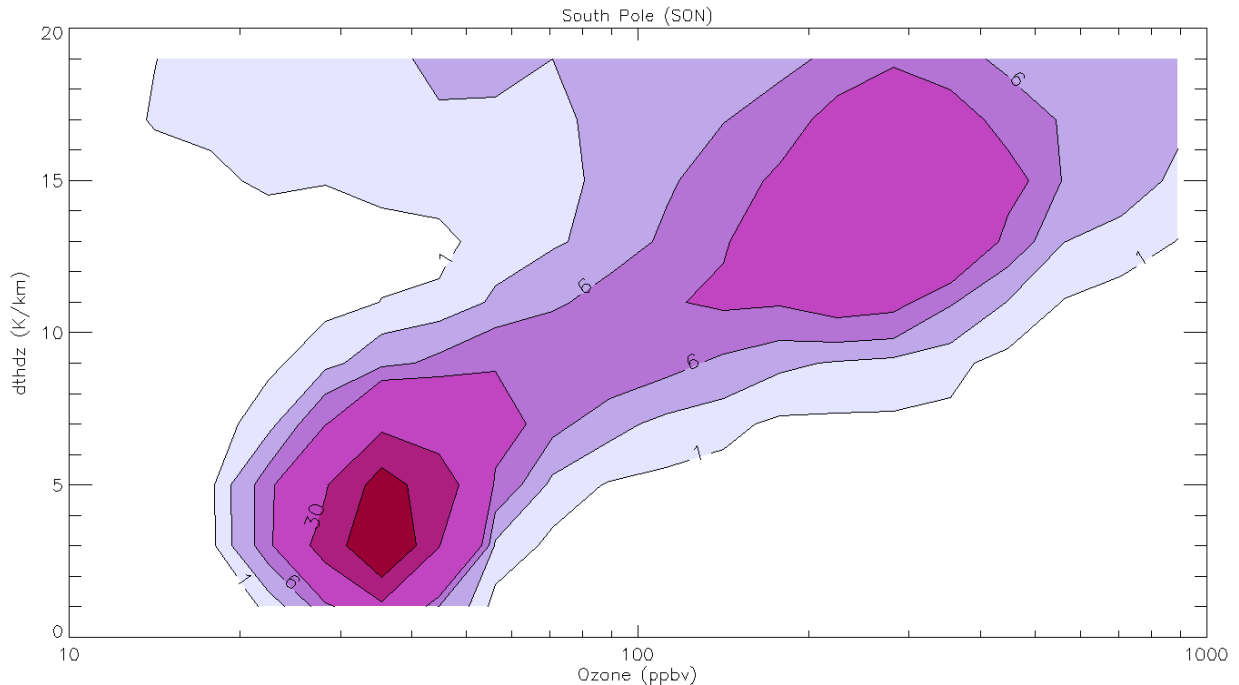


FIG. 5. SON in the South Pole with the bottom 4 km excluded.

that is difficult to identify with the LRT, yet can easily be defined by an increase in O_3 and the 9 K km^{-1} stability threshold. Two apparent maxima can be seen in all panels, one at low stability and low O_3 and the other at high stability and high O_3 concentrations. Yet again, a very pronounced difference between tropospheric and stratospheric air along a positive slope can be seen. These figures are very different from the other two locations, especially in the way there is relatively high stability below 40 ppbv of O_3 . This is likely indicative of a stable boundary layer, where low-tropospheric stability values are high in cold Antarctic temperatures. By factoring out the bottom 4 km of the troposphere (Figure 5), the anomaly largely disappears, confirming that this signal mostly originates from the boundary layer and is not related to UTLS O_3 /stability relationships. Looking at SON (Figure 5), the remaining low amounts of O_3 at high stability (between 40 ppbv and 100 ppbv) are likely indicative of the stratospheric O_3 hole, which is most common during the spring months over Antarctica.

Upon analyzing these 2-D histograms, 9 K km^{-1} appears to be a suitable, seasonally and geographically consistent threshold for separating the troposphere and stratosphere based on the relationship between stability and O_3 composition. It is important to keep in mind that this is a multi-decade average divided trimonthly for each of these stations. High and/or low outlier data possibly exists, which is why comparing these parameters across varying latitudinal locations is important for identifying a univer-

sal threshold. Although this can be fine tuned even further, potentially to a decimal amount, the defining amount provides a general idea where the separation of the UTLS is located and can be applied to individual vertical profiles, as long as stability is calculated.

b. Tropopause Comparison and Evaluation

Now that a stability threshold of 9 K km^{-1} has been established, we can move on to evaluating its performance in individual vertical profiles from each of the three locations. Of the nearly 6000 ozonesonde observations utilized in this study, three profiles were selected in cases where the LRT appears to clearly fail. Next, calculating both the LRT and the 9 K km^{-1} stability threshold tropopause, we can see the difference in where the LRT may identify the transition layer in comparison to stability. By analyzing both defined tropopause layers on top of O_3 concentration, we can examine how these different tropopause definitions perform compared to the vertical gradient of O_3 . Since O_3 is a tracer of stratospheric air, a rapid increase and strong gradient in the UTLS allows us to infer the location of the tropopause transition layer.

Beginning with Boulder, CO, a springtime ozonesonde observation (Figure 6) is chosen due to the relatively high frequency of double tropopause days within this area at this season, offering complexity in the UTLS. The LRT identifies a tropopause located around 11.5 km. While there is an inversion found just below 11 km, this was not

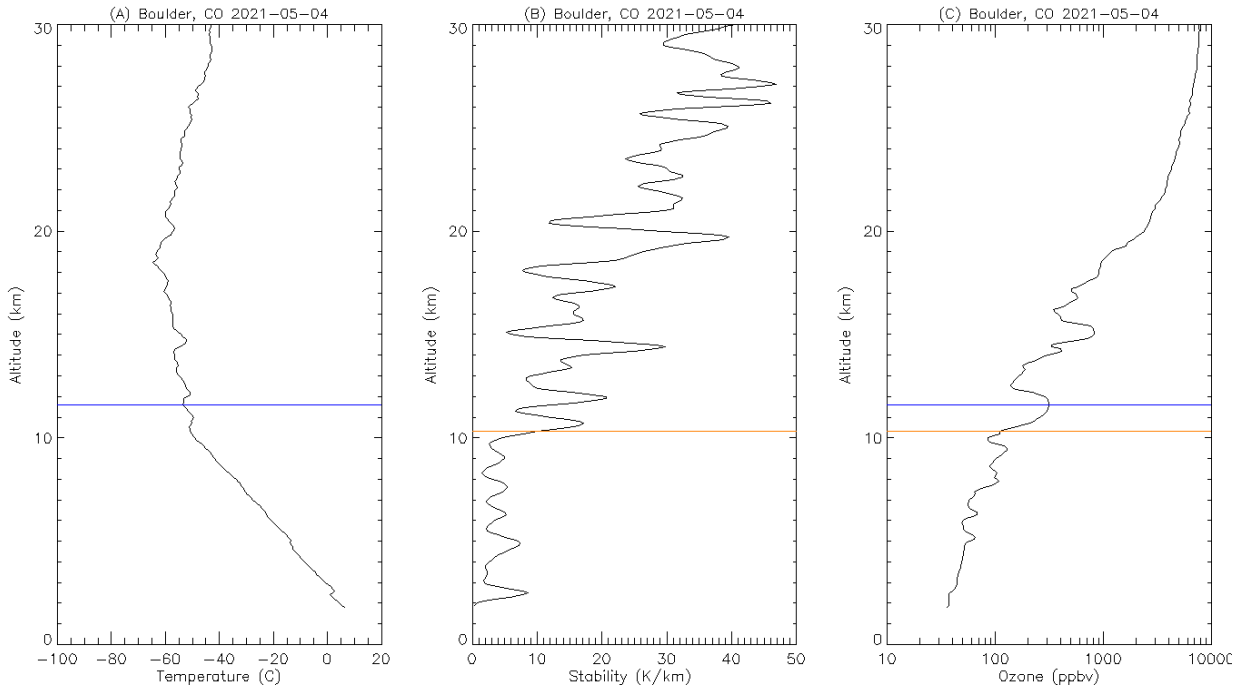


FIG. 6. Three parameter comparison in Boulder, CO on May 4th, 2021. Each panel is divided by variable, featuring: Temperature (A) with the WMO tropopause plotted, stability (B) with the 9 K km^{-1} threshold calculated, and ozone (C) with both the WMO tropopause and stability threshold overlaid for comparison.

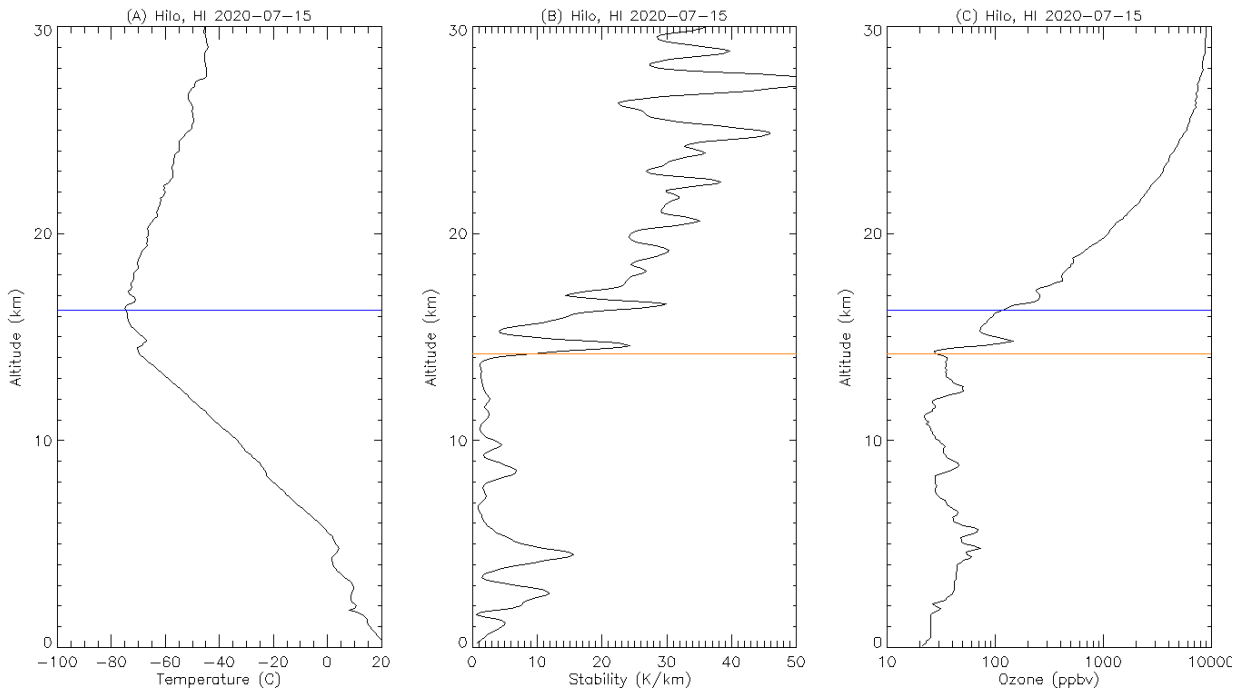


FIG. 7. As in figure 6, but for Hilo, HI on July 15th, 2021.

identified as the tropopause likely because it didn't meet the 2°C km^{-1} lapse-rate definition. Conversely, the stability threshold marked a 9 K km^{-1} oscillation above 10 km in Figure 6b where the first local temperature minimum

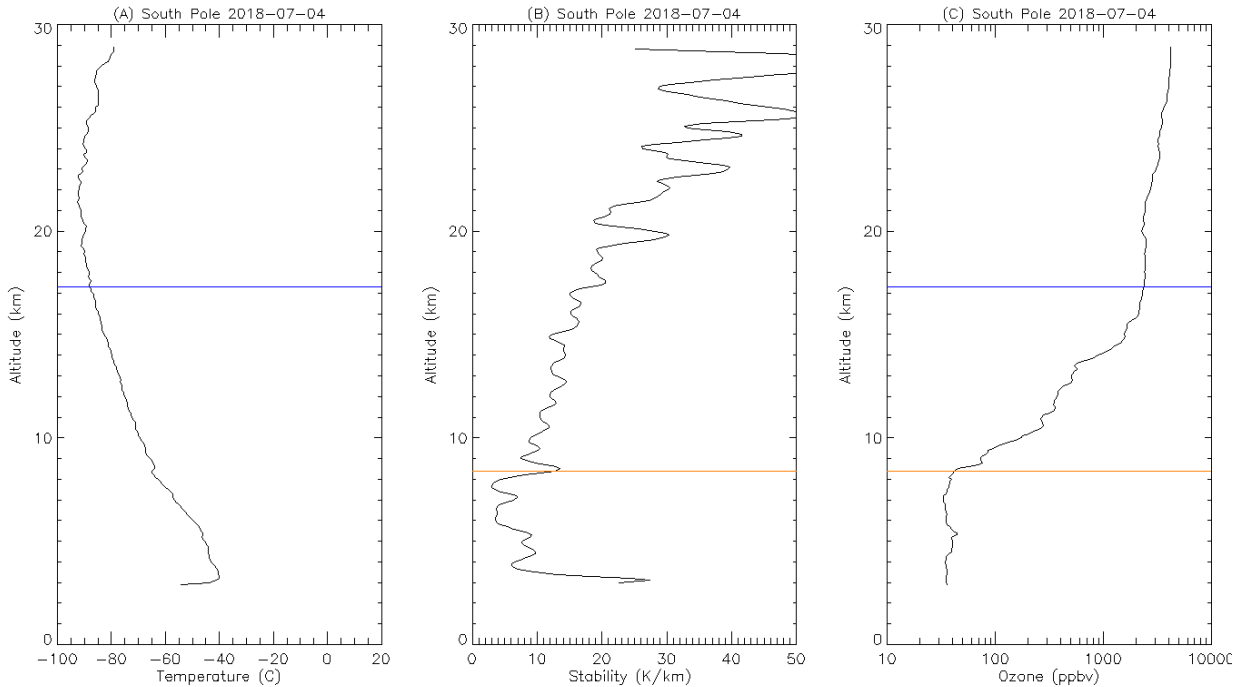


FIG. 8. As in figure 6, but for the Amundsen-Scott South Pole Station on July 4th, 2018.

occurs. This stability-based tropopause corresponds well to a large increase in O_3 (Figure 6c), whereas the LRT occurs at a local O_3 maximum. The increase in O_3 concentration at 10 km suggests that the stability threshold is accurately identifying the tropopause, while the LRT places it 1.5 km too high. This is a significant difference in altitude and can have a profound impact on studies that rely on an accurately-identified tropopause, such as those focused on STE.

Next is Hilo, HI in Figure 7. A hot, July summer month, where an even larger difference between the LRT and stability can be seen. The LRT didn't identify the first temperature inversion near 14 km since it didn't make the 2°C km^{-1} threshold, yet again, but stability caught the transition almost spot-on, as seen in the first large oscillation. Comparing these to O_3 , there it coincided with a large increase as well, marking entrance into the tropopause transition layer. The difference between the two tropopause contours is nearly 2 km, meaning this could have an even larger impact on quantitative studies, as mentioned in the preceding paragraph.

Lastly, we have the South Pole in Figure 8. This was observed on Independence Day, a cold winter month for the region. Because it can be so cold, especially with increasing altitude, the LRT regularly fails during this season. Using the 9 K km^{-1} stability threshold, the entrance of the tropopause can easily be seen in comparison with O_3 at 8.25 km, whereas the LRT is just above 17 km. There is a whole 9 km between each of these markers, but can easily

be solved by approaching from a stability and composition standpoint.

4. Conclusions

Using O_3 measurements and calculations of potential temperature, we examined the relationship between stability and composition in the UTLS with a focus upon the tropopause transition layer. There are many different definitions that can be used adjacent to the topic being researched, but few that can be applied universally. Our goal was to discover a stability threshold contingent upon UTLS O_3 concentration change across the tropical, polar, and extratropical regions. Specifically, we found that 9 K km^{-1} of stability is a reliable marker separating low- O_3 tropospheric air from O_3 -rich stratospheric air. The threshold was shown to work extremely well in all regions, especially where the LRT tropopause can fail, although there can be issues with oscillation below the tropopause that reach 9 K km^{-1} in instances of extremely stable boundary layers. For these types of situations, it is important to look at the threshold in comparison with temperature and/or O_3 , searching for an inversion/slightly isothermal layer corresponding with an increase in O_3 . The development of a universally applicable algorithm will take additional work to ensure it can handle myriad complexities. The relationship between stability and composition established in this study can be applied to conventional

observations, such as what is received from a typical radiosonde, as well as model analyses and forecasts. In doing so, it is important to calculate stability using 100-m averaged vertical profile of $\frac{\partial\theta}{\partial z}$ for consistency.

Although the 9 K km^{-1} stability threshold is ideal and tends to work in situations the LRT may fail, there are several limitations worth highlighting. First, the data obtained in this study from the ESRL Global Monitoring Laboratory only uses 3 locations, though these locations are within climatologically and latitudinally diverse regions. Incorporating data from other locations can be done, but a majority of alternative stations lack consistency and longevity in data. Second, the 9 K km^{-1} marker has not yet been verified to work in models. With time, this can be tested and applied, especially using chemistry-climate model output where composition information is available. Thirdly, as mentioned in the previous paragraph, oscillations exceeding 9 K km^{-1} can happen below the tropopause. This can be worked around by establishing a minimum height the tropopause can be located. Lastly, this threshold requires 100-m averaged profiles and may be sensitive to smoothing. We chose $2\text{-}\sigma$ Gaussian smoothing for the $\frac{\partial\theta}{\partial z}$ calculation to preserve data and create clear, concise profiles.

This study brings forth a latitudinally diverse but ubiquitous understanding of the relationship between stability and composition. The established 9 K km^{-1} threshold is promising and with future work on the development of a complete algorithm, this method could potentially provide better apprehension and accuracy in locating the tropopause transition layer with conventional observations. Further implications could include (but are not limited to) taking an in-depth look at quantifying the tropopause depth and/or sharpness, tracer-tracer analyses, STE contribution, and climate-model inclusion. With the establishment of a universal stability-based tropopause definition, better insight could be provided to the complexity of the UTLS while alleviating confusion surrounding the transition layer.

Acknowledgments. This research has been supported by the National Science Foundation (NSF) under Grant No. AGS-1560419. The authors would like to thank Dr. Daphne LaDue and Alex Marmo for running a great virtual program and prospering, even with the ongoing difficulties of the coronavirus pandemic. An extended thanks is given to the National Weather Center (NWC) for hosting this initiative. Lastly, Lexy would like to specifically thank Emily Tinney, a NWC REU alumni and PhD student at OU/SOM and Dr. Cameron Homeyer, Associate Professor and Director for Graduate Programs at OU/SOM for their amazing mentorship during the course of this summer.

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