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Short Report

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The Formation Mechanisms of Layered Structures in the Subtropical Troposphere Revealed by Integrated Analysis of Sonde and Atmospheric Reanalysis Data

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Abstract

Material tracers such as ozone and water vapor concentration as observed by balloon measurements often show a marked vertical fluctuation. Previous studies examined the formation mechanism of such a “layered structure” mainly by using a correlation analysis between O_3 and potential temperature (θ) as obtained by balloon measurements: if the correlation is high, the vertical wind fluctuation associated with gravity waves is a key. The present study has found a case where this

analysis alone cannot specify the formation mechanism. We thus for the first time adopt a backward trajectory analysis for identifying the formation mechanism. It is clearly shown that this structure was primarily formed by the quasi-horizontal mixing of distinct air masses: an O_3 -poor/ H_2O -rich tropical air mass and an O_3 -rich/ H_2O -poor subtropical air mass. The observed high correlation between O_3 and θ likely results from weak upward and downward motions of these air masses associated with the Hadley circulation rather than vertical wind fluctuations. It is suggested that conventional correlation methods may overestimate the contribution of gravity waves.

Keywords

Layered structure, horizontal mixing, Gravity wave, Backward trajectory analysis, ozonesonde, reanalysis

Statements and Declarations

Competing interests

The authors declare that they have no competing interests.

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1 Introduction

In the troposphere, atmospheric minor constituents (e.g., ozone (O_3) and water-vapor (H_2O)) and meteorological parameters (e.g., potential temperature) often change significantly in the vertical direction with a scale of several hundred meters to several kilometers (e.g., Newell et al. 1996, 1999; Wu et al. 1997): this is sometimes called the “layered structure”.

The cause of layered structure has been discussed mainly from two perspectives: quasi-horizontal mixing and vertical wind fluctuation. Newell et al. (1996, 1999), and Wu et al. (1997) suggested that it was formed by the mixing of different air masses that were quasi-horizontally advected from different regions; for instance, the atmosphere over the tropical ocean has relatively low ozone concentration and high water-vapor concentration. Shiotani et al. (2002) indeed analyzed data from balloon measurements over the equatorial Eastern Pacific and found alternating structures of O_3 -poor ($O_3 -$)/ H_2O -rich ($H_2O +$) layers (hereafter denoted as $< O_3 - / H_2O + >$) and O_3 -rich ($O_3 +$)/ H_2O -poor ($H_2O -$) layers (hereafter denoted as $< O_3 + / H_2O - >$), with each having a thickness of approximately 1-2 km. They also found that the $< O_3 - / H_2O + >$ layer was accompanied by the wind blowing from the ITCZ, suggesting that the observed layered structure was formed by an air mass

54 originating in the tropical region with $\langle O_3 - /H_2O+ \rangle$ being advected and
55 intruding into the subtropical region with $\langle O_3 + /H_2O- \rangle$. Otsuka and Yoden
56 (2005) supported this idea by performing numerical simulations. They also pointed
57 out that the near-equatorial horizontal flow was not strongly constrained by the
58 thermal wind relationship so that it could evolve somewhat independently at different
59 levels, facilitating the formation of strong vertical shear.

60 Vertical wind fluctuations associated with gravity waves (GWs) also produce the
61 vertical anomalies in material tracers such as potential temperature (θ) and
62 ozone/water-vapor concentration given that they have a marked vertical gradient
63 (Holton, 1987). Based on this argument, Pierce and Grant (1998, hereafter referred
64 to as PG98) analyzed the correlation coefficient between ozone mixing ratio ($[O_3]$)
65 and θ , both of which are considered material tracers, using ozonesonde data at a
66 midlatitude station (see Section 3 for details). They regarded the layers with high
67 correlation as those caused by GWs (i.e., vertical wind fluctuations), while the layers
68 with low correlation as those caused by “Rossby waves” (this identification seems
69 vague but is likely based on the argument that quasi-horizontal Rossby-wave motions
70 result in little θ variation). The authors then suggested that more than 60% of
71 layered structures in the upper troposphere and the lower stratosphere in a particular

season were formed by GWs. Thompson et al (2011, hereafter denoted as T11) adopted this method to tropical and subtropical ozonesonde data collected by the SHADOZ project, and found that more than 40% of the cases could be attributed to GWs at some sites.

As outlined above, previous studies discussed the formation mechanism relying on somewhat “indirect” evidence, such as local correlation coefficient analysis of profile observations or numerical simulations. This was partly because the typical vertical scale of the layered structures was too small to be resolved by conventional reanalysis data. In recent years, however, the vertical resolution of reanalysis data has significantly improved; for example, the ERA5 model-level data provided by ECMWF features a vertical resolution of approximately 150-350 m in the troposphere.

In this study, we will demonstrate that such latest reanalysis can be used to directly elucidate the formation mechanism of observed layered structure. Notably, by analyzing radiosonde data taken over the subtropical western Pacific, we have found a case where the conventional correlation analysis alone cannot specify the formation mechanism. A backward trajectory analysis with ERA5 succeeds in clearly revealing that the layered structure is primarily produced by quasi-horizontal mixing of air

masses originating from the tropical and subtropical regions.

The remaining manuscript is organized as follows. Section 2 and Section 3 describe datasets and analysis method, respectively. Section 4 presents the results and examines the formation mechanism using backward trajectory analysis. Section 5 summarizes the main findings, while discussing why the mechanism was difficult to identify with the conventional approach that only used radiosonde data.

2 Data Description

a. Radiosonde data

We use balloon measurement data taken through the Years of the Maritime Continent Boreal Summer Monsoon 2021 campaign (YMC-BSM 2021). Figure 1 shows the balloon launching points. We analyze data from May 27 to June 3, 2021, when both ozonesondes and conventional radiosondes were used for measurements. Data were recorded every second, which corresponds to a vertical resolution of ~ 5 m. Following the previous studies, we analyze data of θ (calculated from the temperature and pressure), relative humidity RH (%), and $[O_3]$ (kg kg^{-1}) for identifying the layered structures. As this study does not consider very small-scale vertical variations, the radiosonde data are smoothed using a 100-meter vertical running mean before the following analysis.

b. Reanalysis data (ERA5-model-level Data)

To analyze the spatiotemporal characteristics of the layered structures, we use model-level data (Hersbach et al. 2017) of ERA5 (Hersbach et al. 2020). The vertical resolution of the data is approximately 150 to 350 m in terms of geopotential height in the troposphere (at altitudes of 2-16 km), which is sufficient for resolving a layered structure with a vertical scale of a few kilometers. Just as for the sonde data, we analyze ERA5 data for θ (K), RH (%), and $[O_3]$ (kg kg^{-1}), where RH is calculated from the specific humidity, pressure and temperature. As the model-levels are on hybrid σ - p coordinate, the data are interpolated to uniform altitude grids where geopotential height (gph) on model levels is calculated following ECMWF (2024) and is regarded as “altitude”.

In section 4, the Ertel potential vorticity on an isentropic surface (Π_θ , hereafter PV) is calculated as follows (c.f., Achatz, 2022):

$$\Pi_\theta = -g(f + \zeta_\theta) \frac{\partial \theta}{\partial p} \quad (1)$$

where g is the gravitational acceleration, f is the Coriolis parameter, and ζ_θ is the relative vorticity on the isentropic surface. Note that the conventional radiosonde data during YMC-BSM 2021 campaign were assimilated into ERA5, whereas the ozonesonde data were not.

3 Analysis Method

a. Correlation Analysis

We revisit the correlation analysis that was proposed by PG98 and T11 for identifying the formation mechanism. First, for any observed quantity x in data from radiosonde measurements or ERA5 (e.g., $[O_3]$ and RH), its vertical anomaly x' associated with the layered structure is defined as

$$x' = \frac{x - \bar{x}}{\bar{x}} \quad (2)$$

where $\bar{x}$ is the background field of a variable defined as the 2500-m vertical running mean.

If the tracer advection associated with vertical wind fluctuations is dominant over advection associated with horizontal wind variations, as is typical for GWs, the vertical ozone anomaly could be estimated (denoted as $[O_3]'_E$) by using θ' as well as $\overline{[O_3]}$ and θ :

$$[O_3]'_E = \theta' \cdot R(z) : R(z) = \left(\frac{1}{\overline{[O_3]}} \frac{\partial \overline{[O_3]}}{\partial z} \right) / \left(\frac{1}{\bar{\theta}} \frac{\partial \bar{\theta}}{\partial z} \right) \quad (3)$$

PG98 and T11 thus identified the layers with $|[O_3]'| > 0.1$ and the correlation coefficient between $[O_3]'$ and $[O_3]'_E$ (hereafter denoted as $r([O_3]', [O_3]'_E)$) being greater > 0.7 as those induced by vertical fluctuations of GWs. In this study, the vertical profiles of $r([O_3]', [O_3]'_E)$ are obtained by computing r over a 5 km

vertical window, shifted by 10 m (50 m) for the radiosonde (ERA5) data. We note, however, that a large $r([O_3]', [O_3]_E')$ does not necessarily guarantee an exact agreement between their absolute values.

b. Backward Trajectory Analysis

As a more direct approach to investigate the formation mechanisms of layered structures, we conduct a backward trajectory analysis using LAGRANTO (Sprenger and Wernli 2015). This tool calculates the trajectories of air parcels by using the three-dimensional wind vectors on model levels (u, v, ω). Note that ω in the ERA5 does not account for subgrid-scale convection transport, such as cumulus convection (Sprenger and Wernli 2015).

4 Results

Figure 2 shows the vertical profiles of $[O_3]'$ and RH' as well as $[O_3]_E'$ and $r([O_3]', [O_3]_E')$ on May 30, 2021, as obtained by radiosonde measurement (Figs. 2a and 2b) and from ERA5 (Figs. 2c and 2d) (the reason why this date was chosen for analysis will be described later). The radiosonde measurements show that both $[O_3]'$ and RH' have large vertical fluctuations with the vertical scales ranging from a few

hundred meters to a few kilometers (Figs. 2a and 2c). Also, anti-correlation between $[O_3]'$ and RH' is observed over a wide vertical range from 4 to 14 km (Fig. 2a). For subsequent discussion, the layer with $[O_3]' > 0.1$ and $RH' < -0.1$ over 200 m (in vertical) is referred to as $< O_3 +/H_2O->$ (shaded in light red), while that with $[O_3]' < -0.1$ and $RH' > 0.1$ is as $< O_3 -/H_2O+>$ (shaded in blue). As noted in Sec. 1, previous studies suggested that such a layered structure was produced by quasi-horizontal mixing of different air masses with different origins (e.g., Newell et al. 1996; Shiotani et al. 2002). By contrast, we also find that $r([O_3]', [O_3]_E')$ is high (~ 0.7) over this altitude region (Fig. 2b). Again, note that the layer with $r > 0.7$ was considered as being formed by vertical wind fluctuations associated with GWs (PG98 and T11).

According to previous studies, these findings thus imply that two seemingly two quite different processes — quasi-horizontal mixing and vertical fluctuations associated with GWs— are simultaneously involved in the formation of the layered structure. There were no other cases where both formation mechanisms are suggested (see Online Resource 1 and 2 for profiles on other days), thus our focus on this particular profile.

Notably, we find that the characteristics of the observed layered structure, such as

the anti-correlation between $[O_3]'$ and RH' and large $r([O_3]', [O_3]_E')$, are quite well reproduced by ERA5 especially for 7-10 km in altitude, though the vertical scale of layered structures is relatively large compared to observation (Fig. 2). In the following, we will focus on the layered structure for this altitude region using ERA5.

Figure 3 shows the latitude-pressure cross sections along $148.5^\circ E$ for (a) $[O_3]'$ and (b) RH' , and the longitude-pressure cross sections along $17.5^\circ N$ for (c) $[O_3]'$ and (d) RH' , at 09:00 UTC on May 30, 2021 as revealed by ERA5 data. The triple-layered structure with $<O_3 + /H_2O-> / <O_3 - /H_2O+> / <O_3 + /H_2O->$ observed in balloon measurements over 7~10 km in altitude (Fig. 2c) extend meridionally over $15-25^\circ N$ and zonally over $143-152^\circ E$. The thickness of each layer is spatially almost uniform, ranging from approximately 0.5 to 1 km (50-100 hPa in pressure).

We also find that these layers move southward and slightly downward with time (see Online Resource 3). Note that the downward-moving wavy structure reminds us of a GW propagation with downward phase progression and upward energy propagation; however, the vertical anomaly in horizontal wind velocity (more specifically, band-pass filtered data for vertical wave lengths between 0.5 and 4.0 km) does not show a clockwise hodograph which is a characteristic of GW with a

downward phase speed and an upward group velocity (c.f., Sato et al., 1997; Ogino et al., 2006) both for the radiosonde and ERA5 data (see Online Resource 4). This finding indicates that GWs are not the cause of the layered structure.

We then next calculate the backward trajectory of the air parcels sitting in the $< O_3 +/H_2O->$ and $< O_3 -/H_2O+>$ layers in Figs. 2c and 2d. As indicated in Fig. 3 (yellow and blue circles for $< O_3 +/H_2O->$ and $< O_3 -/H_2O+>$, respectively), their initial positions are set as follows:

■ Vertical levels : $< O_3 +/H_2O->$: 280, 290, 300, 400, and 410hPa

$< O_3 -/H_2O+>$: 330, 340, 350, 360, and 370hPa

■ Horizontal locations : 3×3 latitude-longitude grid points with the resolution of 0.5° with the center point at 17.5 °N, 148.5 °E (nearest grid point to the balloon launching site)

Backward trajectories are computed for 105 hours, from 09:00 UTC on May 30 to 00:00 UTC on May 26, 2021.

Figure 4 shows the positions of the air parcels as calculated by the backward trajectory analysis, at 00:00 UTC on May 26, 2021 (105 hours prior to the radiosonde observation time), as well as the horizontal distribution of $[O_3]$ (Fig. 4a) and RH (Fig. 4b) averaged over 5-12 km in altitude on that day. Most of the parcels belonging to the $< O_3 +/H_2O->$ layer (red circles) were originally located in the subtropical

region (10-25 °N), which is characterized by high ozone and low water-vapor concentrations. By contrast, most of the parcels in the $< O_3 - /H_2O + >$ layer (blue circles) come from the near-equatorial region (5-15 °N), which is characterized by low ozone and high water-vapor concentrations.

Figure 5a shows the horizontal map of the 105-hour backward trajectories for $< O_3 + /H_2O - >$ (red and magenta lines) and $< O_3 - /H_2O + >$ (blue lines), while Figure 5b displays the surface pressure (black contour) and the geopotential height at 350 hPa in pressure level (red contour) at 21:00 UTC on May 28, which corresponds to an intermediate time during the trajectory analysis. We see that the air parcels belonging to $< O_3 - /H_2O + >$ are advected from the near-equatorial region (5-15 °N) by anticyclonic flow, as visualized by the contour of 8,620 m over the region 10-23 °N and 140-147 °E (Fig. 5b). In contrast, most of the parcels in $< O_3 + /H_2O - >$ are found to be advected from the region north of 20 °N along the northerly wind in the region sandwiched between the anticyclone at (10-23 °N, 140-147 °E) and the strong cyclone at 15-23 °N, 156-166 °E (Fig. 5b).

To demonstrate the importance of anticyclonic flow for the formation of $< O_3 - /H_2O + >$ layer, Figure 6 shows the time series of ozone concentration on the 338-K isentropic surface, which corresponds to the vertical level of $< O_3 - /H_2O + >$

(see Fig. 2c). The near-tropical air mass with relatively low $[O_3]$ (indicated by red circle) around $10-15^\circ N$, $140-155^\circ E$ at 09:00 UTC on May 26 is advected northward (see Fig. 6a), with an elongated filamentary structure, to approximately $25^\circ N$ by 21:00 UTC on May 28 (see Fig. 6f). Subsequently, this region moves southward toward the observation site ($17.5^\circ N$, $148.5^\circ E$) by 09:00 UTC on May 30 (see Fig. 6i).

The intrusion of tropical air mass is also visualized by the movement of a low PV patch with < 0.3 PVU (see Online Resource 5). The cause of the northward movement around May 26 associated with a filamentary structure may be related with some dynamical instability, although the detailed mechanism has yet to be determined. On the other hand, the subsequent anticyclonic, returning motion into the tropics may be explained by the PV conservation: As the air mass moves northward, the relative vorticity decreases and produces an anticyclonic circulation to conserve its PV.

5 Discussion and Concluding Remarks

Our analysis has indicated that the triple-layered structure observed in the present case is very likely caused by quasi-horizontal mixing of air masses which had

originally different ozone/water-vapor concentrations, rather than by vertical fluctuations associated with GWs. The importance of horizontal mixing is also supported by the finding that the air masses themselves move downward with the motion of layers (Online Resource 3): If this structure were produced by GWs, the tracers (air parcels) would merely oscillate vertically.

This basically agrees with Shiotani et al. (2002)'s idea that the tropical air mass characterized by $\langle O_3 - /H_2O + \rangle$ intrudes into the subtropical region, contributing to the formation of a layered structure. Note that such intrusion over a narrow altitude region is possible presumably because the vertical scale of horizontal flow is very small near the tropics (Otsuka and Yoden, 2005): indeed, the Rossby height (fL/N ; L is horizontal scale and N is static stability ($\sim 10^{-2} \text{ s}^{-1}$), which is the height scale of the influence of an PV patch, is $\sim 2 \text{ km}$ for the air mass with $L = 500 \text{ km}$ at 20°N (c.f., Fig. 6), being consistent with the vertical scale of the observed layer.

However, these results raise a question: why is the $r([O_3]', [O_3]_E)$ so large (as shown in Fig. 2) given that this quantity was considered as a signal of vertical fluctuations? To address this issue, Figure 7 presents the latitude-pressure cross section of the backward trajectories, as well as the θ distribution averaged over $130^\circ\text{--}160^\circ \text{E}$ (contours and color shading) at 00:00 UTC on May 26 (105 hour prior to the

measurement time). As already shown, the air masses belonging to the $< O_3 - /H_2O+ >$ layer mostly originate in the tropical region. Here, we note that their trajectories at an early stage are accompanied by upward motion in the tropical region. Considering that the lower atmosphere has relatively lower θ (see contours in Fig. 7), these air masses (again with $< O_3 - /H_2O+ >$) tend to have low θ . This is opposite for the air masses belonging to the $< O_3 + /H_2O- >$; they descend from the extratropical upper troposphere (relatively high θ region) before being quasi-horizontally advected to the observation site. The resultant positive correlation between $[O_3]'$ and θ' is likely responsible for the positive correlation between $[O_3]'$ and $[O_3]'_E$ (see Eq. (3)) even though their actual values do not necessarily match each other.

To summarize, this study is the first to provide a new, more direct approach to clarify the formation mechanism of layered structure with the aid of latest reanalysis data including the backward trajectory calculation.

Although ERA5 is found to have a limitation such that it resolves a layered structure with a scale greater than a few kilometers, our approach greatly contrasts with the previous studies (e.g., PG98 and T11) which reported only a correlation analysis between different quantities obtained from balloon measurements. Notably,

we have demonstrated that there is a case where quasi-horizontal mixing is primarily important even though $r([O_3]', [O_3]_E')$, is large. In this perspective, PG98 and T11 might have overestimated the contribution of GWs for the formation process. Indeed, the tropical upward and subtropical downward motion, which are likely a key for producing large $r([O_3]', [O_3]_E')$ for the layered structure in the present case, may reflect a general feature of Hadley circulation. We are now trying to conduct more statistical analysis to examine how often similar cases do exist.

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Figure Legends

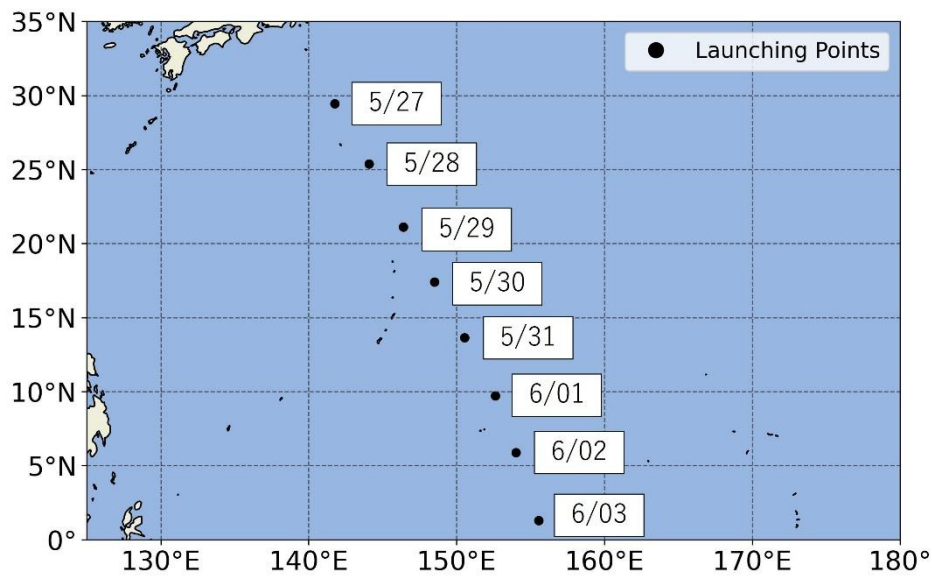


Fig. 1 Dates and locations of balloon measurements for the YMC-BSM 2021 campaign

for the period from May 27 to June 3, 2021.

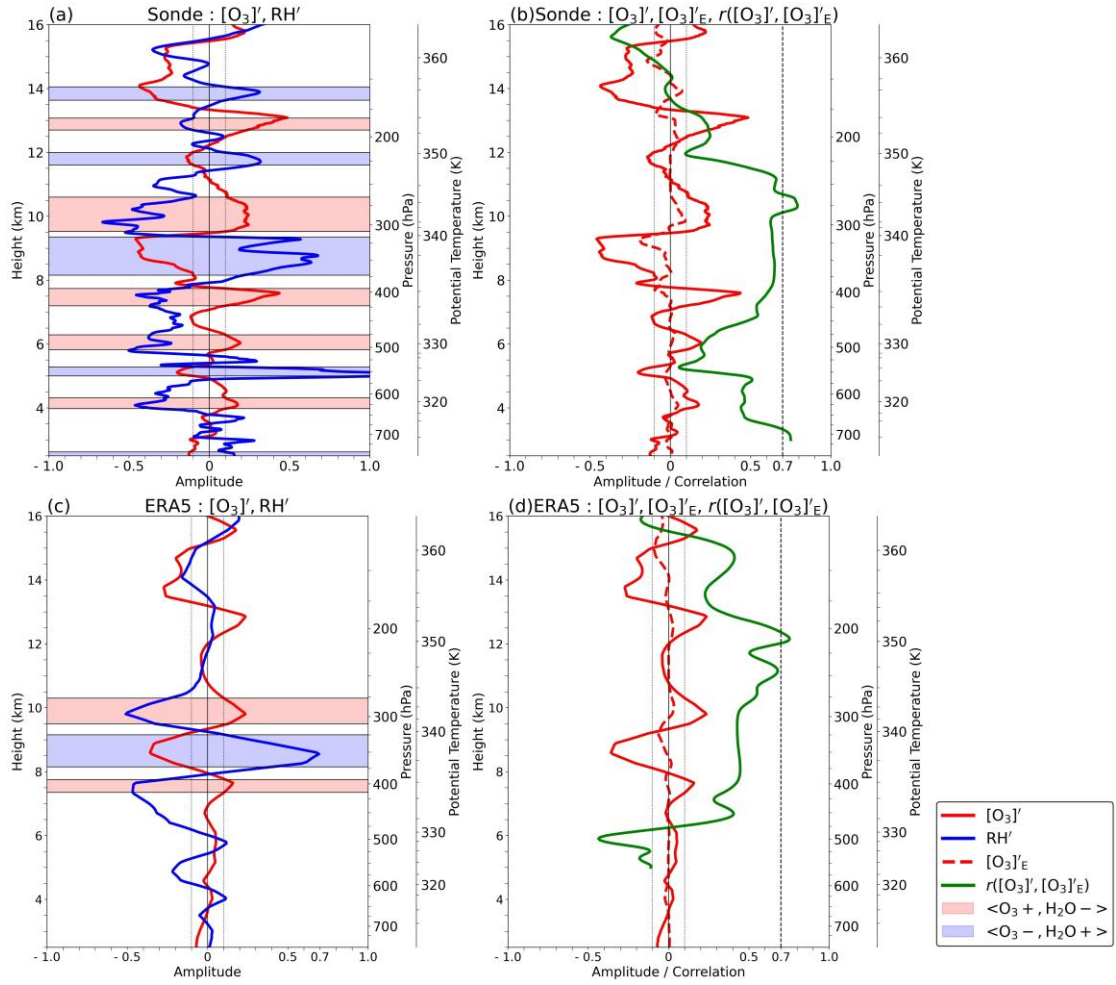


Fig. 2 Vertical profiles of (a, c) $[O_3]'$ (red lines) and RH' (blue lines) and (b, d) $[O_3]'$ (red lines), $[O_3]'_E$ (red dashed line), and the correlation coefficient between $[O_3]'$ and $[O_3]'_E$, $r([O_3]', [O_3]'_E)$, as calculated over the 5km window. See text (Section 2) for the details for the definition of each variable. Panels (a) and (b) are the results from balloon measurements (at approximately 17.5 °N and 148.5 °E and at 09:39 UTC on May 30, 2021), while panels (c) and (d) are the result from ERA5 model-level data at the nearest grid point/time. Red and blue shaded areas represent $\langle O_3 + , H_2O - \rangle$ and $\langle O_3 - , H_2O + \rangle$, respectively. Only layers with a thickness of 200 m or more are showed.

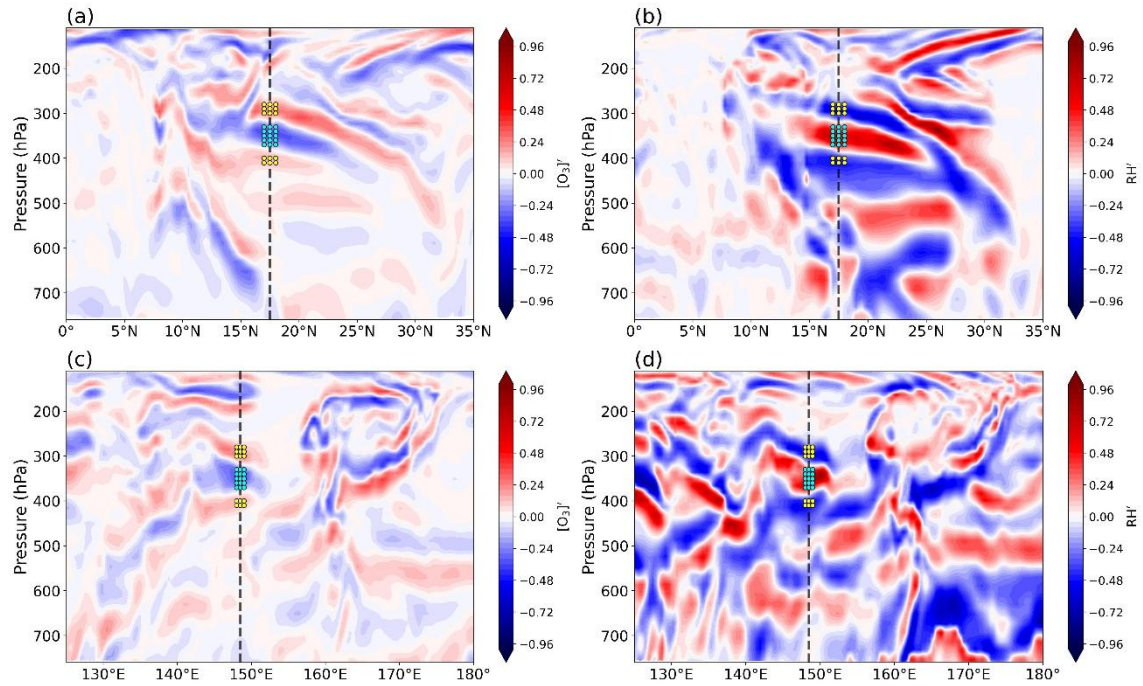
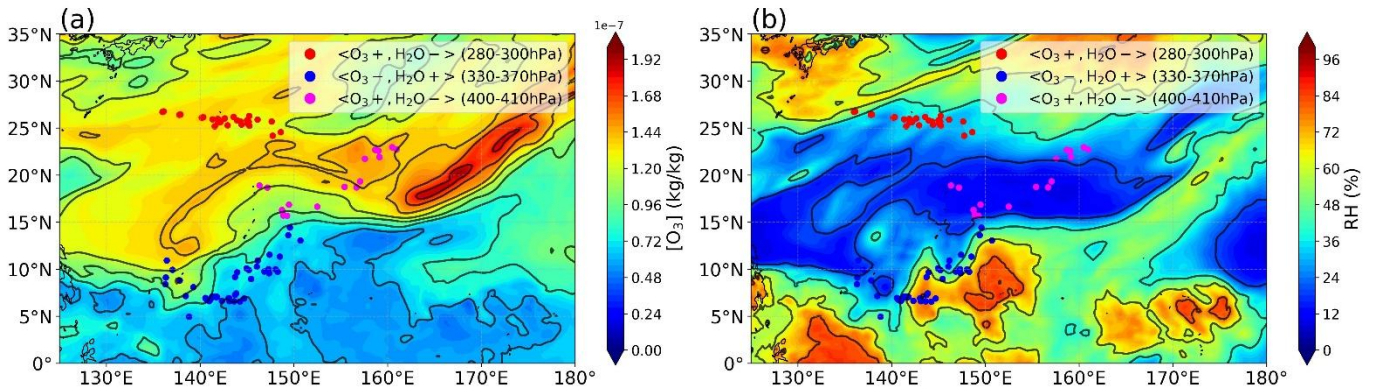


Fig. 3 (a-b) Latitude-pressure cross sections at 148.5°E and (c-d) longitude-pressure cross sections at 17.5°N for $[O_3]'$ (left panels) and RH' (right panels) at 09:00 UTC on May 30, 2021, as derived from ERA5 data. The vertical dashed lines indicate the location of the observation site (17.5°N, 148.5°E). The yellow and blue circles correspond to the initial positions of the backward trajectory calculation for $\langle O_3 + ,H_2O - \rangle$ (yellow) and $\langle O_3 - ,H_2O + \rangle$ (blue), respectively.



388

389 **Fig. 4** Horizontal distribution of (a) $[O_3]$ and (b) RH averaged over the vertical region
 390 of 5-12 km in altitude, at 00:00 UTC on May 26, 2021 (105 hours prior to the
 391 observation time), as derived from ERA5 data. Red, magenta, and blue circles
 392 indicate the positions of the air parcels which belong to $<O_3 + ,H_2O->$ (280-300
 393 hPa), $<O_3 -,H_2O+>$ (330-370 hPa), and $<O_3 + ,H_2O->$ (400-410 hPa),
 394 respectively, at the initial time of backward trajectory calculation (i.e., 00:00 UTC
 395 on May 26, 2021).

396

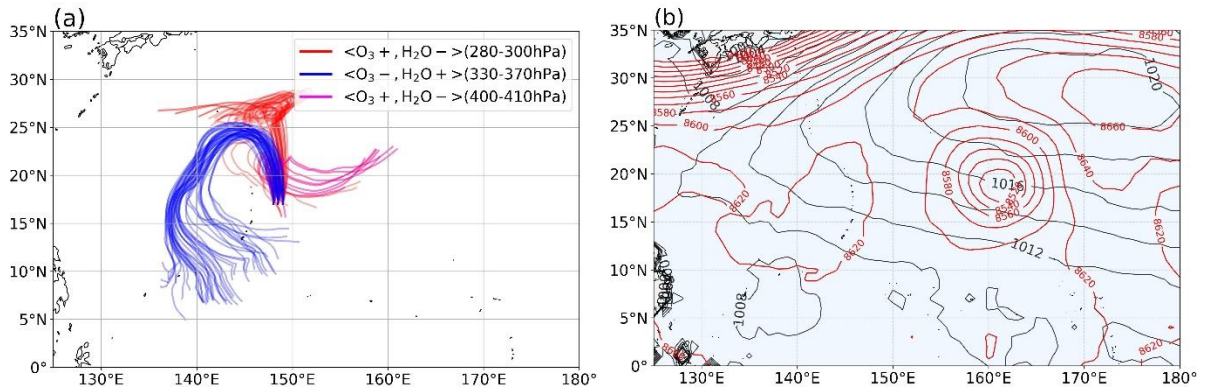


Fig. 5 Horizontal distribution of (a) the 105-hour backward trajectories and (b) the surface

pressure (black contour; contour interval of 2 hPa) and geopotential height at 350

hPa in pressure level (red contour; contour interval of 20m) at 21:00 UTC on May

28, 2021, which corresponds to an intermediate time during the trajectory analysis.

For panel (a), red, magenta, and blue curves denote the trajectories that start from

the $\langle O_3 + , H_2O - \rangle$ at 280-300 hPa, the $\langle O_3 - , H_2O + \rangle$ at 330-370 hPa, and

the $\langle O_3 + , H_2O - \rangle$ at 400-410 hPa, respectively.

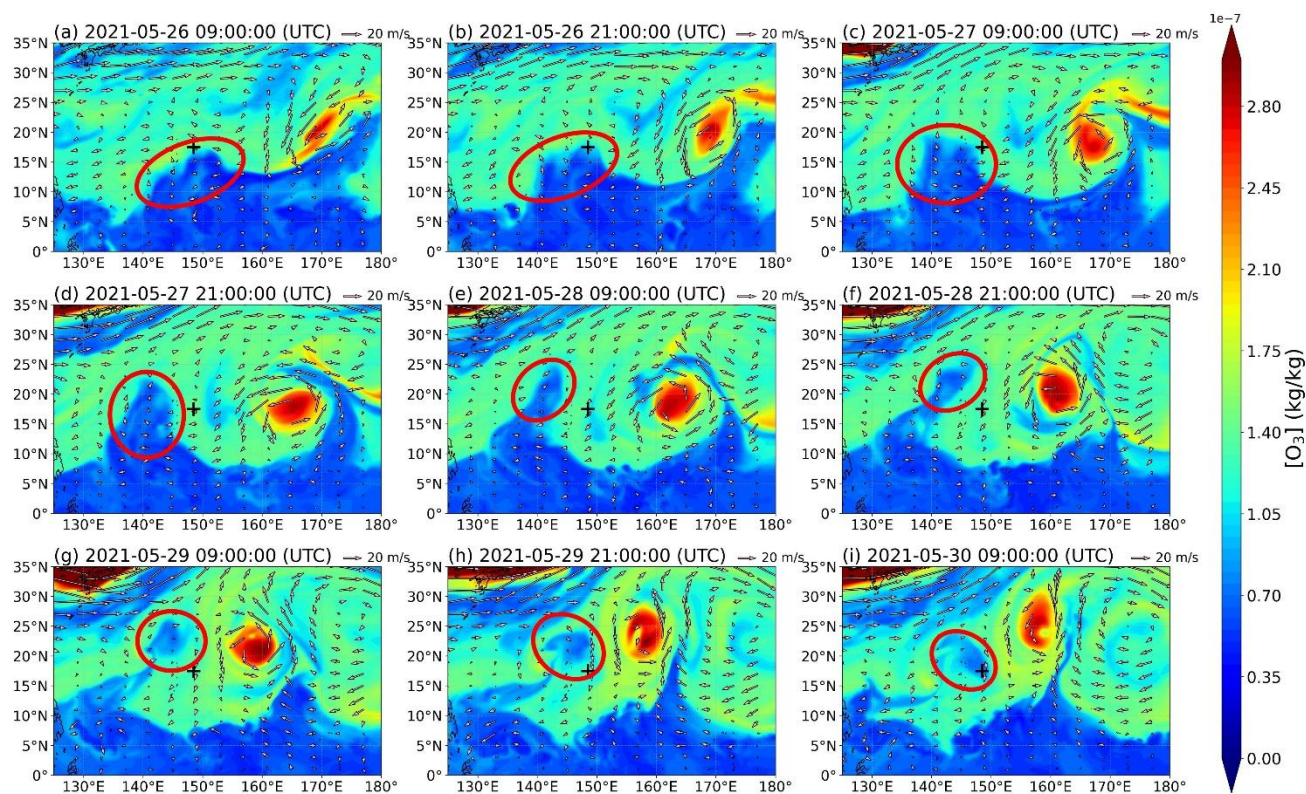


Fig. 6 Time series of horizontal distribution in $[O_3]$ concentration on the 338 K isentropic surface from 09:00 UTC on May 26 to 09:00 UTC on May 30, at 12-hour intervals, as revealed by ERA5 data. Arrows indicate horizontal wind vectors. The black plus sign in each panel denotes the location site (17.5°N , 148.5°E). The red ellipses highlight the movement of $\langle O_3 - ,H_2O+ \rangle$ air mass focused on in this study.

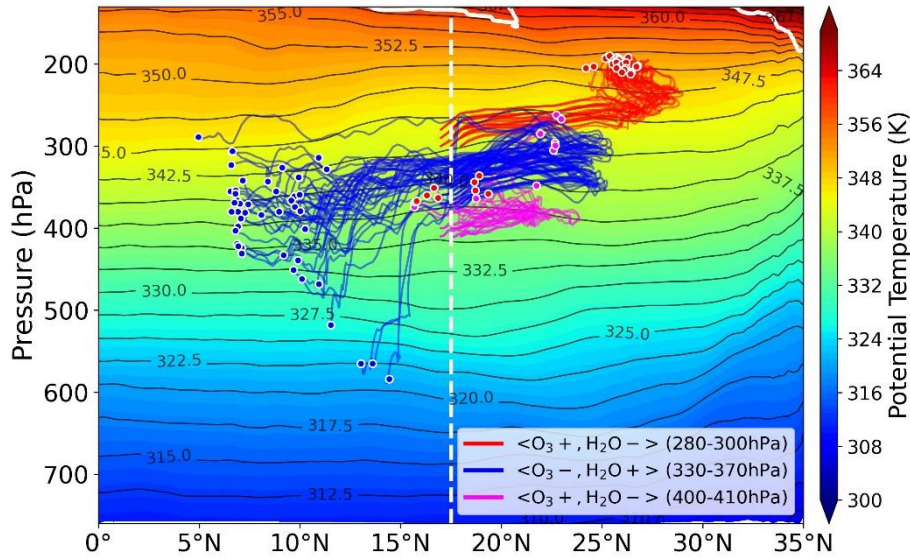


Fig. 7 Latitude-pressure cross-section of backward trajectories (solid curves; color allocation is the same as Fig. 5) and the potential temperature (color shading and contours; contour interval of 2.5 K) averaged over 130-160 °E in longitude, as derived from the model-level ERA5 data at 00:00 UTC on May 26, 2021. White solid curves denote the contour of 1.5 PVU as an indicator of tropopause. The vertical white dashed line indicates the latitude of the observation site (17.5 °N).

Supplementary Files

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- [ESM3.mp4](#)
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