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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 $PM_{2.5}$ 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_3SPD) 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_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 $SO4^{2-}$ and $NO3^-$ among O_3SPD, $PM_{2.5}$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_5PD, less S was oxidized into $SO4^{2-}$during $PM_{2.5}$SPD and less N was oxidized into NO_3^- during O_3SPD. 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_2O_2, O_3, OH or NO_2) of SO_2 and NOx in GEOS-Chem? Can pathways be different among O_3SPD, $PM_{2.5}$SPD and O_3&$PM_{2.5}$PD?
- In Fig.9, I'm confused about the totally different diffusion profile in $SO4^{2-}$ relative to $NO3^-$and $NH4^+$. In the PBL, air pollutants are supposed to diffuse following concentration gradients. For $NO3^-$ and $NH4^+$, strong chemical production happened in upper layers (913-771 hPa), where diffusion contributions at this altitude were negative, meaning the diffusion of new-generated $NO3^-$ and $NH4^+$ diffused through PBL. It is reasonable. However, $SO4^{2-}$ 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 $SO4^{2-}$ 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_3SPD, PM_5SPD 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_3SPD 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?