## March 20, 2022

## Reviewer 1 (Reviewer's comments in black and our responses in red)

General comments:

The study conducted by Lin et al. shed some new light on the mechanism for the occurrence of the haze extreme. In the revised manuscript, the authors have added some critical information, such as the missing tables and the new observation dataset of PBL height, to further support their conclusions. And most of concerns raised by the referees have been addressed. However, there are still some language errors in the current version and the authors should examine the text more carefully to avoid these problems.

We are grateful to the positive comments to our manuscript by this reviewer and have fully addressed the issues raised by this reviewer below.

For example, Line 347, 'at the group level' should be 'at the ground level'. Done.

Lines 347-348, the collapse of atmospheric boundary layer will lead to pollution accumulation rather than the vertical dilution for PM. We modified the statement as "Note that both the photochemical production and PBL evolution contribute to PM accumulation at the ground level, since the PBL development during the daytime leads to vertical dilution" (Lines 346-348).

We also found other unclear statements/typos, which were modified/corrected as below:

Lines 258-261: The statement was modified to "The input of the PBL height for the both clean and aged-BC cases were based on ceilometer measurements, showing that the PBL height increases by about 700~900 m from the aged-BC cases to the clean cases".

Line 475: Section no. "3.5" should be "3.4".

What's more, it is important to include some discussion to strengthen the reliability of the model simulation results in the manuscript. Here are some observational evidences for the impact of aerosol-PBL interaction on near-surface haze pollution on different time scales.
1. Dong et al., 2017. Opposite long-term trends in aerosols between low and high altitudes: a testimony to the aerosol–PBL feedback, Atmos. Chem. Phys., 17, 7997–8009.
2. Huang et al., 2018. Impact of Aerosol-PBL Interaction on Haze Pollution: Multiyear Observational Evidences in North China. Geophysical Research Letters, 45, 8596–8603.
3. Su et al., 2020. The significant impact of aerosol vertical structure on lower atmosphere stability and its critical role in aerosol–planetary boundary layer (PBL) interactions. Atmos. Chem. Phys., 20, 3713–3724.

We have added some discussions about the reliability of the model simulation results in the

manuscript as below:

Lines 387-390: The extent of warming in the upper boundary layer and cooling at the surface due to the aerosol effect simulated at Beijing in this study are consistent with the observational analysis on North China by Huang et al. (2018), suggesting that our simulations can well reproduce the aerosol radiative effect under severe regional haze condition.

Lines 411-418: The significant aerosol-PBL interaction and its impact on surface air pollution revealed in our simulation sensitivity studies are also evident in multiple observation-based studies in China (Dong et al., 2017; Huang et al., 2018; Su et al., 2020). However, there might exist certain uncertainties in evaluating the aerosol impacts on PBL development based our simulation experiments as previous observational analysis like Dong et al. (2017) and Su et al. (2020) has pointed out that the aerosol-PBL interaction also varies with the aerosol vertical structure but an exponential decreasing aerosol profile was assumed and fixed in our simulations.

Lines 470-473: The significant role of BC in atmospheric heating is also evident in long-term observations, e.g., Huang et al. (2018) has also proven that the heating in the atmosphere was mainly caused by absorbing aerosols like BC.