

Signature of a tropical Pacific cyclone in the composition of the upper troposphere over Socorro, NM

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Introduction

This supplement contains figures and discussion to support the conclusions of the paper by Minschwaner et al [2015]. It is focused primarily on two topics: comparison of ozone vertical profiles between the MLS satellite instrument and Socorro ozonesondes, and interpretation of low relative humidity observed in the same air masses with low ozone.

Text S1.

It should be noted that detailed comparisons of the datasets are not the primary focus of our analysis, and that the main purpose for using MLS data in the paper is to provide context for the interpretation of the Socorro ozonesonde observations. However, this context is valid only to the extent that the two datasets are consistent with each other. The difficulties in comparing satellite data with balloon data mainly involve co-location (both spatial and temporal), sampling, and averaging. As discussed by Livesey *et al.* [2015], there are important considerations when comparing vertical profiles of mixing ratio from MLS to profiles measured with higher vertical resolution. Since MLS Level 2 data describe a piecewise linear representation of vertical profiles at fixed pressure levels, the high resolution ozonesonde profile must be interpolated to the MLS retrieval

grid using a least-squares fitting procedure before applying the appropriate averaging kernels to produce a simulated MLS profile. In reality, the full MLS averaging kernels are complicated two-dimensional quantities reflecting the tomographic nature of MLS retrievals, but for the purposes of individual profile comparisons, representative mean vertical averaging kernels are available for each retrieved data product.

Figure S1 shows the Socorro raw ozonesonde vertical profile from 12 Aug, 2015, along with a simulated MLS ozone profile derived from the gridded ozonesonde values. Also shown is the measured MLS profile closest to Socorro on that day (located at 34.1N, 113W, about 500 km west of Socorro), and the a priori profile used for the measurement retrieval. The measurement times are nearly coincident (20.37 UT for MLS, 20.3-20.6 UT for the ozonesonde between 10 and 15 km altitude).

The simulated profile includes the effects of averaging kernels on differences between the gridded ozonesonde values and the a priori ozone profile [Livesey *et al.*, 2015], and can be considered a “best estimate” of what MLS should have seen if the raw ozonesonde data are taken as an exact description of the true atmospheric state. Figure S1 indicates good agreement between the simulated MLS profile from the ozonesonde and the nearest measurement from MLS. While there are some difference in the exact shape of the low ozone region between 383 and 147 hPa, both profiles show minimum values between 15 and 30 ppbv, and the large deviation of the MLS measurements from the a priori (up to 70% smaller) provides a good indication that MLS can detect anomalies such as this in the upper troposphere.

Another method that makes use of MLS data to detect and track ozone anomalies is the reverse domain-filling (RDF) trajectory analysis outlined by Manney *et al.* [1998, 2009]. Using this method, we generated vertical profiles based on five-day back trajectories and observed MLS ozone fields. The trajectories were initialized in a $1^\circ \times 1^\circ$ box around Socorro (e.g., Figure 3) and at 100 potential temperature (Θ) layers equally spaced in $\log(\Theta)$. After going back 5 days to the origination points of these trajectories, the ozone mixing ratio is determined using MLS version 4 ozone fields interpolated to the trajectory locations. This provides an indication of what might be observed if the ozone field from 5 days earlier was passively transported over Socorro on the date of the ozonesonde flight at 18 UT (very close to the typical sounding times). Figure S2 shows the results for 9 August, 2015, in which all of the RDF profiles display low-ozone signatures consistent with the ozonesonde profile for that day.

Text S2.

Calculations of water vapor amounts were carried out using temperatures along a cluster of five-day back trajectories centered on Socorro, such as those shown in Figure 3. The air parcels were assumed to be at 80% relative humidity at the trajectory origination points on 8 Aug, five days prior to the terminal date of 12 Aug. The corresponding water vapor mixing ratios are then determined by the temperatures at these origination points. Water vapor mixing ratios were conserved along trajectories, except if the temperature along a parcel forward trajectory fell below the saturation point, at which point excess water was removed and relative humidity fixed at 100% until subsequent trajectory temperatures rose above the new saturation point. This approach is similar to the water vapor simulations described by Dessler and Sherwood [2000].

Figure S3 shows air parcel pressure and relative humidity as a function of time over the forward parcel trajectories. Pressures initially start near 200 hPa and descend over time to near 250 hPa. Evidence of wave activity is apparent in some parcels, particularly as indicated by quasi-periodic vertical displacements during days 1 and 2. The final relative humidity is generally between 5% and 20%, consistent with the Socorro relative humidity near 11 km shown in Figure 4. Final results were not significantly sensitive to the initial value of 80% relative humidity. Roughly one-third of the parcels reached saturation within the initial 12 hours of the forward trajectory, and the largest decreases in relative humidity for most parcels occurred during day 1 and between days 2 and 4. Humidity values near days 2 and 3, when air parcels were closest to Hilo, are in the range of 20%-50% and these are broadly consistent with the Hilo humidity profile from Figure 4.

References

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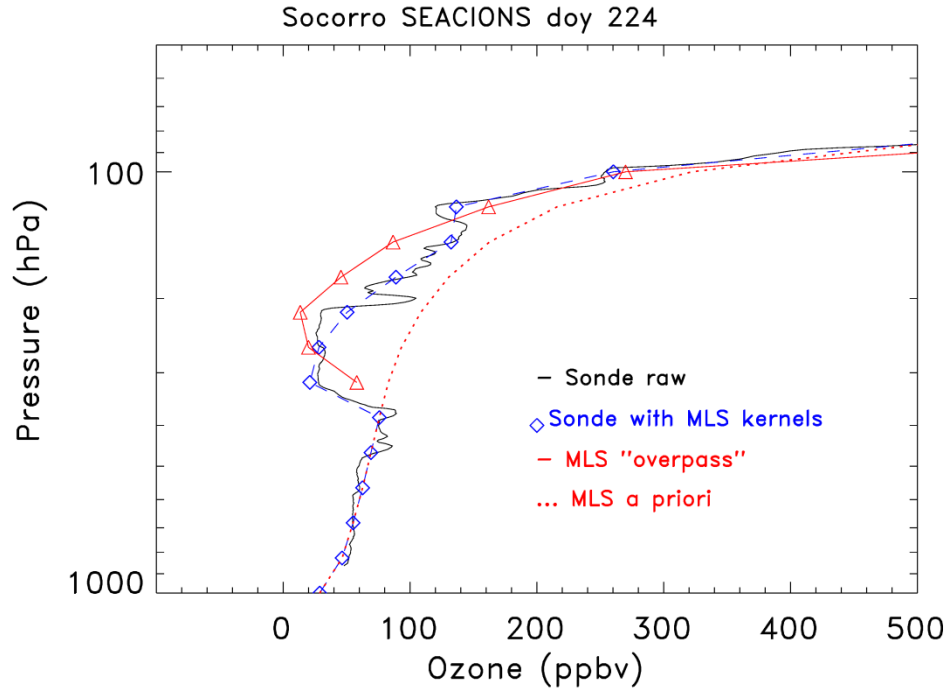


Figure S1. Ozone vertical profiles measured on 12 August, 2013 from the Socorro ozonesonde (solid black), simulated MLS using ozonesonde data on MLS retrieval grid and averaging kernels (blue triangles), nearest MLS profile to Socorro (red triangles, measurement centered at 34.1°N, 113°W), and a priori ozone profile used for this MLS retrieval (red dotted).

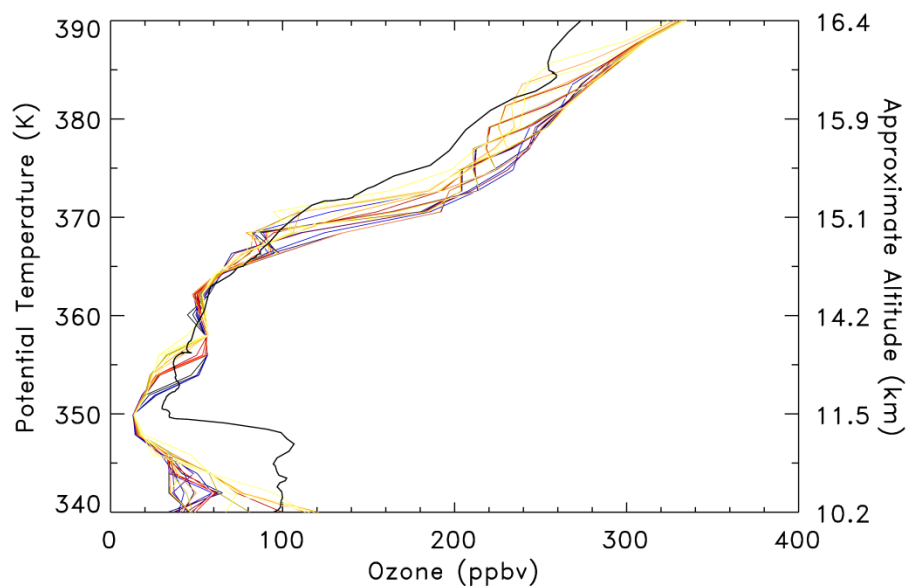


Figure S2. Cluster of simulated ozone profiles over Socorro for 9 Aug, 2013, using the reverse domain filling technique and gridded ozone observations from MLS from 4 Aug, 2013 (color curves). The observed profile from 9 Aug is shown in black.

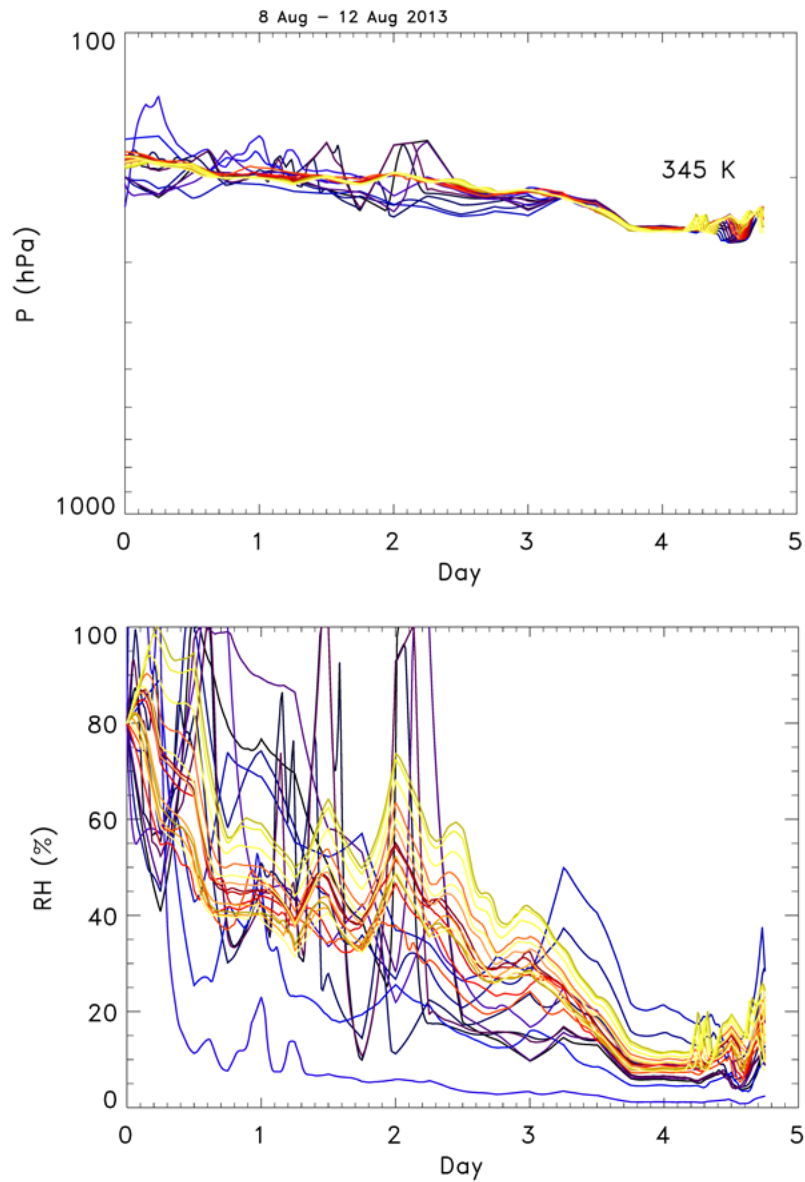


Figure S3. (Top) Variation in pressure along 5-day back trajectories initialized on the 345 K theta level from Socorro during the period 8 August to 12 August, 2013. (Bottom) Variation in relative humidity along the same trajectories, based on temperatures and assuming initial RH values of 80%.