Dear Editors and Referees:

Thank you very much for your review and comments concerning our manuscript entitled "Elevated 3D structures of PM_{2.5} and impact of complex terrain-forcing circulations on heavy haze pollution over Sichuan Basin, China" [MS No.: acp-2020-1161]. Those comments are all valuable and helpful for revising and improving the manuscript. We have studied comments carefully and have accordingly made the revisions. Revised parts are highlighted with Track Changes in the revised manuscript. In the following we quoted each review question in the square brackets and added our response after each paragraph.

Response to Referee #1

[The paper analyzes an episode with high concentrations of PM2.5 in the Sichuan Basin (China), combining observations and numerical simulations. The paper is potentially interesting, in particular for the peculiar interaction between meso and local circulations and pollutant emissions, which leads to the formation of an elevated pollutant layer. However, the discussion of the results should be improved before the paper can be accepted for publication.]

Response 1: Many thanks for your encouraging comments. We have revised the manuscript accordingly. All the revisions have been highlighted with Track Changes in the revised manuscript. The point-by-point responses to the reviewer's comments are as follows.

General comments

[1. A general meteorological overview of the event, including a synoptic characterization, is missing in the paper.]

Response 2: Following the referee's comment, We have plotted the 700hPa geopotential heights and wind vectors in three stages (newly added Figure 3) over SCB and the surrounding regions with the meteorology analysis data of ERA-Interim.

We also characterized the overview of the synoptic conditions in the revised Sect. 2.4 as follows:

"The meteorological overview of the haze event was characterized with the 700hPa fields of geopotential heights and wind vectors (Fig. 3). A trough in the mid-latitude westerlies moved eastwards from the eastern edge of TP to the western SBC margin during the haze formation stage P1, the trough of low pressure was evolved over the SCB region during the haze maintenance stage P2, and the westerly trough shifted out the SCB region with the low-pressure system disappearing in the haze dissipation stage P3 (Fig. 3). The changes of atmospheric circulations in the formation, maintenance and dissipation stages reflected the meteorological modulation on heavy haze development over SCB in associated with the effect of TP topography on the westerlies. "



Figure 3. The 700 hPa geopotential height fields and wind vectors averaged during (a) P1, (b) P2 and (c) P3 stages with the trough line (brown line) and low-pressure center (L). The SCB was outlined with the red solid lines.

From the formation to the maintenance and the dissipation periods of haze pollution, the near-suface prevailing northeasterly winds strengthened gradually over SCB. During the formation and maintenance stage, the surface winds were weak $(1.4-1.7 \text{ m s}^{-1})$ over SCB, which was insufficient to dispel the air pollutants, but to continuously accumulate PM_{2.5} locally from light to heavy pollution conditions (Fig. 7a, Fig. 7b). By the dissipation period, the northeasterly winds intensified and removed PM_{2.5} from SCB (Fig. 7c).

[2. The Authors adopt a grid ratio of 1:4, while an odd grid ratio is recommended because for even values interpolation errors arise due to the nature of Arakawa C-grid staggering. The authors should at least discuss this choice.]

Response 3: Thanks for the referee's suggestion. In the revised manuscript, we have accordingly added the following discussions in the revised Sect. 2.3:

"Considering the complex terrain underlying over the SCB's deep basin and surrounding plateaus and mountains in Southwest China, we adopted a grid ratio of 1:4 for simulation experiments with precisely defined horizontal resolution in the study. It should be pointed out that the even grid ratio may cause the interpolation errors at the nested-domains boundary conditions due to the nature of Arakawa C-grid staggering."

[3. The Authors say that the "vertical turbulent diffusion coefficient of the boundary layer was reduced". This aspect should be better discussed, since it might significantly affect the results.]

Response 4: Following the referee's comments, we have added the below discussions into the revised Sect. 2.3.

"High PM_{2.5} levels in the atmosphere could significantly reduce the near-ground solar radiation for the stable atmospheric stratification, which decreases vertical turbulent diffusion in the boundary layer (Wang et al., 2019), that is an important mechanism for severe haze pollution formation with the explosive growth of PM_{2.5} (Zhong et al., 2018). The overestimated vertical diffusion capacity under poor air quality conditions (Ren et al., 2019) causes the deviation of air pollutants concentrations simulated in air quality model (Wang et al., 2018). In this study, the vertical turbulent diffusion coefficient of the atmospheric boundary layer was cut a

half down for better simulation of the 3D structures of PM_{2.5} during the heavy air pollution over the SCB region."

References

Wang, L., Liu, J., Gao, Z., Li, Y., Huang, M., Fan, S., Zhang, X., Yang, Y., Miao, S., Zou, H., Sun, Y., Chen, Y., and Yang, T.: Vertical observations of the atmospheric boundary layer structure over Beijing urban area during air pollution episodes, Atmos. Chem. Phys., 19, 6949–6967, https://doi.org/10.5194/acp-19-6949-2019, 2019.

Zhong, J., Zhang, X., Dong, Y., Wang, Y., Liu, C., Wang, J., Zhang, Y., and Che, H.: Feedback effects of boundary-layer meteorological factors on cumulative explosive growth of PM_{2.5} during winter heavy pollution episodes in Beijing from 2013 to 2016, Atmos. Chem. Phys., 18, 247–258, https://doi.org/10.5194/acp-18-247-2018, 2018.

Ren, Y., Zhang, H., Wei, W., Wu, B., Liu, J., Cai, X., and Song, Y.: Comparison of the turbulence structure during light and heavy haze pollution episodes, Atmospheric Research, 230, 0169-8095, https://doi.org/10.1016/j.atmosres.2019.104645, 2019.

Wang, H., Peng, Y., Zhang, X., Liu, H., Zhang, M., Che, H., Cheng, Y., and Zheng, Y.: Contributions to the explosive growth of PM_{2.5} mass due to aerosol–radiation feedback and decrease in turbulent diffusion during a red alert heavy haze in Beijing–Tianjin–Hebei, China, Atmos. Chem. Phys., 18, 17717–17733, https://doi.org/10.5194/acp-18-17717-2018, 2018.

[4. No information about the vertical discretization is given. An adequate vertical resolution is fundamental to evaluate the thermal stratification over complex terrain.]

Response 5: Thanks for the referee's comments. The information about the vertical discretization is added in the revised manuscript (lines 116-118) as follows:

"An adequate vertical resolution is fundamental to evaluate the thermal stratification over complex terrain. Therefore, 35 vertical layers were set with the fine resolutions of 30–120 m in the boundary layer."

[5. The Authors propose a series of statistical indexes for evaluating model results, both for meteorological variables and PM2.5. From these statistical indexes it is difficult to judge the performance of the model, regarding in particular the time evolution of observed and simulated variables. I strongly suggest to show some representative time series to better evaluate the model performance at some representative location.]

Response 6: Following the referee's suggestion, the hourly variations of $PM_{2.5}$ concentrations, 2 m air temperature, surface relative humidity and near-surface wind speed in Chengdu (site 1), Suining (site 10) and Zigong (site 13) were shown in Figures S1 and S2 in the supplement of manuscript. The comparisons between observation and simulation also were evaluated with the reasonable WRF-Chem modeling performance.



Figure S1. Hourly variations of observed (black curves) and simulated (red curves) $PM_{2.5}$ concentrations respectively in (a) Chengdu (site 1), (b) Suining (site 10) and (c) Zigong (site 13) during the haze pollution episode.



Figure S2. Hourly variations of observed (black curves) and simulated (red curves) 2 m air temperature, surface relative humidity and wind speed results respectively in (a) Chengdu (site 1), (b) Suining (site 10) and (c) Zigong (site 13) during the haze pollution episode in 2017.

[6. Figure 4 presents a comparison between the vertical profiles of potential temperature, wind speed and relative humidity from observations and model results. Also in this case it is difficult to evaluate model results, since only mean profiles and the variation range over the entire period are presented. I suggest to show also some representative profiles at some specific hours. In particular, it would be interesting to evaluate how the WRF model is able to capture the vertical temperature profile, since atmospheric stability is crucial for pollutant dispersion. In many points in the paper a temperature inversion is cited, but the simulation of this temperature inversion is

never discussed. For example, at lines 243-250, "thermo-dynamical structures" and "stable stratification" are cited, but, without a representative figure, it is difficult to follow the discussion of the results.]

Response 7: Following the referee's suggestions, the vertical air temperature profiles were evaluated with the comparisons of vertical air temperature profiles between observation and simulation during different haze periods at (a) 11:00 p.m. on 2 January, (b) 05:00 a.m. on 3 January, (c) 02:00 p.m. on 3 January, (d) 02:00 p.m. on 4 January, (e) 08:00 p.m. on 4 January, (f) 05:00 p.m. on 5 January, (g) 08:00 a.m. on 6 January, (h) 11:00 a.m. on 6 January and (i) 11:00 a.m. on 7 January 2017. (Figure S3 in the supplement of manuscript) with the following description added in the revised Sect. 3.1:

"Comparing with the observed air temperature, the WRF-Chem simulations were evaluated to reasonably capture the vertical temperature profiles for understanding atmospheric stability in the vertical thermo-dynamical structures in the boundary layer over SCB (Fig. S3)."

We have clarified the description of "thermo-dynamical structures" and "stable stratification" into the revised Sect. 3.3.

"The potential temperature vertical gradients (Fig. 5), which is used for assessing atmospheric stability, were estimated respectively with 4.0 K/km, 7.8 K/km and 5.2 K/km in the boundary layer during the formation, maintenance and the dissipation periods of haze pollution with near-surface strong temperature inversion (Fig. S3), presenting the thermo-dynamical structure with stable stratification in the atmospheric boundary layer weakening air pollutant dispersion."



Figure S3. Comparisons of vertical profiles of air temperature between observation (black curves) and simulation (red curves) at (a) 11:00 p.m. on 2 January, (b) 05:00 a.m. on 3 January, (c) 02:00 p.m. on 3 January, (d) 02:00 p.m. on 4 January, (e) 08:00 p.m. on 4 January, (f) 05:00 p.m. on 5 January, (g) 08:00 a.m. on 6 January, (h) 11:00 a.m. on 6 January and (i) 11:00 a.m. on 7 January 2017.

[7. Although the paper is rather well written, a review by a native English speaker would be beneficial.]

Response 8: Thanks for your positive comments. A native English speaker has reviewed the paper to improve the language.

Specific comments:

[Page 2, line 79: "Section 2 introduced...". Here and in other parts of the paper I would use the present tense (when referring to tables, figures...).]

Response 9: Thanks for the careful review, we have changed with the present tense (when referring to tables, figures...).

[Figures 7 and 8: the location of the cross sections should be indicated in Fig. 1.]

Response 10: We have indicated the location of the cross sections in the modified Figure 1.



Figure 1. (Left panel) three nesting domains D1, D2 and D3 of WRF-Chem simulation with the terrain heights (m in a.s.l.) and (right panel) the location of 18 urban observation sites (black dots, Table 1) including site 1 (Chengdu) with the intensive sounding observations and site 15 (Ya'an) with the ground-based MPL detection in SCB with the surrounding Tibetan Plateau (TP), Yunnan-Guizhou Plateau (YGP), Mountains Daba (Mt. Daba) and Wu (Mt. Wu) in Southwest China. The red dash lines indicate the location of the cross sections respectively along 30.67° N and 104.02° E.