Comment on acp-2022-557
Anonymous Referee #2

Referee comment on "Composited analyses of the chemical and physical characteristics of co-polluted days by ozone and PM2.5 over 2013-2020 in the Beijing–Tianjin–Hebei region" by Huibin Dai et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2022-557-RC2, 2022

In recent years, decreases in PM$_{2.5}$ but increases in O$_3$ over eastern China make the co-occurrences of PM$_{2.5}$ and O$_3$ polluted days (O$_3$&PM$_{2.5}$PD) an important issue related to human health. In this work, Dai et al. explored the chemical and synoptic characteristics of O$_3$&PM$_{2.5}$PD in Beijing-Tianjin-Hebei (BTH) region within a GEOS-Chem framework. They provided comprehensive analysis and concrete details in the differences among PM$_{2.5}$ alone polluted days (PM$_{2.5}$SPD), O$_3$ alone polluted days (O$_3$SPD) and O$_3$&PM$_{2.5}$PD. Results are novel and of scientific significance. I would like to suggest publication after addressing my comments below:

Major Concerns:

- I suggest authors to separate Section 3.3 into two or three parts, where the chemical characteristics, vertical profile and process analysis are described respectively. The current demonstration looks not very logistic and thus makes it hard to follow.
- Section 3.2, GEOS-Chem still significantly underestimates peak PM$_{2.5}$ concentrations as shown in Fig. 3d. Which PM$_{2.5}$ components dominate such underestimates? I’m worried that GEOS-Chem incapacity in simulating peak PM$_{2.5}$ could significantly influence the following analysis related to the differences in SO$_4^{2-}$ and NO$_3^-$ among O$_3$SPD, PM$_{2.5}$SPD and O$_3$&PM$_{2.5}$PD. At least more evaluation and discussions are necessary.
- Lines 351-354 and Fig. 6, compared to O$_3$&PM$_{2.5}$PD, less S was oxidized into SO$_4^{2-}$ during PM$_{2.5}$SPD and less N was oxidized into NO$_3^-$ during O$_3$SPD. Such differences also reflected in the PM2.5 components in Fig. 6. Are there any explanations about that? In addition, I’m curious what are the dominant oxidation pathways (e.g. SO$_2$ oxidation through H$_2$O$_2$, O$_3$, OH or NO$_2$) of SO$_2$ and NOx in GEOS-Chem? Can pathways be different among O$_3$SPD, PM$_{2.5}$SPD and O$_3$&PM$_{2.5}$PD?
- In Fig.9, I’m confused about the totally different diffusion profile in SO$_4^{2-}$ relative to NO$_3^-$ and NH$_4^+$. In the PBL, air pollutants are supposed to diffuse following concentration gradients. For NO$_3^-$ and NH$_4^+$, strong chemical production happened in upper layers (913-771 hPa), where diffusion contributions at this altitude were negative, meaning the diffusion of new-generated NO$_3^-$ and NH$_4^+$ diffused through PBL.
It is reasonable. However, \( \text{SO}_4^{2-} \) diffusion were still positive at altitude where chemical production was strong, which seems against the concentration gradients. It might also be related to the constant \( \text{SO}_4^{2-} \) profile in Fig. 8, which is interesting but I could not find clear explanations in this manuscript.

- I suggest authors to summarize some highlights logistically in conclusions, e.g. what are the major differences in chemical mechanisms among O\(_3\)SPD, PM\(_2.5\)SPD and O\(_3\)&PM\(_{2.5}\)PD? What meteorological factors or synoptic patterns drives the differences? Also, although authors made very comprehensive analysis, one important question remained not very clear to me: Why O\(_3\)&PM\(_{2.5}\)PD only occurred at part of the O\(_3\)SPD or PM\(_{2.5}\)SPD? Which one among chemical mechanisms, vertical profile and meteorology drives the differences?

Specific Comments:

- Lines 48-49: Natural sources also have significant contributions to PM\(_{2.5}\).
- Line 61: 'observations' should not be capitalized.
- Lines 334-342: I suggest authors to add a table or figure in the main text or supplementary to show the OH evaluation.
- Line 548: From the traditional synoptic definition, WPSH in eastern China should be regions with 500hPa geopotential height larger than 5880 m (or larger than 1520 m at 850hPa). I don’t think the high pressure here is WPSH.
- Line 553: Northeast Cold Vortex is not necessary to abbreviate since it no longer appeared in the manuscript.
- Figure 12 and S10: I wonder could the synoptic patterns be clearer if using anomalies rather than absolute values?