Response to Reviewer #1:

We are grateful to the reviewer for the professional comments. According to these comments, we have carefully revised the manuscript again. Additional work has been carried out to run a chemical transport model and actually show the dynamical transport processes of air pollutants. 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

My comments have been addressed partially in the revised version. The revised manuscript has improved as compared with the first submission. However, there are still issues that I consider fundamental which were not fully satisfied.

Response: We appreciate the positive evaluation of our efforts, and faithfully accept the major criticism of our previous revision. We have simulated the air pollution transport processes by the WRF-Chem model to fulfill the gap between meteorology and air pollution concentration. And the manuscript is revised accordingly.

Major comments

[R1.1] *Although the authors give some explanations as to why they did not choose the chemical transport model (e.g., WRF-Chem) for their simulations, their WRF results do not explain the formation of pollution in cases 1 and 2 well in my view, probably because the observed PM2.5 distributions (Fig. 4) are not necessarily due to the dynamical mechanisms proposed by the authors, and therefore, the use of chemical transport models could be a good support to explain these dynamical causes. For example, in Figs. 9a i-iv of case 2, their spatial fields of wind and divergence are similar, but their PM2.5 distributions (Figs. 4b i-iv) are clearly different. A similar pattern is also found in Figure 8a i-iv. These may be better explained if the results of the chemical transport model are used.*

Response: Yes, there is indeed a gap between the modeled meteorological fields and the observed $PM_{2.5}$ fields shown in the manuscript. Most importantly, the meteorological fields are not correspondent to the $PM_{2.5}$ pollution distributions apparently. Therefore, we have accepted this criticism and employed the WRF-Chem model to analyze the dynamical causes of the pollution formation in Case-1 and Case-2.

We add a figure in the new version of the manuscript to show the simulation results, as new Fig. 10. It shows that wind convergence leads to the pollutants accumulation, e.g., Fig.10a vs b, and Fig.10e vs f, for Case-1 and Case-2. The concentration increment fields are presented in Fig. 10c&g, and the patterns of $PM_{2.5}$ horizontal advection integrated over this period are shown in Fig. 10d&h. Their spatial distribution manifests a good correspondence. Quantitatively, the dynamical advection process contributes 27%-80% to the concentration increases during the pollution development period of these two cases. These results demonstrate clearly that airflow convergence plays a dominant role in the regional air pollution formation of the wind shear category.

New Fig. 10 and the detailed analysis added in Lines 412-444 of the revised manuscript are presented below.

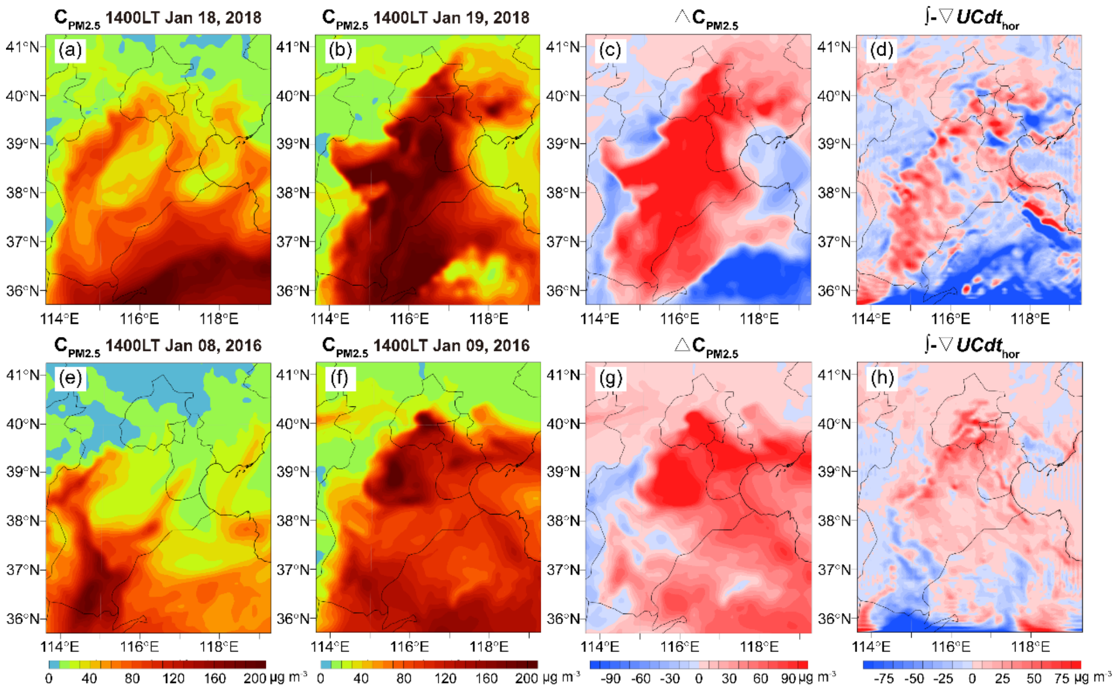

Figure 10. Simulated near-surface $PM_{2.5}$ concentrations (a-b, e-f) at two instants during the pollution formation-maintenance stage and their difference (c, g), as well as the temporal integration of the $PM_{2.5}$ horizontal advection term over this stage (d, h) for Case-1 (upper) and Case-2 (lower) respectively.

"To provide explicit support to the above explanation between the dynamical convergence feature and the pollution development, we adopt a chemical transport model (WRF-Chem) to simulate the $PM_{2.5}$ pollution process and directly quantify the advection term in the $PM_{2.5}$ concentration prognostic equation, i.e.:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \left(\vec{U}c\right)_{adv} + \nabla \cdot (K_e \nabla c)_{diff} + E_{emiss} + S_{sink} + R_{chem}, \qquad (1)$$

where c is $PM_{2.5}$ concentration, $\vec{U}$ is the wind vector, K_e is the turbulent diffusion coefficient. The first term on the right side of the equation represents the advection process both horizontally and vertically. The second term is turbulent diffusion, and the last three terms represent emissions, deposition and chemical reactions, respectively. The present study pays attention to the horizontal advection, which is considered of most important effect on the pollution development for the wind shear category. Details of the model configuration and validation are described in the supplementary material (Text S1, Fig. S4, and Table S2). The simulations of Case-1 and Case-2 well reproduce the $PM_{2.5}$ pollution concentration patterns and their evolution. Their pollution formation and maintenance stages are discussed here. For Case-1, the simulated near-surface $PM_{2.5}$ fields at 14:00 of both January 18 and January 19, 2018, as well as their difference are displayed in Fig. 10a-c, indicating that the air pollution aggravates and spreads eastward. The temporal integration of the $PM_{2.5}$ horizontal advection term over this period (Fig. 10d) agrees well with the concentration increment pattern in Fig. 10c, demonstrating the crucial role of the dynamical convergence in the development of $PM_{2.5}$ pollution. The contribution of the horizontal advection term on the total increment of $PM_{2.5}$ concentration during this period over most of this region is very high, e.g., at Handan, Shijiazhuang, Baoding, and Tianjin, the contribution ranges 40%-85%. For Case-2, heavy pollution is transferred to the north and east from January 08 to January 09, 2016 (Fig. 10e-g). Similar to Case-1, the advection term integrated over the pollution formation-maintenance period (Fig. 10h) presents good agreement with the $PM_{2.5}$ increment pattern (Fig. 10g). Quantitatively, this term contributes to total concentration accumulation as high as 27%-80% in the pollution process, especially in Beijing, Tianjin, and Baoding. This result is also consistent with those in previous works (Jiang et al., 2015; Chang et al., 2019; Jin et al., 2020). The above analysis indicates that, the airflow convergence AIB does not sharply confine the pollution air mass, but provides a circumstance or structure for pollutants transporting/accumulating along or nearby this zone. Because of the dynamical property, the concentration fields of the wind shear category pollution are more variable in space and time."

[R1.2] *Also Figures 5 and 6 in the revised version are still very unclear, making it difficult for the reader to get the appropriate information. Please re-plot these figures with the same color bar and with high resolution for better comparison.*

Response: Accepted. The figures have been re-plotted using the same color bar and with higher resolution in the revised manuscript.

Minor comments

[R1.3] *Line 56. Should be "Petäjä et al., 2016", not "Petaja et al., 2016".*

Response: We are sorry for this mistake. "Petaja et al., 2016" has been corrected to "Petäjä et al., 2016" in Line 38 of the revised manuscript.

[R1.4] *Line 93. Please specific the figure number in the supplement material for the emission spatial distribution.*

Response: Accepted. The figure number "Fig. S1" in the supplementary material for the emission spatial distribution has been specified in Line 73 of the revised manuscript.

[R1.5] *Line 435. Can you explain how the reader can see such a low-pressure trough?*

Response: The low-pressure trough is shown in Fig. 6a, presenting a narrow area extending from a low-pressure system with the surface isobar opening to the north. We have added the word "(refer to Fig. 6a)" in Line 367 of the revised manuscript to make the reader clearly see the low-pressure trough.

***[R1.6]** Line 612. Should be "The present study focuses on the characteristic of mesoscale PBL structures"?*

Response: Yes. This sentence has been corrected in Line 557 of the revised manuscript.

References

Chang, X., Wang, S.X., Zhao, B., Xing, J., Liu, X.X., Wei, L., Song, Y., Wu, W.J., Cai, S.Y., Zheng, H.T., Ding, D. and Zheng, M.: Contributions of inter-city and regional transport to PM2.5 concentrations in the Beijing-Tianjin-Hebei region and its implications on regional joint air pollution control, Sci. Total Environ. 660, 1191-1200, doi:10.1016/j.scitotenv.2018.12.474, 2019.

Jiang, C., Wang, H., Zhao, T., Li, T., Che, H.: Modeling study of PM2.5 pollutant transport across cities in China's Jing–Jin–Ji region during a severe haze episode in December 2013. Atmos. Chem. Phys. 15, 2969–2983, doi:10.5194/acp-15-5803-2015, 2015.

Jin, X. P., Cai, X. H., Yu, M. Y., Song, Y., Wang, X. S., Kang, L. and Zhang, H. S.: Diagnostic analysis of wintertime PM2.5 pollution in the North China Plain: The impacts of regional transport and atmospheric boundary layer variation. Atmos. Environ., 224, 117346, doi: 10.1016/j.atmosenv.2020.117346, 2020.