

## Response to referee#1's comments for manuscript

The authors would like to thank the substantial comments and suggestions from the referees, which significantly helped improve the quality of this manuscript. We have revised the manuscript carefully based on the comments and suggestions of the reviewer. More details of the revision can be found in the revised manuscript as well as the point-to-point response as follows (all authors' responses here are in blue).

In this paper, ozone changes in the middle atmosphere around sudden stratospheric warming (SSW) and early final stratospheric warming (FSW) events are analyzed. MERRA-2 data are used to disentangle the different dynamical and chemical processes affecting ozone in the stratosphere and mesosphere. MERRA-2 data are evaluated against observations of GROMOS-C and MLS, and the good qualitative agreement in the ozone anomalies between GROMOS-C, MLS, and MERRA-2 below 0.1 hPa justify the use of MERRA-2 for the analysis of dynamical versus chemical processes. This is an interesting analysis, and the approach used to disentangle advection, turbulence, and chemistry is to my knowledge novel. In this sense, the paper brings new aspects to our understanding of these large disturbances of middle atmosphere dynamics; as SSWs are known to affect the whole atmosphere from the troposphere to the ionosphere, understanding its drivers and impacts is of course very important. However, I found the paper in parts difficult to follow. In particular how ozone is implemented in MERRA-2, and how it depends on the different chemical and dynamical terms is unclear (Section 2.3). As this is a prerequisite to understand the analysis and interpret the results, this should be clarified, and I have listed more specific comments to this issue as Major points below. I also have a rather long list of minor comments mostly regarding unclear wording listed below.

### Major comments:

1. Lines 111-112: in the stratosphere, odd oxygen is dominated by ozone, but in the upper mesosphere, it is dominated by atomic oxygen. This has to be taken into account when comparing MERRA-2 ozone to GROMOS-C and MLS, and presumably can explain the much higher values of MERRA-2 in the upper mesosphere.

We completely agree that this distinction in atmospheric composition between the stratosphere and upper mesosphere must be carefully considered when interpreting and comparing ozone data from different sources. The revised manuscript is going to add this information about MERRA2 ozone in the model section.

2. Lines 111-114: I don't understand the relationship between the different models here. As I understand your description, MERRA-2 uses tendencies of  $O_x$  (not ozone) from the GEOS CTM as ozone tendencies. This would explain the very high ozone values of ozone in the upper mesosphere, as  $O_x$  (and  $O_x$  tendencies) is significantly higher there, than ozone. But why are the assimilated meteorological data from GMAO used here, not from MERRA-2? I presume that you mean that these are used within the GEOS-CTM, not within MERRA-2, but this is not clear. Also, if the GMAO meteorological data are used to derive the ozone tendencies than used in MERRA-2, that would imply that the resulting ozone fields in MERRA-2 are inconsistent with dynamics of MERRA-2. I don't think this is the case, but can you please clarify?

Ozone tendency: these datasets are assimilated with the Goddard Earth Observing System Model, version 5 (GEOS-5) by using odd-oxygen mixing ratio as its prognostic variable. This includes an odd-oxygen family transport model that provides the ozone concentration necessary for solar absorption. The vertically integrated ozone tendency is given as following equation. In addition, the revised manuscript cites two publications that use the ozone tendency from MERRA-2 to investigate the polar stratospheric ozone and provide a description of the datasets.

Lubis, S. W., Silverman, V., Matthes, K., Harnik, N., Omrani, N.-E., and Wahl, S.: How does downward planetary wave coupling affect polar stratospheric ozone in the Arctic winter stratosphere?, *Atmospheric Chemistry and Physics*, 17, 2437–2458, 2017.

Bosilovich, M. G.: MERRA-2: Initial evaluation of the climate, National Aeronautics and Space Administration, Goddard Space Flight Center, 2015. <https://gmao.gsfc.nasa.gov/pubs/docs/Bosilovich785.pdf>

3. Line 115: what is vertically integrated here – ozone, or the ozone tendency? Vertically integrated ozone would be total ozone; as you are discussing ozone profiles here, is it possible that you mean “vertically resolved”, not

“vertically integrated”?

The model uses an odd oxygen mixing ratio, as its prognostic variable. It is the vertically integrated ozone tendency.

4. Line 117: shouldn't the left-hand side be the total derivative, not a partial derivative?

The left-hand side is a partial derivative. <https://gmao.gsfc.nasa.gov/pubs/docs/Bosilovich785.pdf>

5. Line 121: can you explain in a bit more detail how ANA refers to assimilation of ozone? Also, is this done within MERRA-2, or within the GEOS CTM?

Ozone is analyzed and so can change due to ozone increments or due to increments in atmospheric dry mass. We report only the total analysis contribution. To compare the tendencies with the total tendency from the states, a conversion factor of 1.65 mol/mol must be applied to the tendencies. <https://gmao.gsfc.nasa.gov/pubs/docs/Bosilovich785.pdf>

6. Line 189 and Section 4: in my view, the value of the GROMOS-C (and MLS) data is that the evaluation of the performance of MERRA-2 ozone in relation to the FSW/SSW events; the good qualitative agreement is the justification to use MERRA-2 to analyze the dynamics versus chemistry in a later step. This should be made very clear here.

We will add this justification as suggested by the reviewer: In this section, our analysis reveals a qualitative agreement between MERRA-2 ozone data and observations from GROMOS-C and MLS instruments during FSW/SSW events. This agreement serves as a robust justification for employing MERRA-2 data to explore the dynamics versus chemistry relationship in subsequent steps of our research, providing confidence in the reliability of MERRA-2 ozone data for our analytical purposes.

7. Line 198: If I understood correctly how ozone is implemented in MERRA-2 (description in Sec. 2.3), this is  $O_x$ , not  $O_3$ ; in the stratosphere and lowermost mesosphere, the difference is negligible, but in the upper mesosphere, there is significantly more  $O_x$  than  $O_3$  – this presumably explains the very high values of MERRA-2 “ $O_3$ ” shown in Figure 3 c) and f). If this is correct, MERRA-2 ozone can not be used above 0.1 hPa. Please clarify.

Changed: The results indicate a good agreement between MERRA-2 (below 0.1 hPa) and MLS with GROMOS-C observations. However, due to the complexity of altered dynamics in the winter polar regions introducing extra uncertainties into numerical models and data assimilation systems (Wargan et al., 2017), ozone VMRs exhibit dramatic variability (in Fig.3b, e) in the mesosphere from MERRA-2.

8. Lines 374 and following, Discussion and conclusions: Please be more precise which data you used, and what for. You used MERRA-2 temperatures and wind fields to identify SSWs. You probably did not use MLS wind fields for this as stated here, as MLS does not observe winds(?). You used MLS and GROMOS-C ozone to evaluate MERRA-2 ozone fields, and ozone anomalies, and justify its use for analyzing the dynamical and chemical drivers of the ozone changes. Please clarify this here.

Changed: In this paper, we use MERRA-2 reanalysis data to identify the SSW and FSW events by analyzing zonal wind fields and polar temperatures covering the period from 2004 to 2022. A qualitative agreement in ozone between MERRA-2 and observations from GROMOS-C and MLS instruments during FSW/SSW events provides confidence in the reliability of MERRA-2 data to investigate the driving mechanisms of polar ozone dynamics and chemistry.

#### Minor comments:

1. Lines 13-15: it is not clear what “this response pattern” refers to here. Maybe better “FSW events are associated with ...”

Changed: The pattern of ozone anomalies for FSW events is associated with the combined effects of dynamical and chemical terms, which reflect the photochemical processes counteracted partially by positive horizontal eddy transport, in particular in the middle stratosphere.

- Line 16: which chemistry-climate model? In the paper, model results are shown from MERRA-2 whose ozone product is based on a chemistry-transport model. No chemistry-climate model results are shown.

Changed: Here, we contrast results from the ozone continuity equation using MERRA-2 reanalysis data and direct ozone tendency based on the odd-oxygen family transport model to quantify the impact of dynamical and chemical processes on ozone anomalies during SSW and FSW events.

- Line 15-17: this sentence should come after the sentence ending in line 10, to clarify where the results discussed in lines 7 and following come from. Else it is not clear where “the underlying dynamical and chemical mechanism” discussed in the sentence starting in line 10 comes from.

Changed

- Line 26: SSW events (plural)

Changed

- Line 29: Observed FSW events . . . . depend (plural)

Changed

- Line 31: atmospheric species, not atmosphere species

Changed

- Lines 32-33: “. . . ozone plays the most important role in the coupling between chemistry, radiation, and dynamical processes in the stratosphere and lower mesosphere. “ Ozone radiative heating and cooling peaks at the stratopause; in the upper mesosphere, heating by O<sub>2</sub> becomes important as well.

Changed: ozone plays the most important role in the coupling between chemistry, radiation, and dynamical processes in the stratosphere and lower mesosphere. Ozone radiative heating and cooling peaks at the stratopause, in the upper mesosphere, heating by oxygen becomes important as well.

- Line 23-45: There are less studies of the impact of SSWs on mesospheric ozone, but there is some literature about this as well, e.g., Tweedy et al., JGR, 2023; Smith-Johnsen et al., JASTP, 2018. These should be discussed here as well.

Added: Tweedy et al. (2013) use output from SD-WACCM to explore the evolution of secondary ozone in the mesosphere during SSWs associated with anomalous vertical residual motion and consistent with photochemical equilibrium governing the mesosphere-lower thermosphere (MLT) nighttime ozone. Smith-Johnsen et al. (2018) investigates the cause of the mesospheric nighttime ozone increase during the 2002 Southern Hemisphere winter which is attributed largely to enhanced upwelling and the associated cooling of the altitude region in conjunction with the wind reversal.

- Line 61: In addition, we show . . .

Changed

- Line 61-63: this is stating the obvious – as total ozone is dominated by the amount of ozone in the lower stratosphere, anything affecting lower stratosphere ozone will have a correlating response in total ozone.

In addition, we show that polar ozone anomalies in the lower stratosphere mainly predominantly governed by the horizontal eddy effect and vertical advection transport processes exhibit a strong correlation with polar total column ozone corresponding to both types of events.

11. Line 75: using instead of leveraging

Changed

12. Line 80: and instead of which

Changed

13. Line 80-82: are you using the same retrieval and calibration version as in Fernandez et al (2015)?

Yes, we use the same retrieval and calibration version for the GROMOS-C.

14. Line 84: instrument, not instruments (?)

Changed: instrument

15. Line 88-89: please clarify what depends on the pressure here – the ozone profile, not the 240 GHz microwave band

Changed: The ozone profile is retrieved using the 240 GHz microwave band, which extends from 261 hPa to 0.0215 hPa for recommended scientific applications.

16. Line 93: available instead of applicable

Changed

17. Line 135: X(dyn) consists of three terms, not four

X(dyn) consists of four terms: the horizontal and vertical advection, horizontal and vertical eddy transport effects

18. Line 139: in this equation, one bracket is missing, probably at the end

Changed

19. Lines 164-165: I would say the westerly starts to weaken in 10-1 hPa already a few days before the warming. During the warming, the wind reverses quickly to easterly, and stays like this for at least 30 days below 1 hPa, but reverses back above that.

Below approximately 0.1 hPa, the westerly wind rapidly weakens lags - 10 days and then switches to an easterly wind after the SSW onset (lags 0 days) at 10 hPa in Fig.1a. The easterly wind stays like this for at least 30 days below 1 hPa but reverses back above that.

20. Line 165-166: I think you mean the westerly winds return after approximately 15 days? However, only above 1 hPa

Changed: The easterly wind returns after approximately 15 days at 10 hPa. After around 20 days of SSW onset, wind at 0.1 hPa reverses to westerly with a maximum speed of 80 m/s and stays like this for at least 20 days.

21. Line 168: . . . . and cooling in the mesosphere above 0.1 hPa, which seems to onset a few days before the warming?

Changed: The temperature fields undergo alterations in conjunction with the wind field weakening.

22. Line 168: In Fig. 1b) . . . please state here that now you are discussing FSWs, not SSWs. Note that the westerlies begin to weaken at lag -10 as well (similar to SSWs), and even reverse above 0.1 hPa before the event.

In Fig.1b, the zonal-mean zonal wind at 60°N and 10 hPa during the FSW event is easterly with lags 50 days until the early summer and does not reverse to westerly. We emphasize the reversal of wind at 10 hPa.

23. Line 170: at the stratopause. Temperatures in the lower stratosphere also increase strongly, but there is cooling in the upper mesosphere.

Added: Temperatures in the lower stratosphere also increase strongly, but there is cooling in the upper mesosphere.

24. Line 173: the mean climatology of all years, or of all years without SSWs/FSWs? If SSW years are included in the climatology, that will diminish the anomalies somewhat.

The mean climatology is all years with SSW/FSW events. Although SSW years are included in the climatology, still appear the anomalies somewhat due to the high occurrence of SSW in the northern hemisphere.

25. Line 174: as shown in Fig. 2.

Changed

26. Line 181: in Fig. 2a?

Changed

27. Line 183: what does it mean that you have significant anomalies in  $w^*$  extending to lag -30 before FSWs – those winters are significantly different to other winters much earlier?

FSWs evolve relatively slowly and result from the sustained lack of stratospheric wave driving, leading to the gradual strengthening and cooling of the vortex. However, the small wave driving sometimes exists starting several weeks before FSW onset such as the minor warming in the winters. This is different from SSWs, as the wave driving during SSW changes much more abruptly during onset. Yes, it means that those winters are different to other winters much earlier.

28. Line 187-188: the lasting  $w^*$  anomalies after the FSWs at and below 1 hPa are very small though

Changed

29. Line 196-197: in which altitude range?

Changed: The results indicate a good agreement between MERRA-2 (below 0.1 hPa) and MLS with GROMOS-C observations.

30. Line 204: erase “with” before descending downward

Changed

31. Lines 205-206: ... before the FSW onset, which is stronger than before the onset of the SSW events.

Changed

32. Line 211: Climatological for all years, or for only those without SSW/FSW events? Please clarify.

Changed: Seasonal changes in ozone tendencies from the eddy effect, advection transport, and chemical loss and production processes based on MERRA-2 reanalysis data for the period 2004-2021 are shown in Fig.5.

33. Line 251-252: how does that explain the difference between 5 and 6?

We mainly compare the difference between  $\bar{\chi}_t$  and  $TOT$ ,  $\bar{S}$  and  $CHM$ .

34. Line 252-254: I agree that it is important to understand the interplay between dynamics and chemistry, which is particularly difficult during strong disturbances of the atmospheric dynamics like SSWs and FSWs. Still, I think the wording here “one of the keys to improving our understanding” is too strong. I would argue instead that SSWs are periods of known stratosphere-troposphere coupling, and that a better understanding of SSWs, and better representation in chemistry-climate models, therefore has the potential to improve medium-range weather forecasts during high-latitude winter.

Changed: Determining the ozone transport mechanisms during stratospheric extreme events is a better understanding of stratospheric processes and ozone variability in stratosphere chemistry-climate models, and better representation in chemistry-climate models, therefore has the potential to improve medium-range weather forecasts during high-latitude winter.

35. Figure 7: I would say this figure shows essentially the same behavior as 3, though with less noise due to the better sampling; the figure and the discussion of it, are not really necessary, as they repeat things already discussed. In my view, the main use of Figures 3 and 4 is to justify the use of MERRA-2 data for the analysis of dynamics versus chemistry; it is not necessary to do this again.

Thank you for your perspective on the similarity in behavior between Figure 7 and Figure 4. Figures 3 and 4 primarily illustrate ozone variability at a single polar station and its comparison with GROMOS-C and MLS datasets. Figure 7 serves a distinct purpose. Figure 7 presents ozone anomalies in the polar regions (70-90N) to correspond with the dynamic and chemical processes discussed in the subsequent section. It aims to provide insight into anomalous ozone tendencies during both types of events, providing a broader perspective on ozone behavior across the polar regions during these events. In summary, Figure 7 complements Figures 3 and 4 by focusing on ozone anomalies in the broader polar regions, facilitating a deeper analysis of dynamic and chemical processes influencing ozone variability during specific events.

36. Figure 8: here you use the absolute derivative for TOT, DYN and CHM. This is not consistent with the notation in equation 1, where all are given as partial derivatives. From the setup of equation 1, I think the correct use would be to denote TOT with total derivatives, DYN and CHM with partial derivatives; anyway this should be done in a consistent way throughout the manuscript.

Thanks for your valuable comment. We have fixed the denotation in Figure 8.

37. Lines 332-334: the sentence is missing a verb.

Changed: The positive TCO anomalies after SSW events span a period exceeding 40 days analyzing data from ERA5 and MERRA-2 reanalysis data, MLS, or comprehensive GCMs such as WACCM over the polar regions

38. Lines 336-337: as TCO is dominated by the lower stratosphere, changes in lower stratosphere ozone will map directly into TCO.

Added: As TCO is dominated by the lower stratosphere, changes in lower stratosphere ozone will map directly into TCO.

39. Line 341: 30-90°N, not 60-90°N.

Changed: We calculate TCO tendency anomalies in the northern hemisphere (30 - 90° N) during SSW and FSW events using MERRA-2 in Fig. 10.