Response to Reviewer #1:

We are grateful for the positive evaluation and comment from Reviewer #1. Based on these suggestions, we have carefully revised the manuscript. There are three major changes: (1) The reasons for using the WRF model rather than the WRF-Chem model are discussed; (2) The PBL height evolution in both observation and simulation is presented and analyzed; (3) The vertical cross-sections of potential temperature during Case-1 and Case-2 are added in the supplementary material. In addition, the manuscript structure is improved as suggested by Reviewer #2, by moving Fig.12 and related descriptions into the Introduction, and deleting Fig. 7 and the paragraph "Frontal category". The numbering of all figures is changed accordingly.

The response to each comment is listed below. The original comments are in *blue and italic*, our replies are in normal font. Bracketed numbers are used for referee comments (e.g., ***[R1.1]***).

Summary

The manuscript investigated the three-dimensional PBL structures under various pollution types in the North China Plain (NCP) by using the WRF model during autumn and winter of seven years (2014-2020). They proposed three pollution PBL types (frontal category, wind shear category, and topographic obstruction pollution category) and investigated the two main types of wind shear category and topographic obstruction category through case studies in this paper. Such work is a good supplement to the synoptic-scale and boundary-layer scale studies and I believe it will be of interest to the community of atmospheric pollution and boundary-layer meteorology. Overall, the paper is logically structured and well written. However, some details and explanations on methods and data need to provide to justify and support the conclusions. Thereby, I suggest a major revision before the paper can be accepted by Atmospheric Chemistry and Physics. My detailed comments are listed below.

Response: We thank the reviewer for the positive evaluation and comment on this manuscript. The manuscript has been revised accordingly.

Major comments

[R1.1] *My first concern is about the use of the WRF model. Given this study is focused on the different types of aerosol pollution cases, then using the atmospheric chemical transport model WRF-Chem or WRF-CMAQ to simulate these pollution events sounds more plausible than the pure-meteorological model WRF. Otherwise, it is difficult to convince the reader that these pollution cases are reasonably captured without evaluating the performance of simulating $PM_{2.5}$ concentration. Moreover, the interaction between aerosols and boundary layer can modify the PBL thermal and* *dynamic structures, so I wonder if the pure-meteorological model WRF is suitable for investigating such pollution cases. The authors at least give some discussions on this.*

Response: We thank the reviewer for this very critical comment. We have adopted the suggestion and added an explanation to our research method in the revised manuscript. The reasons for using only the WRF model are as follows.

Generally, air pollutant emission, meteorological condition and chemistry, three of them are determinants of air pollution. The present study focuses on the mesoscale PBL structures under pollution conditions, and we try to combine the strength/advantage of both observation facts and numerical simulation capacity to investigate this issue. The densely distributed network of monitoring stations provides reliable $PM_{2.5}$ pollution facts. WRF model provides boundary layer meteorology information. A chemical transport model (e.g., WRF-Chem or WRF-CMAQ) can of course simulate the whole process from meteorology to pollutants transport/diffusion and chemical transformation. But the uncertainties caused by emission inventory, chemical mechanism, and meteorology conditions may complicate the simulation results together (e.g., Travis et al., 2016; Bouarar et al., 2019; Wang et al., 2021). Our current work isolates the boundary layer meteorology simulation from other factors, and evaluates the model intensively by observation data. Therefore, this study relies more on observations, but utilizes ultimately the capacity of the meteorological model to reveal the three-dimensional structure of PBL when pollution occurs.

We admit that, by the present method, the interaction between aerosols and boundary layer properties cannot be analyzed. However, the modification of aerosols to the PBL structures is a special issue to be discussed. The present study focuses on the more traditional part: the impact of meteorology on $PM_{2.5}$ pollution.

The relevant discussion added in Lines 612-630 of the revised manuscript is presented below.

"The present study focuses on the characteristic mesoscale PBL structures under pollution conditions, and emphasizes their role in shaping regional pollution patterns. The analysis of pollution evolution is based on the $PM_{2.5}$ concentration fields interpolated or diagnosed from monitoring data, relying on densely distributed stations. However, the PBL spatial structure is presented by numerical simulation, due to the scarcity and limitation of sounding data. Evaluation from the spatial-temporal variation of the surface meteorological field and PBL vertical structure indicates that the model performance is good. WRF can capture mesoscale systems and AIBs, as well as their overall evolution process and diurnal variation. It should be noted that, it is still difficult to reproduce the precise timing of the buildup and breakup as well as the exact location and range of these systems. This deficiency should be concerned seriously when simulated meteorological fields are used to drive air quality models, since a small position bias and time deviation of the AIBs can significantly alter pollution levels at a certain site (Seaman, 2000; McNider and Pour-Biazar, 2020). Accurate capture of mesoscale AIBs is a necessary prerequisite for reliable simulation of pollution evolution. Besides, successful reproduction and forecast of air quality by the chemical transport models also involves other factors, such as the accuracy of source inventories and the complexity of chemical mechanisms, which are beyond the scope of this study. The aim of the present work is to provide a clear cognition of these typical PBL structures reproduced by numerical simulations. This goal is achieved satisfactorily."

[R1.2] *Since PBL height is a key parameter in characterizing the PBL structures and the pollution formation mechanism, I am afraid that the authors fail to present this diagnosed variable in the whole manuscript, either for simulation or observation. Moreover, I suggest the author present the vertical cross-sections of potential temperature (like Figure 7) for wind shear category and topographic obstruction category in the supplementary materials to justify that those cases do not belong to the first frontal category.*

Response: We thank the reviewer for these suggestions. The PBL height has been presented and analyzed in the revised manuscript, including the comparison between the observations and simulations in Lines 367-370, 372-373, 379-382 and 387-389, and its relationship with wind and temperature structures in Lines 400-401, 441-443, 457-459, 468-469, 504-507 and 517-521. Meanwhile, the PBL height has been indicated in the vertical cross-sections of wind divergence and potential temperature (new Figs. 7-11) to better support the above explanations.

The vertical cross-sections of potential temperature during Case-1 and Case-2 have been shown in the supplementary material, which illustrates that there is no significant discontinuity in the atmospheric thermal structure and demonstrates their non-frontal characteristics.

For your convenience, the added sentences on describing the PBL height and the supplementary cross-sections of potential temperature (Figs. S2-S3) are presented below.

"As for Case-1, the model successfully reproduces the thermal structure evolution in the pollution formation-maintenance period, while the final uplift of the inversion layer and the growth of PBL are not well captured with an underestimation of about 200-300 m. The correlation coefficient (R) between simulated and observed PBL height is about 0.68 ($p<0.01$). During Case-2, observed and simulated PBL heights show a consistent evolution with a correlation coefficient as high as 0.78 ($p<0.01$). Both of their PBL heights are lower during the pollution formation-maintenance stage and increase by more than 1000 m in the diffusion stage. In Case-3, the PBL height is characterized by typical diurnal variations during the polluted period, and begins to abruptly develop in the evening of October 12, 2014, associated with the cold air mass and strong wind, both in observation and simulation ($R=0.81$, $p<0.01$)."

"During the pollution formation-maintenance stage of Case-1, the vertical section across the surface convergence belt shows that the depth of the convergence layer did not exceed 1000 m, with a compensating divergence layer immediately above it, being consistent with the evolution of the PBL (Fig. 8b, i-iv). In the process of pollution diffusion, a northeast wind divergence layer was relatively thin with a thickness of no more than 600 m (Fig. 8b-c, v), implying that the removal of pollutants only occurred within the PBL. As for the south-north wind shear mode, the vertical cross-sections of this special convergence zone exhibited a depth extending upwards for more than 3000 m, with a peak between 1000 m and 2000 m above the PBL top (Fig. 9b, i-iv). During Case-3, a deep, well-mixed warm PBL (with a height of more than 1000 m) has formed in the southern plain while a cold air mass capped by strong inversion (at the height of about 600-1000 m) still remained in the northern piedmont area in the afternoon.”

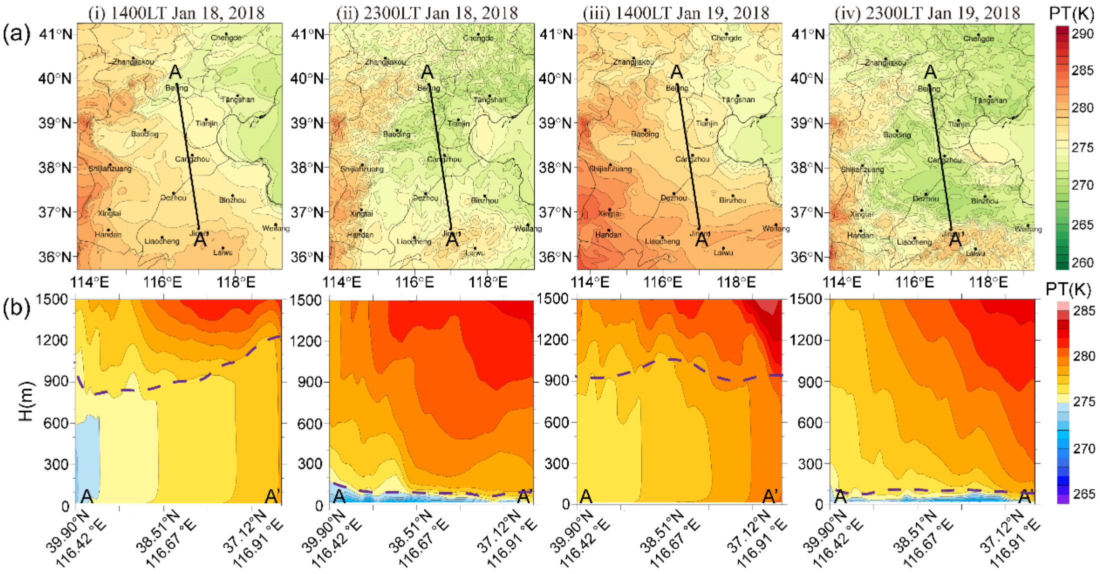

Figure S2. (a) Surface spatial distributions and (b) vertical cross-sections of the simulated potential temperature at the pollution stages of (i) formation, (ii-iv) maintenance, and (v) diffusion during representative Case-1 under west-southwest wind shear mode. The black lines in (a) indicate the section lines in (b). The purple dashed lines in (b) indicate the PBL heights.

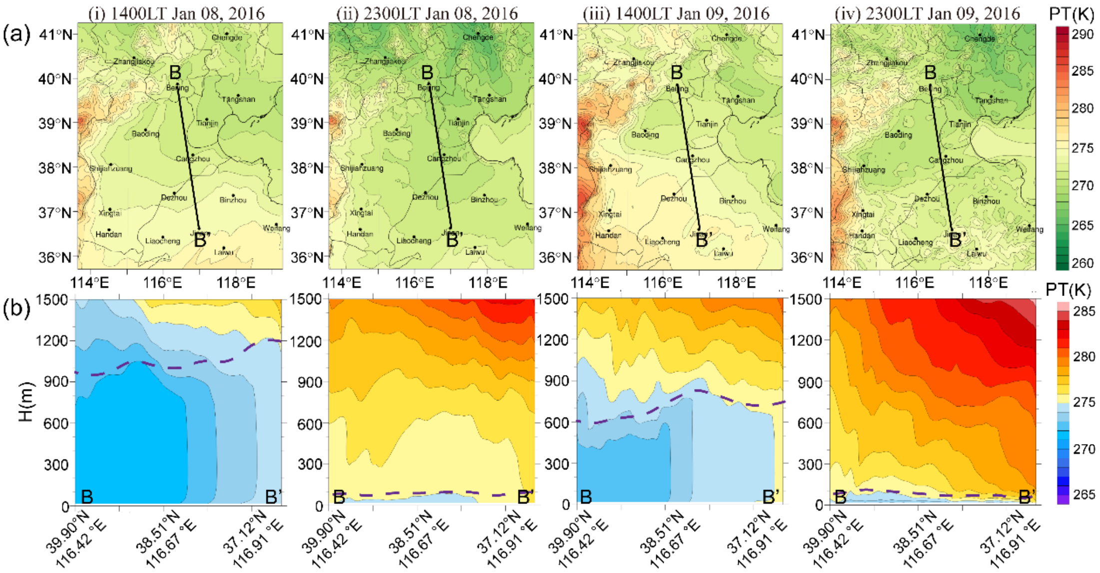

Figure S3. Same as Fig. S2, but for representative Case-2 under south-north wind shear mode.

Minor comments

[R1.3] Lines 1-2. I suggest the author give the study period in this sentence, otherwise, this sentence will be inaccurate.

Response: Accepted. The study period has been added in Line 2 of the revised manuscript.

[R1.4] Line 36. Should be "Petäjä et al., 2016".

Response: "Petaja, 2016" has been corrected to "Petäjä et al., 2016" in Line 56 of the revised manuscript.

[R1.5] Line 100. Should be "from December 25, 2017, to January 24, 2018".

Response: We are sorry for this mistake. It has been corrected in Line 171 of the revised manuscript.

[R1.6] Line 103. Please give the full name of LT and UTC when they appeared for the first time.

Response: The full names of LT and UTC (i.e., Local Time = Universal Time Coordinated + 8) have been given in Lines 174-175 of the revised manuscript.

[R1.7] Lines 107-108. What does the original data mean here?

Response: The original data refers to raw data directly measured by radiosonde soundings, which has higher vertical resolution than publicly available data from the Wyoming University, USA (http://weather.uwyo.edu.html). The related explanation has been added in Lines 179-181 of the revised manuscript.

[R1.8] Lines 115-116. Could you show the comparison of the observational and simulated PBL depth?

Response: The observational and simulated PBL heights during these pollution episodes have been superimposed on new Fig. 7 for comparison, and the relevant descriptions are added in the revised manuscript in Lines 367-370, 372-373, 379-382 and 387-389, as follows.

"As for Case-1, the model successfully reproduces the thermal structure evolution in the pollution formation-maintenance period, while the final uplift of the inversion layer and the growth of PBL are not well captured with an underestimation of about 200-300 m. The correlation coefficient (R) between simulated and observed PBL height is about 0.68 ($p<0.01$). During Case-2, observed and simulated PBL heights show a consistent evolution with a correlation coefficient as high as 0.78 ($p<0.01$). Both of their PBL heights are lower during the pollution formation-maintenance stage and increase by more than 1000 m in the diffusion stage. In Case-3, the PBL height is characterized by typical diurnal variations during the polluted period, and begins to abruptly develop in the evening of October 12, 2014, associated with the cold air mass and strong wind, both in observation and simulation ($R=0.81$, $p<0.01$).”

[R1.9] *Lines 131-133. I wonder if the vertical grid resolution is enough to resolve the PBL structure. It is better to give the detailed height of the model level within 2 km?*

Response: The detailed heights of the model level within 2 km are as follows: 9 m, 25 m, 50 m, 85 m, 120 m, 160 m, 200 m, 240 m, 290 m, 350 m, 420 m, 500 m, 580 m, 660 m, 740 m, 820 m, 900 m, 980 m, 1080 m, 1200 m, 1350 m, 1550 m, 1700m, 1850 m, and 2000 m. They are listed in Section 2.2 in Lines 205-208 of the revised manuscript.

[R1.10] *Line 148. The authors do not mention this study period in section 2.1.*

Response: The study period of Case-3 (October 7–12, 2014) corresponds to the routine radiosonde sounding period, which has been stated in Lines 177-179 of the revised manuscript.

[R1.11] *Figure 2. I am wondering why the authors present $PM_{2.5}$ concentrations at different sites for these three cases?*

Response: The spatial patterns of these three pollution cases are different, therefore we respectively choose the corresponding sites to reflect their unique distribution characteristics. For example, the pollution during Case-2 is severe in the south and relative lighter in the north, so the southern sites (such as Liaocheng and Xingtai) and northern sites (such as Chengde and Beijing) are presented for comparison; while for Case3, since the heavy pollution is mainly concentrated in the front of the mountains, the sites near the mountains (e.g. Shijiazhuang and Baoding) and far away from the mountains (e.g. Binzhou and Dezhou) are selected to highlight this feature. In the same way, sites such as Handan and Shijiazhuang and sites such as Cangzhou Binzhou are chosen in Case-1 to reflect the pollution expansion from the piedmont and the southwestern part to the middle and eastern area.

[R1.12] *Figure 3. Please state the figure represents observation data in the caption.*

Response: We have rewritten the figure caption in the revised manuscript in Lines 273-275, and indicated that the $PM_{2.5}$ concentration fields are derived from spatial interpolation of observation data.

[R1.13] *Figure 4. The figure looks very unclear. I think it should be re-plotted with making the wind vector line thinner.*

Response: Accepted. The figure has been re-plotted and the wind vectors have been set thinner in the revised manuscript.

***[R1.14]** Table 1. Give the units of those presented variables.*

Response: The units of the potential temperature (K) and wind speed (m s^{-1}) have been added in Table 1 in the revised manuscript.

***[R1.15]** Figure 6. Again, it seems that there is an intensive GPS sounding observation during October 7–12, 2014, but the author did not mention such observation in section*

Response: During October 7–12, 2014, the intensive GPS sounding observation is absent, and thus the routine sounding data are collected. This statement has been added in Section 2.1 in Lines 177-179 and in the figure caption in Lines 344-345.

***[R1.16]** Line 314. Should be "5 &8".*
Line 315 and Figure 7. Why do the authors present the results at 1500 LT and 2200 LT in this front category, but illustrate them at 1400 LT and 2300 LT for other categories? It is better to keep consistent.
Line 322, "Figs. 5 &8" is different from the description of the figure caption, please check and keep consistent.
Line 324. No Fig.7c-d, please add them in figure 7.

Response: According to the suggestions of Reviewer #2, the paragraph "Frontal category" and the corresponding Fig. 7 in the original manuscript have been removed, because the "frontal category" is discussed by a previous study (Jin et al., 2021) rather than the present work. We declare this research background and review the characteristics of the frontal category pollution in the Introduction in Lines 112-118 of the revised manuscript.

***[R1.16]** Line 325-326. It is difficult to see the change of the PBL height; I suggest the authors add the diagnosed PBL height in Figure 7 and other figures (e.g., Fig. 8, 9, 10, 11) to better support their explanations.*

Response: Accepted. We have superimposed the PBL heights on the vertical cross-sections of potential temperature and wind divergence, i.e., new Figs. 7-11 and updated the figure captions in the revised manuscript. The improved figures better illustrate the evolution of the PBL thermal and dynamic structures during these pollution cases.

***[R1.17]** Line 420. Should be PBL height in Jinan had increased to 1100 m.*

Response: Corrected as suggested.

References

Bouarar, I., Brasseur, G., Petersen, K., Granier, C., Fan, Q., Wang, X.M., Wang, L.L., Ji, D. S., Liu, Z.R., Xie, Y., Gao, W., and Elguindi, N.: Influence of anthropogenic emission inventories on simulations of air quality in China during winter and summer 2010. Atmos. Environ. 198, 236–256. https://doi.org/10.1016/j.atmosenv.2018.10.043, 2019.

Jin, X. P., Cai, X. H., Yu, M. Y., Wang, X. S., Song, Y., Kang, L., Zhang, H. S. and Zhu, T.: Mesoscale structure of the atmospheric boundary layer and its impact on regional air pollution: A case study, Atmos. Environ., 258 563 , doi:10.1016/j.atmosenv.2021.118511, 2021.

McNider, R. T. and Pour-Biazar, A.: Meteorological modeling relevant to mesoscale and regional air quality applications: a review, J. Air Waste Manage. Assoc., 70, 2-43, doi:10.1080/10962247.2019.1694602, 2020.

Seaman, N. L.: Meteorological modeling for air-quality assessments. Atmos. Environ. 34 (12–14):2231–59, doi:10.1016/S1352-2310(99)00466-5., 2000.

Travis, K. R., Jacob, D. J., Fisher, J. A., Kim, P. S., Marais, E. A., Zhu, L., Yu, K., Miller, C. C., Yantosca, R. M., Sulprizio, M. P., Thompson, A. M., Wennberg, P. O., Crounse, J. D., St Clair, J. M., Cohen, R. C., Laughner, J. L., Dibb, J. E., Hall, S. R., Ullmann, K., Wolfe, G. M., Pollack, I. B., Peischl, J., Neuman, J. A., and Zhou, X. L.: Why do models overestimate surface ozone in the Southeast United States?, Atmos. Chem. Phys., 16, 13561-13577, doi:10.5194/acp-16-13561-2016,2016.

Wang, W. G., Liu, M. Y., Wang, T. T., Song, Y., Zhou, L., Cao, J. J., Hu, J. N., Tang, G. G., Chen, Z., Li, Z. J., Xu, Z. Y., Peng, C., Lian, C. F., Chen, Y., Pan, Y. P., Zhang, Y. H., Sun, Y. L., Li, W. J., Zhu, T., Tian, H. Z., and Ge, M. F.: Sulfate formation is dominated by manganese-catalyzed oxidation of SO2 on aerosol surfaces during haze events, Nat. Commun., 12, doi:10.1038/s41467-021-22091-6,2021.