Anonymous Referee #1

General comments:

- ***This manuscript provided an interesting study investigating the factors that affect the WRF-Chem performance of diurnal cycle of surface $PM_{2.5}$ concentrations in East China. This study suggested that PBL mixing coefficient is the key factor controlling the WRFChem model performance instead of PBL height and the diurnal cycle and injection height of emissions. This manuscript points out the importance of improving the PBL mixing process in WRF-Chem to achieve better results of diurnal $PM_{2.5}$ cycle. The topic is applicable for Atmospheric Chemistry and Physics. The text is concisely written and well documented. This study has comprehensive analysis and detailed explanation/discussion.***

We thank the reviewer for the detailed and constructive comments. They are very helpful for improving the quality of the manuscript.

In the revised manuscript, we added a few new figures in the supporting material to support some statements in the text and to address the review comments. Specifically, the evaluation of model performance in spatial distribution of surface $PM_{2.5}$ concentration is added. The PBL height is evaluated with the climatological estimate derived from the air sounding observations. More information about how to calculate the contribution from each process to surface $PM_{2.5}$ concentration is added in the methodology section. Other text and figures have also been revised as the reviewer suggested.

Major comments:

- ***This manuscript only discussed the normalized diurnal amplitude (i.e, DI) from observations and WRF-Chem simulations, but lacked the evaluation of model performance of actual $PM_{2.5}$ concentrations in East China.***

First of all, this paper focuses on the modeling of diurnal variation of surface $PM_{2.5}$. The evaluation of WRF-Chem simulated daily or monthly mean surface $PM_{2.5}$ has been conducted by previous studies (e.g., Gong et al., 2007; Ding et al., 2013; Gao et al., 2014; Chen et al., 2014; Zhao et al., 2014; Zhang B et al., 2015; Huang et al., 2016). The modeling biases of daily or monthly mean surface $PM_{2.5}$ can be affected by many other factors besides the boundary mixing, therefore beyond the scope of this study. In addition, besides focusing on the modeling of diurnal variation, we also investigated the impact of diurnal variation on daily mean concentration in the manuscript, and provided evaluation of actual monthly mean surface $PM_{2.5}$ at all stations over East China in Fig. 12. Fig. 12 shows the control simulation CTL1 significantly overestimates the observed surface $PM_{2.5}$ concentration with the normalized mean biases (NMB) of 22% (winter) - 109% (summer) on regional average. In the sensitivity experiment EXP1 with increased nighttime boundary mixing, the NMB is reduced to 7% (winter) - 38% (summer) on regional average. Therefore, we do have some discussion about the evaluation of actual surface $PM_{2.5}$ concentration over East China, although it is not the focus of this study. Now we also show

the spatial distribution of modeling biases of surface $PM_{2.5}$ concentration in the four months from the experiments CTL1, CTL2, CTL3, EXP1 and EXP2 compared to the observations in Fig S9. We add more discussion in the text as

"The model overestimates largely the monthly mean surface $PM_{2.5}$ at the stations of East China in the seasons other than winter from the control experiments. These modeling biases are significantly reduced at most stations of East China (Fig. S15 in the supporting material) in the sensitivity experiments."

- ***The comparison of monthly mean $PM_{2.5}$ concentrations between CTL1 and EXP1 (Figure 12) suggested that WRF-Chem had moderate model performance in winter (Jan) and poor performance in other 3 seasons (Apr, Jul, and Oct) even after increasing the PBL mixing coefficient. Note in winter the PBL is usually shallow and if we assume the MEIC emissions are accurate, my hypothesis is that the accuracy of PBL height simulations dominated the model performance of surface $PM_{2.5}$ in these 3 seasons. We cannot rule out that the PBL height was significantly underestimated in WRF-Chem, while increasing the PBL mixing could slightly improve the surface $PM_{2.5}$ simulations. The current manuscript claimed that the mixing coefficient is more important than the PBL height, but it did not show any comparison of PBL height from observations and simulations. I suggested the authors added 1) evaluate $PM_{2.5}$ simulations especially the spatial distribution with observations; 2) evaluate the WRF-Chem simulated PBL height with sonde or LIDAR observations to rule out the possibility that PBL height is more important.***

Fig. 12 shows that the control simulation CTL1 significantly overestimates the surface $PM_{2.5}$ concentration with the normalized mean biases (NMB) of 22% (winter) - 109% (summer) on regional average compared to the observations. In the sensitivity experiment EXP1 with increased nighttime boundary mixing, the NMB is reduced to 7% (winter) – 38% (summer) on regional average. Therefore, we would not agree that the performance in seasons other than winter with increasing nighttime boundary mixing is judged as poor. Emery et al. (2017) summarized many modeling applications in air quality studies and established a criterion for model evaluation. They concluded that the NMB< ±15% for surface $PM_{2.5}$ on regional average can be set as the best goal that a model can be expected to achieve. Currently, only one-third of modeling applications reached. The NMB< ±30% for surface $PM_{2.5}$ can be viewed as the acceptable performance of a model. Therefore, in our study, in terms of monthly mean surface $PM_{2.5}$ concentration averaged over East China, the sensitivity modeling performance with the increasing nighttime boundary mixing is acceptable in all seasons (it is a little worse than the criteria in summer), compared to the control modeling performance that is only acceptable in winter. As the reviewer suggested, now we also show the spatial distribution of modeling biases of surface $PM_{2.5}$ concentration in the four months from the experiments CTL1, CTL2, CTL3, EXP1 and EXP2 compared to the observations in Fig S15. We add more discussion in the revised manuscript as

"The model overestimates largely the monthly mean surface $PM_{2.5}$ at the stations of East China in the seasons other than winter from the control experiments. These modeling biases are significantly reduced at most stations of East China (Fig. S15 in the supporting material) in the sensitivity experiments."

We agree with the reviewer that the PBL height is very important in determining the PBL mixing. We are sorry to make the conclusion misleading. We did not intend to rule out the importance of modeling PBL height reasonably. Now, we revise the statement in the text, such as

in the key points "Besides the PBL height, PBL mixing coefficient is also the key factor controlling the simulated diurnal cycle of surface $PM_{2.5}$ concentration in WRF-Chem"

in the abstract "Besides the PBL height, the PBL mixing coefficient is found as the critical factor determining the PBL mixing of pollutants in WRF-Chem. With reasonable PBL height, the increase of lower limit of PBL mixing coefficient during the night can significantly reduce the modeling biases in diurnal $PM_{2.5}$ and also the mean concentrations, particularly at the major cities of East China."

in the summary "The analysis indicates that although PBL height is an important factor to reflect the PBL mixing strength, the PBL mixing process is more explicitly controlled by the PBL mixing coefficient instead of the PBL height in WRF-Chem, particularly during the night."

in the discussion "However, this study reveals that the PBL mixing flux is also critical in addition to the PBL height in terms of understanding the mixing of pollutants within PBL, particularly during the night, which can not only significantly affect the diurnal variation but also the daily mean of surface pollutant concentration."

In order to evaluate the simulated PBL heights, the long-term averaged PBL heights derived from the air sounding observations at four cities (Hangzhou, Nanjing, Shanghai, Anqing) provided in Guo et al. (2016) are used for comparison. Now Fig. S11 is added to show the comparison of simulation and observation-based estimation of PBL heights at 8 am and 8 pm (local time) at four stations. In general, throughout the four seasons, the CTL3 with the YSU scheme simulates reasonable PBL heights in the early morning and night, while the CTL1 and CTL2 with the MYNN scheme overestimate the PBL heights compared to the derived values. Therefore, the positive modeling biases of surface $PM_{2.5}$ concentration during the night is not due to the model underestimation of the PBL heights, instead that it is likely due to the underestimation of PBL mixing coefficient even with reasonable PBL height. Now, more discussion is added into the revised manuscript as

"The simulated PBL heights are evaluated with the long-term averaged PBL heights, primarily for 8 am and 8 pm local time, derived based on the air sounding observations available at four stations of East China as reported by Guo et al. (2016) (Fig. S11 in the supporting material). In general, throughout the four seasons, the CTL3 with the YSU scheme simulates reasonable PBL heights in the early morning and night, while the CTL1 and CTL2 with the MYNN scheme overestimate the PBL heights compared to the derived

values. The comparison between simulations and observations (Fig. 2 and 3) suggests the positive modeling biases of DI during the night may be partly due to the underestimation of the PBL mixing during the night, which cannot be explained by the modeling biases of PBL heights during the night."

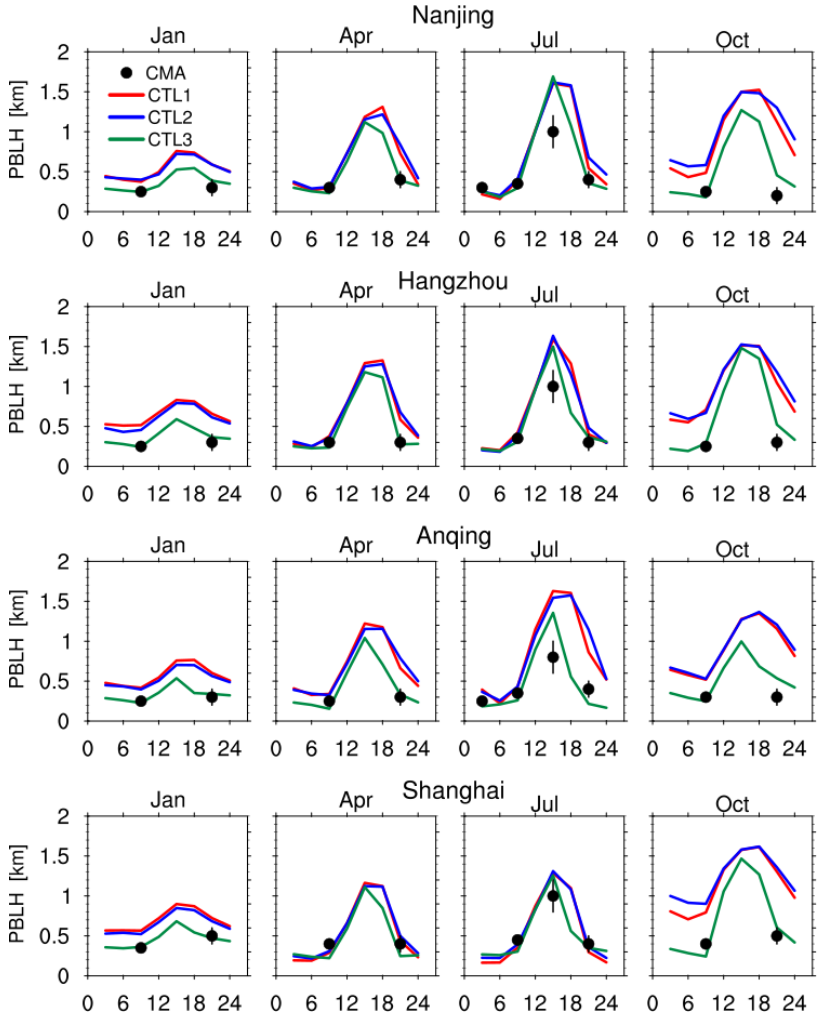

Figure S11. Diurnal variation of PBL height within 24-hour averaged at four stations in the cities of Nanjing, Hangzhou, Anqing, and Shanghai, respectively, for January, April, July, and October of 2018 from the experiments CTL1, CTL2, and CTL3. The long-term PBL heights at specific time derived from the air sounding observations at the corresponding stations are also shown as the black solid circle.

Specific comments:

- ***line 48: 'significantly overestimated' the $PM_{2.5}$ concentrations compared with observations?***

Sorry for the confusion. Now the sentence is revised as "…, and is significantly overestimated against the observation during the night".

- ***lines 72: The format of reference such as 'Davidson C I et al.' should be 'Davidson et al.'. Please correct all the references based on ACP bibliography requirement.***

Thanks for your suggestion. Now most references cited are corrected, except for those published in the same year and with first authors having the same surname. For those references, in order to distinguish them, abbreviations of first name are retained, for example, "Liu M et al., 2018" and "Liu T et al., 2018".

- ***line 94: Should 'Hu et al. (2017)' be 'Hu et al. (2016)'?***

Corrected as suggested.

- ***line 96: 'CAMQ' should be 'CMAQ'***

Corrected as suggested.

- ***line 294: In spring (Figure 2), I don't see two peaks of DI from observations. There is only one peak around 8 am in the morning. Similarly, the 'two peaks' in Oct is also not very clear. If the black dots are centered on 8 am, only one peak exists.***

Thanks for correction. Now it is revised as "In spring and autumn, the observed diurnal variation of DI is similar, showing the peak during the night, and reaching the minimum in the afternoon".

- ***line 305: I think the Figure S1 should be moved to the main article. It provided the spatial evaluation of DI from observations and simulations.***

As we discussed in the manuscript, the result shown in Fig. S1 is consistent with that in Fig. 2. There is no much additional information provided by Fig. S1. In order to keep the manuscript more concise, we decide to still keep Fig. S1 in the supporting material for the readers who are interested.

- ***line 328-329: I don't quite understand how the contribution was calculated. Looks like it is a unique function in the USTC version of WRF-Chem. Please add further explanation here.***

Yes, it is an added function in the USTC version of WRF-Chem in this study. We have mentioned briefly in the Methodology as "Particularly, in order to understand the modeling mechanisms driving the diurnal variations of surface $PM_{2.5}$ concentration over East China, this study updates the USTC version of WRF-Chem to include the diagnosis of contribution to surface $PM_{2.5}$ concentration from individual process including transport, emission, dry and wet deposition, PBL mixing, and chemical production/loss through estimating the difference of surface $PM_{2.5}$ concentration before and after individual process during the simulation.".

Now, we add more detailed description of the process contribution estimation in the Methodology as "More specifically, the contribution of each process is estimated in the following formula:

$$\boldsymbol{CT_{P,S,T} = C_{P,S,T} - C_{P,S,T0}}$$

where $\boldsymbol{C_{P,S,T0}}$and $\boldsymbol{C_{P,S,T}}$ represent the concentration of species *S* before (model time *T0*) and after (model time *T*), respectively, the process P. Therefore, $\boldsymbol{CT_{P,S,T}}$ represents the contribution of the process *P* to the change of concentration of species *S* during the time period (*T*-*T0*). For example, if *C0* and *C* represent the surface concentrations of $PM_{2.5}$ before (*T0*) and after (*T*), respectively, the PBL mixing, the contribution (*CT*) of PBL mixing to the change of surface concentrations of $PM_{2.5}$ during the time period (*T*-*T0*) can be estimated as (*C*-*C0*). The overall contribution during a specific time period (e.g., one day) can be obtained through integrating $\boldsymbol{CT_{P,S,T}}$ for that time period."

- ***line 332: Similar as above, please explain how the tendency was calculated.***

We add clarification in the revised manuscript as "The 3-hourly tendency (the difference between the current time and 3-hour ago) of surface $PM_{2.5}$ concentration is also shown."

- ***Line 355: Figure 5 shows the chemical composition of $PM_{2.5}$ simulated by WRF-Chem. Are there observations available to verify the accuracy of WRF-Chem?***

Very few observations of chemical composition of $PM_{2.5}$ at multiple stations over East China are publicly available, particularly for the simulation period of this study. Therefore, we acknowledged this need in the manuscript and suggested that the long-term measurements of $PM_{2.5}$ components at multiple stations are needed to further investigate the characteristics of diurnal variation of $PM_{2.5}$.

In addition, in the conclusion of this study, we discussed that the PBL mixing of the primary $PM_{2.5}$ determines the modelled diurnal variation of surface $PM_{2.5}$ concentration and may contribute to the modeling biases over East China. Although the observation of $PM_{2.5}$ components is not available to evaluate the diurnal variation of primary $PM_{2.5}$, the simulated diurnal variation of surface mixing ratio of CO that is normally used to represent the primary pollutant is compared with the observations (Fig. S19 in the supporting material). The results from experiments with enhanced nighttime PBL mixing are more consistent with the observations compared to the control experiments, which supports the findings about $PM_{2.5}$.

We searched the literatures, and found some observations about surface OC concentrations at Nanjing in April of 2015 (Wang, et al., 2016). We compared our simulated results with their observations at Nanjing and also found the control simulations overestimate nighttime surface OC concentrations, and the sensitivity experiments produce more consistent results (Fig. R1).

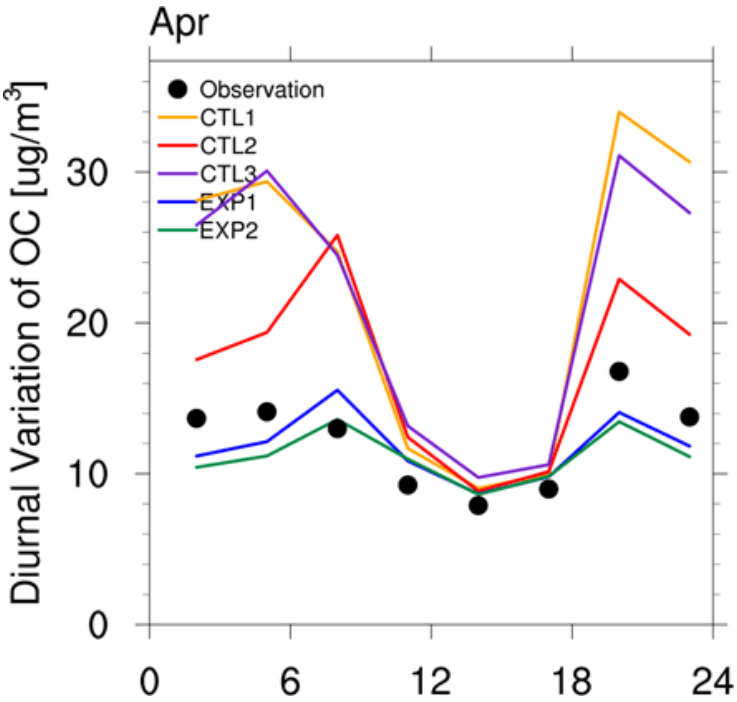

Figure R1. Diurnal variation of surface OC concentrations within 24-hour at Nanjing averaged in April. The modeling results are from the experiments in this study for 2018, and the observations are for 2015 obtained from Wang et al. (2016).

- ***Line 358: What are 'OM' and 'OIN'? I guess OM is equal to OC in Figure 5, while OIN is the total of NH4, NO3, and SO4?***

Sorry for the confusion. OC is represented as OM in WRF-Chem. OIN represents the unidentified aerosol species other than OC, BC, SO4, NH4, and NO3 in emissions, which are composed mostly of minerals in emissions. OC in Figure 5 and Figure 9 have been corrected as OM and the explanation of OIN is added in the revised manuscript "OIN represents the unidentified aerosol species other than OM, BC, sulfate, ammonium, and nitrate in emissions if any, which are composed mostly of minerals in emissions in this study.".

- ***Line 378-379: More vertical layers in the lower atmosphere could also better simulate the PBL height, which influence the surface $PM_{2.5}$ concentrations. The authors should evaluate the PBL height with observations (if available) or at least make sure the PBL heights simulated in all WRF-Chem runs are comparable.***

Yes, the configuration of vertical layers could affect the simulation of PBL height. In fact, we have shown the comparison of PBL heights from the simulations with different vertical configuration in Fig. 6 in the manuscript. As we can see that the difference in PBLH between CTL1 and CTL2 is very small. In addition, now, we add the evaluation of PBLH from different experiments with the long-term averaged PBL heights derived from the air sounding observations at four cities (Hangzhou, Nanjing, Shanghai, Anqing) provided in

Guo et al. (2016) in the revised manuscript (Fig. S11). Now, in the revised manuscript, Fig. S11 shows that the PBLH from the experiments with different vertical configurations is comparable. The details can be found in our response to your comment above.

- ***Line 412-413: As above, this statement is only valid if the PBL heights simulated in CTL1-3 runs are comparable.***

First of all, the PBL height and PBL mixing are related instead of discrepant. This statement only means that the PBL mixing between CTL3 and CTL2 is different. It is not necessary to conclude that the PBL heights between them are comparable or different. More detailed analysis about the reason of different PBL mixing is discussed in section 3.2.2. The comparison between the PBL heights from CTL1-3 is shown in Fig. 6 and Fig. S11 in the revised manuscript. More discussion is added as in the response to your comments above.

- ***Line 434: Hard to tell from the figure, but I think the PBL height from CTL 1-3 are substantially different. For instance, at 8 am in Apr with the maximum surface $PM_{2.5}$ simulated, CTL 3 has much lower PBL height as compared with CTL1 and 2. Again, if observations such as LIDAR are available, it will be great to see which run has the better PBL height. Same as in Figure 7, I suggest plotting all the PBL height from WRF-Chem runs in one figure to see the difference.***

See our response to your comments above. Now Fig. S11 is added in the revised manuscript for direct comparison of PBLH among all the experiments and observation derived dataset. The PBLH is comparable between CTL1 and CTL2, while it is true that the PBLH is different between CTL2 and CLT3. In fact, we discussed about their different PBLH in the manuscript as "The difference between CTL2 and CTL3 is consistent with the analysis about the simulated diurnal variation of surface $PM_{2.5}$ concentration, further demonstrating that the WRF-Chem simulated diurnal variation of surface $PM_{2.5}$ concentration is not explicitly controlled by the PBL height instead by the PBL mixing coefficient. For example, in autumn the PBL height during the night is lower in CTL3 than in CTL2, while the DI during the night is lower in CTL3 than in CLT2 (Fig. 3) due to the higher PBL mixing coefficient during the night in CTL3 than in CTL2.".

We add more discussion about the PBLH among the experiments in the revised manuscript as "The CTL3 simulates similar PBL height during the daytime but lower values during the night, particularly in October. The simulated PBL heights are evaluated with the long-term averaged PBL heights, primarily for 8 am and 8 pm local time, derived from the air sounding observations available at the four stations of East China as reported by Guo et al. (2016) (Fig. S11 in the supporting material). In general, throughout the four seasons, the CTL3 with the YSU scheme simulates reasonable PBL heights in the early morning and night, while the CTL1 and CTL2 with the MYNN scheme overestimate the PBL heights compared to the derived values."

- ***Line 474: Any reference or data to support the 5 m2/s rate is reasonable?***

The one of the key points of this study is that the PBL mixing during the night over East China may be underestimated by WRF-Chem. Increasing of PBL mixing during the night can significantly reduce the modeling biases of surface $PM_{2.5}$ concentration and also the modeling sensitivity to the PBL configuration. The exact value of PBL mixing coefficient cannot be obtained by this study. The lower limit rate of 5 m^2/s was selected to show the sensitivity. We acknowledged in the manuscript as "It is noteworthy that the lower limit parameter of 5 m^2/s is entirely empirical. It is selected to represent the moderate mixing strength between the full PBL mixing and no PBL mixing. A few other values such as 1 m^2/s and 10 m^2/s are also tested. The results do not change the conclusion found in this study and therefore are not shown."

- ***Line 575-576: Does MEIC inventory treat power plants as point sources? For instance, US EPA has lat/lon information and hourly emission rate to process power plants as point sources in SMOKE. If not, how to support this argument?***

Yes, the power plant emissions in the MEIC inventory are treated as point sources. As shown in Figure R2, the power plant emissions of SO_2 and $PM_{2.5}$, for example, in the MEIC inventory are distributed discretely.

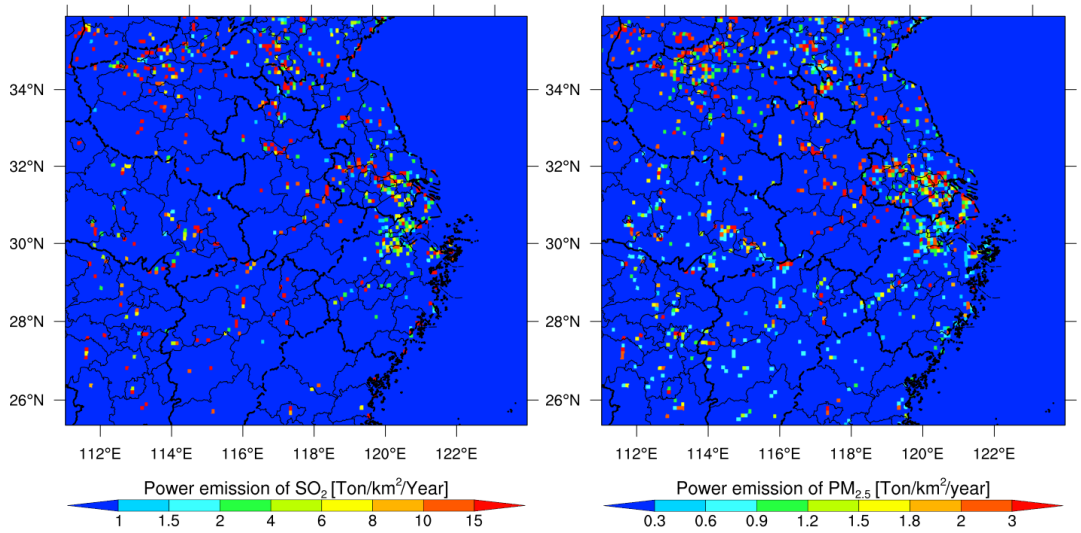

Figure R2. Spatial distribution of power plant emissions of SO_2 and $PM_{2.5}$ from the MEIC inventory.

- ***Line 588: The current version of Section 4 is too long. A concise summary of the paper is needed. I suggest the authors to revise this session.***

Thanks for your suggestion. The Section 4 is now split into two sections, Section 4 (Summary) and Section 5 (Discussion) in the revised manuscript. The summary section is more concise in the revised manuscript.

- ***Line 1183: The unit is %?***

Yes, it is. Now it is clarified.

- ***Line 1187: Plots in Figure 1a are small and hard to see the details. Please remove the black box and symbols for cities in NOx and SO2 plots.***

Figure 1a is revised following your suggestion.

- ***Line 1245: Surprised to see the chemistry contributed so little in the surface $PM_{2.5}$ concentrations. Does 'chemistry' stand for chemical evolution such as formation of SOA?***

Based on Fig. 4, we can only say the relative contribution from chemistry to the change of $PM_{2.5}$ concentration is small compared to the processes of emission, transport, and PBL mixing. As we respond to your comment above, if *C0* and *C* represent the surface concentrations of $PM_{2.5}$ before (*T0*) and after (*T*), respectively, the chemical production/loss of aerosols, the contribution (*CT*) of chemistry to the change of surface concentrations of $PM_{2.5}$ during the time period (*T-T0*) is estimated as (*C-C0*). Therefore, the chemistry contribution includes all the chemical evolution such as the secondary production. However, as we mentioned in the manuscript, the WRF-Chem simulations conducted in this study do not consider the SOA production that still has large uncertainties in mechanisms.

The relatively small contribution from chemical production may be due to that the stations are mostly urban and suburban areas, where the surface $PM_{2.5}$ concentrations are dominated by the primary emissions. We checked that the chemical contribution to the surface $PM_{2.5}$ concentration over the rural areas can be comparable to transport, and larger than emission.

- ***Line 1373: A map of data in Figure 12 is needed, maybe in the SI to show the spatial performance of WRF-Chem.***

In fact, we have shown the observational sites in Fig. 1a. Now we clarify it in the caption of Fig. 12. For the spatial performance of model, now we add Fig. S15 in the supporting material to show the spatial distribution of modeling biases of surface $PM_{2.5}$ concentration in the four months from the experiments CTL1, CTL2, CTL3, EXP1 and EXP2 compared to the observations. Please see our response to your comments above for details.

Anonymous Referee #2

General comments:

- ***This study investigates the simulation of diurnal variation of surface $PM_{2.5}$ concentration over East China in WRF-Chem. The authors test sensitive of model simulations to PBL configuration, PBL mixing coefficient, emission diurnal variation and injection height, etc. It is found that diurnal variation of surface $PM_{2.5}$ is mostly sensitive to PBL mixing coefficient, while diurnal cycle and injection height of anthropogenic emission has smaller impacts than PBL mixing coefficient. It is a nice model sensitivity study. However, the evaluation of the model performance is simply based on surface $PM_{2.5}$ observations. As discussed in the manuscript, the diurnal variation of surface $PM_{2.5}$ is impacted by emission, PBL mixing and transport. It will make the results more convincing by including more model evaluation on the simulation of aerosol and meteorological variables, such as temperature, moisture, wind, stability, PBL height, aerosol speciation, vertical distribution of aerosols, etc.***

We thank the reviewer for the detailed and constructive comments. They are very helpful for improving the quality of the manuscript.

In the revised manuscript, we added a few new figures in the supporting material to support some statements in the text and to address the review comments. Specifically, the evaluation of model performance in some associated meteorological fields, such as temperature, wind, and PBL height, is added. The observed vertical profiles of aerosol are not available for evaluation, and are discussed in the revised manuscript. The publicly available aerosol speciation observations are few over East China. We evaluated the diurnal variation of CO as the representative primary pollutant. In this response, we found some data about OC during other period and added here as the reference. The information about how to calculate the PBL mixing coefficient is briefly described in the methodology section. Other text and figures have also been revised as the reviewer suggested.

Specific comments:

- ***L78: and precipitation.***

Revised as suggested.

- ***L136: What about Liu M et al. (2018)? What are they findings?***

Liu, M et al. (2018) used the nested GEOS-Chem CTM version 9-02 and WRF/CMAQ v5.0.1 to simulate NO2, $PM_{2.5}$, and other pollutants over China in October–December 2013. They found that the air quality model (WRF-CMAQ v5.0.1) also overestimated the surface concentration of $PM_{2.5}$ during the nighttime in October-December, 2013. They speculated that the overestimation is due to the weak PBL mixing in the nighttime, and claimed that the newer version of CMAQ v5.1 driven by WRF v3.7 revised the PBL mixing scheme (ACM2) and might reduce the nighttime biases. According to the technical documentation

of CMAQ v5.1, the PBL mixing scheme (ACM2) in the previous versions produce too weak mixing under stable atmospheric conditions due to the assumption of the same value for the eddy diffusivity of momentum (K_m) and heat (K_h) and the unity Prandtl number (Pr = Km/Kh). In CMAQ v5.1 driven by WRF v3.7, the ACM2 estimates and applies different eddy diffusivities for momentum (K_m) and heat (K_h) and develop new stability functions for both momentum and heat for stable conditions, so the deficiency in boundary mixing under stable atmospheric condition may be improved.

To verify the effect of this modification, we conduct two experiments use ACM2 PBL schemes in WRF-Chem v3.5 (ACM2.v3.5) and WRF-Chem v4.0 (ACM2.v4.0), respectively, over East China for October of 2018. As shown in Figure R3, the PBL mixing coefficients in ACM2.v4.0 are enhanced compare to that in ACM2.v3.5, especially during night. In addition, the simulated surface $PM_{2.5}$ concentrations from ACM2.v4.0 are reduced during night compared to ACM2.v3.5 (Fig. R4). However, the model still significantly overestimates the surface $PM_{2.5}$ concentration comparing to the observations (Fig. R4). We add the discussion in the revised manuscript as "Liu M et al. (2018) found that the air quality model (WRF-CMAQ v5.0.1) also overestimated the surface concentration of $PM_{2.5}$ during the nighttime in October-December, 2013. They speculated that the overestimation is due to the weak PBL mixing in the nighttime, and claimed that the newer version of CMAQ v5.1 driven by WRF v3.7 revised the PBL mixing scheme (ACM2) and might reduce the nighttime biases. To verify this, two experiments are conducted using the ACM2 PBL scheme with WRF-Chem v3.5 and WRF-Chem v4.0, respectively, over East China for October of 2018. The results showed that the PBL mixing of ACM2 scheme is enhanced in v4.0 compared to v3.5 especially during the night, and the simulated nighttime surface $PM_{2.5}$ concentrations are reduced to some extent in v4.0 compared to v3.5 (not shown). However, the simulation still significantly overestimates the surface $PM_{2.5}$ concentration during the night. Therefore, the changes of PBL schemes and vertical configurations within the PBL can affect the simulated DI but cannot improve the simulations to reproduce the observations."

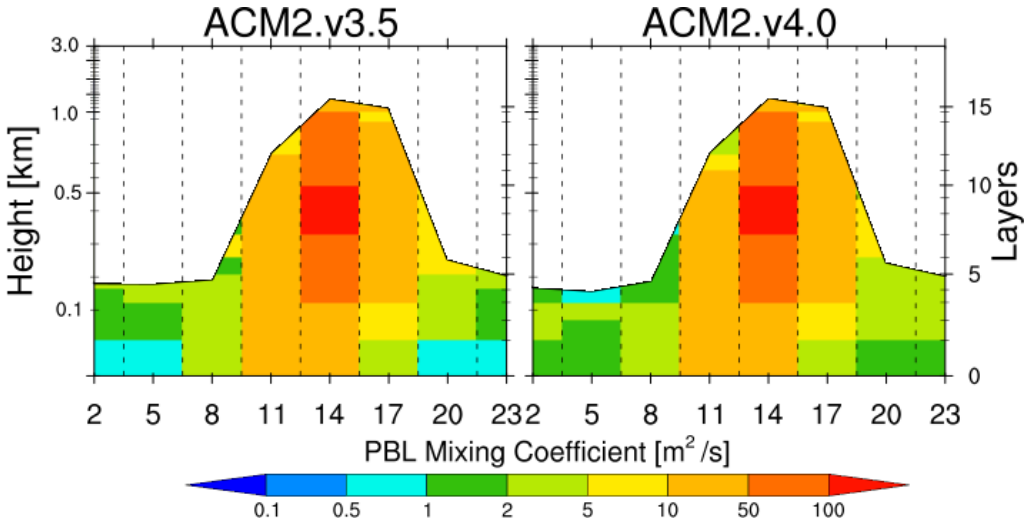

Figure R3. Diurnal variation of PBLH and PBL mixing coefficient below PBLH averaged over Hefei for October of 2018 from the experiments ACM2.v3.5, ACM2.v4.0.

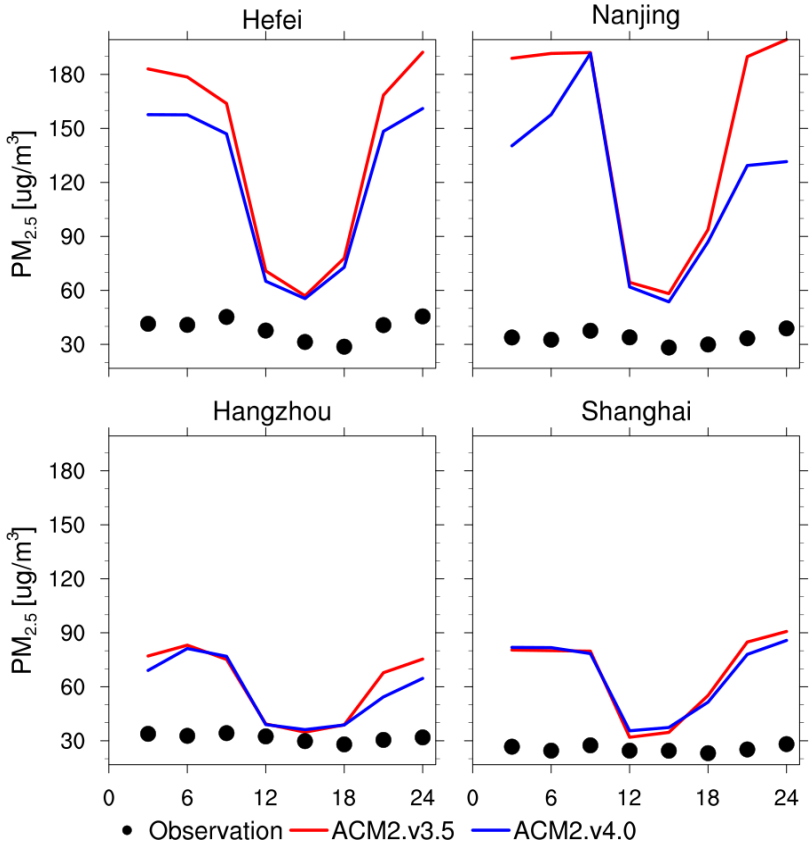

Figure R4. Diurnal variation of surface $PM_{2.5}$ concentrations within 24-hour averaged over four cities (Hefei, Nanjing, Hangzhou, Shanghai) for October of 2018 from the experiments ACM2.v3.5, ACM2.v4.0 and observations.

- ***L233: Which emission (anthropogenic emission, biomass burning, dust or others) is***

the primary contributor(s) to the surface $PM_{2.5}$ over East China in different season?
As shown in Fig. 5, over East China, the dominant emission for surface $PM_{2.5}$ concentration in all seasons are from anthropogenic emission.

- ***L325-327: How does the model simulate the diurnal cycle of temperature, moisture, wind, stability and PBL height? Could the biases in model simulated meteorological variables contribute to the bias in diurnal cycle of surface $PM_{2.5}$?***

Yes, the basic meteorological fields are important for simulating air pollutants. We didn't evaluate them because our simulations are nudged to the reanalysis and WRF simulations has been widely evaluated over China in previous studies. Following your suggestion, now we add Fig. S6-S11 in the revised manuscript about evaluating the simulated wind, temperature, and PBL height. We also add the discussion in the revised manuscript as "In order to understand the possible reasons for this modeling biases, some basic meteorological fields are evaluated with available observations. Since the modeled winds at the layers above the PBL are nudged towards the reanalysis data, the large-scale circulation can be well simulated. The winds at 850 hPa for each season are compared with the NCEP Final reanalysis dataset and ERA5 reanalysis dataset (https://rda.ucar.edu/datasets/ds630.0/, last access: 28 December 2019) (Fig. S6 in the supporting material). The simulated wind circulation is highly correlated with the two reanalysis datasets with the spatial correlation coefficients of 0.9-0.97 over East China. The simulated temperature at 2-m is also evaluated with the available observations at the stations of East China (Fig. S7 and Fig. S8 in the supporting material). The model captures the diurnal variation of near-surface temperature very well over East China. For near surface winds, although the model generally overestimates the observed values by less than 10%, the simulated diurnal variation is generally consistent with the observations over East China (Fig. S9 and Fig. S10 in the supporting material). As the evaluation shows, the basic meteorological fields are generally simulated reasonably. The characteristics associated with the PBL mixing are further investigated below."
And "The simulated PBL heights are evaluated with the long-term averaged PBL heights, primarily for 8 am and 8 pm local time, derived from the air sounding observations available at four stations of East China as reported in Guo et al. (2016) (Fig. S11 in the supporting material). In general, throughout the four seasons, the CTL3 with the YSU scheme simulates reasonable PBL heights in the early morning and night, while the CTL1 and CTL2 with the MYNN scheme overestimate the PBL heights compared to the derived values. The comparison between simulations and observations (Fig. 2 and 3) suggests the positive modeling biases of DI during the night may be partly due to the underestimation of the PBL mixing during the night, which cannot be explained by the modeling biases of PBL heights during the night."

- ***L356-357: Is there any aerosol speciation data available to evaluate the model***

performance?

Very few observations of chemical composition of $PM_{2.5}$ at multiple stations over East China are publicly available, particularly for the simulation period of this study. Therefore, we acknowledged this need in the manuscript and suggested that the long-term measurements of $PM_{2.5}$ components at multiple stations are needed to further investigate the characteristics of diurnal variation of $PM_{2.5}$.

In addition, in the conclusion of this study, we discussed that the PBL mixing of the primary $PM_{2.5}$ determines the modelled diurnal variation of surface $PM_{2.5}$ concentration and may contribute to the modeling biases over East China. Although the observation of $PM_{2.5}$ components is not available to evaluate the diurnal variation of primary $PM_{2.5}$, the simulated diurnal variation of surface mixing ratio of CO that is normally used to represent the primary pollutant is compared with the observations (Fig. S19 in the supporting material). The results from experiments with enhanced nighttime PBL mixing are more consistent with the observations compared to the control experiments, which supports the findings about $PM_{2.5}$.

We searched the literatures, and found some observations about surface OC concentrations at Nanjing in April of 2015 (Wang, et al., 2016). We compared our simulated results with their observations at Nanjing and also found the control simulations overestimate nighttime surface OC concentrations, and the sensitivity experiments produce more consistent results (Fig. R1).

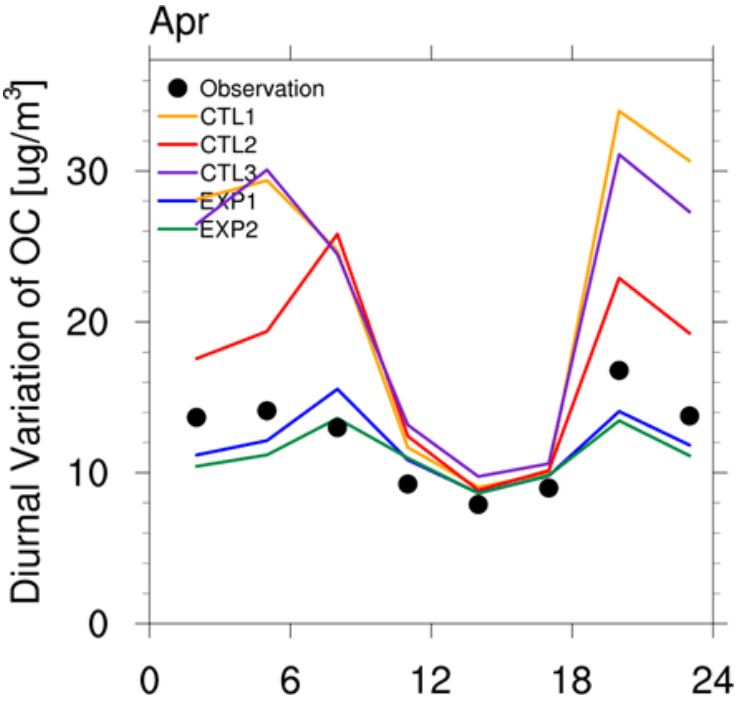

Figure R1. Diurnal variation of surface OC concentrations within 24-hour at Nanjing averaged in April. The modeling results are from the experiments in this study for 2018, and the observations are for 2015 obtained from Wang et al. (2016).

- ***L430: How is PBL mixing coefficient calculated?***

The calculations of PBL mixing coefficient are different in different turbulence closure type of PBL schemes. Now we add more description in the revised manuscript as "Since this study focuses on understanding the PBL mixing impact, the calculation of PBL mixing coefficient within the MYNN2 and YSU PBL schemes is briefly described here. In the local closure PBL scheme MYNN, the PBL mixing coefficient is calculated following Mellor et al. (1982):

$$K_{h,m} = lqS_{h,m}$$

where l is the mixing-length scale, S_h and S_m are stability functions, q is related to the turbulent kinetic energy (TKE) in the following formula:

$$\mathrm{q} = (2 * TKE)^{1/2}$$

In the non-local closure PBL scheme YSU, the momentum mixing coefficient K_m is formulated following Hong et al. (2006):

$$K_m = kw_s z(1 - \frac{z}{h})^p$$

where p is the profile shape exponent taken to be 2, k is the von-karman constant, z is the height from the surface and h is PBL height. For the eddy mixing coefficient for temperature and moisture K_h can be estimated from K_m with the relationship of the *Prandtl* number as in Noh et al. (2003):

$$\mathrm{Pr} = K_m/K_h$$

$$\mathrm{Pr} = 1 + (\mathrm{Pr}_0 - 1)\exp[\frac{-3(z-\varepsilon h)^2}{h^2}]$$

Two additional sensitivity experiments (EXP1 and EXP2, Table 1) are also conducted corresponding to the experiments CTL1 and CTL2, respectively, except that the PBL mixing coefficient is modified (see details in Section 3.2.2)."

- ***L364: Is there any in-situ observation of the vertical distribution of aerosols in the boundary layer? The CALIPSO data may be useful to validate the simulated aerosol profiles.***

It would be great if there are in-situ observed vertical profiles of pollutants over cities to evaluate the simulations, particularly for below 200 m and during the night. However, as we are aware, there is no dataset publicly available for evaluation of our simulations over East China. It is encouraged in the discussion section as "Therefore, this study suggests that the long-term measurements of $PM_{2.5}$ components at more stations and the in-situ measurements of vertical profiles of $PM_{2.5}$ concentration within PBL during the night are needed to further investigate the characteristics of diurnal variation of $PM_{2.5}$".

CALIPSO retrievals are useful, particularly during the night. However, over the urban area such as East China with a lot of tall buildings, the retrievals near the surface (< 100 m) are mostly contaminated by the surface reflection signals. We did check the CALIPSO retrievals. Few of the vertical profiles near the surface is valid.

- ***Figure 4: What is the unit of each variable? And what is the black line?***

In Fig. 4, the contribution and tendency are normalized values by monthly mean surface $PM_{2.5}$ concentration for each month. The original units of contribution and tendency are ug/m^3. After normalization, they are relative values as the ratios. The black line is the 3-hourly relative tendency of surface $PM_{2.5}$ concentrations. It is now clarified in the caption of Fig. 4 as "Relative contribution (normalized by monthly mean surface $PM_{2.5}$ concentration for each month) to surface $PM_{2.5}$ concentration every 3-hour from individual process (transport, emission, dry and wet deposition, PBL mixing, chemical production/loss) averaged over Hefei for January, April, July, and October of 2018 from the experiments CTL1, CTL2, and CTL3. The 3-hourly relative tendency of surface $PM_{2.5}$ concentration is also shown as the black line."

Anonymous Referee #3

General comments:

- ***This study is focused on one of the key uncertainties in modeling and forecasting of air pollution, the parameterization of turbulent mixing of chemical species and its impact on hourly variability of the modeled concentrations of fine particulate matter ($PM_{2.5}$). The sensitivity of the $PM_{2.5}$ simulations to the diurnal cycle and vertical distribution of the anthropogenic emissions is analyzed here as well. The modeling study deploys one of the widely used atmospheric chemistry models - WRF-CHEM. A number of WRFCHEM model simulations are conducted over East China for all the seasons, year of accurate simulation of diurnal variability of the ground level $PM_{2.5}$ is crucial for air quality forecasting applications. It is great to see that this topic is addressed by such rigorous modeling study. This study deserves a publication, but I have reservations on the interpretation of some of the results and conclusions presented here. I suggest addressing the following comments before a final publication in ACP.***

We thank the reviewer for the detailed and constructive comments. They are very helpful for improving the quality of the manuscript. In the revised manuscript, we add the discussion about using the simple modification to enhance the nighttime PBL mixing and its difference from the existing scheme in WRF-Chem. We add more clarification about the model and emission configurations. Other text and figures have also been revised as the reviewer suggested.

Major comments:

- ***The authors show that setting a minimum exchange coefficient for chemicals in WRFCHEM improves the simulation results, especially in winter. Actually the WRF-CHEM model has already included this feature for many years. In the community version of the model the exchange coefficients (ECs) that are used for mixing of the chemical species are modified based on the anthropogenic CO and primary $PM_{2.5}$ emissions. This simple parameterization isn't perfect, but it was designed to help with the strong accumulation of air pollutants near surface, when the modeled boundary layers are too shallow. Why didn't the authors use the existing parameterization in WRF-CHEM? Instead they set the lower limit of the ECs everywhere in the model grid.***

Yes, we noticed that this parameterization is in the community version of WRF-Chem and also in our USTC version of WRF-Chem. Although it is included in WRF-Chem for a few years, we didn't notice any publications about its application, particularly over China. We didn't find the reference for this parameterization in the code as well. If the reviewer can provide the reference, we'd like to cite it.

In addition, it is only for gases if the MOSAIC or MADE/SORGAM aerosol schemes are used because it does not couple with the aerosol activation scheme even in the latest version of WRF-Chem (v4.1), although it can be modified to be compatible with the MOSAIC scheme. This parameterization treats the enhancement of exchange coefficient up to half number of model vertical layers, which is beyond the PBL in most cases during the night and may not be suitable. We prefer adjusting the coefficient only within PBLH. This

parameterization also assumes the PBL mixing is only enhanced in the region with intense emission due to urban island effect. For example, Fig. R5a and 5b show the spatial distributions of anthropogenic emissions of $PM_{2.5}$ and CO exceeding the threshold defined inside of the parameterization. They occur mostly over the big cities of East China. We acknowledged this urban effect in our discussion section, and in fact are working on this issue. However, we noticed that the issue of PBL mixing during the night may not only occur over these urban areas. Therefore, in this study, we omitted this modification and simply adjusted the minimum value of coefficient within PBL height everywhere. It is noteworthy that our study intended to conduct the sensitivity experiments to raise this issue in using WRF-Chem to simulate surface $PM_{2.5}$ over East China and provide the suggestion about potential influential factors, instead of to provide a simple empirical parameterization. Now, we add this discussion in the revised manuscript as "In fact, in WRF-Chem, there is an existing empirical parameterization to enhance the PBL mixing of pollutants in urban area based on the strength of anthropogenic emissions. However, it is only applied to gas pollutants if the MOSAIC aerosol scheme is selected as this study. It also tends to enhance the mixing up to half number of model vertical layers, which is beyond the PBL in most cases during the night. In this study, in order to examine the sensitivity of simulated DI to the PBL mixing coefficient, the sensitivity experiments, EXP1 and EXP2, are conducted corresponding to CTL1 and CTL2, respectively, through setting the lower limit of PBL mixing coefficient from 0.1 m2/s (default in the publically released version of WRF-Chem) to 5 m2/s within the PBL, which is applied to both gas and aerosol pollutants."

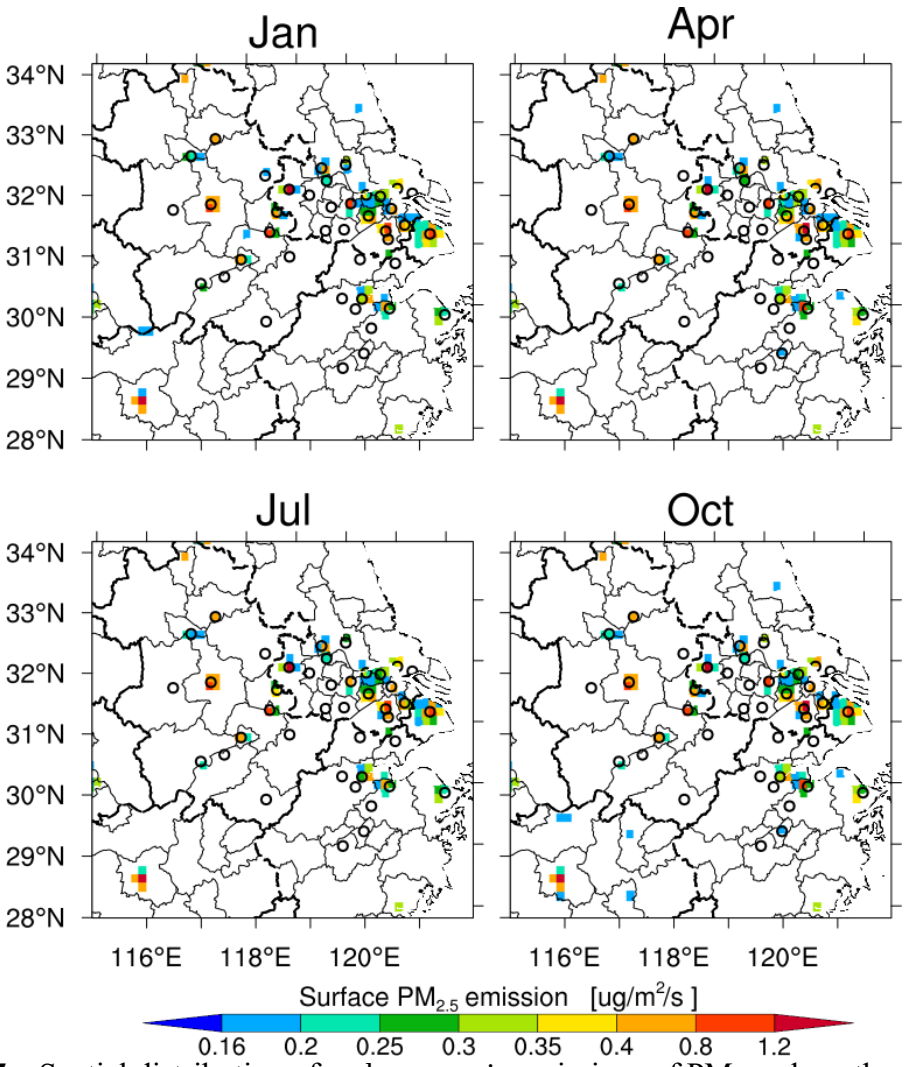

Figure R5a. Spatial distribution of anthropogenic emissions of $PM_{2.5}$ where the exchange coefficient will be modified if using the current parameterization in WRF-CHEM.

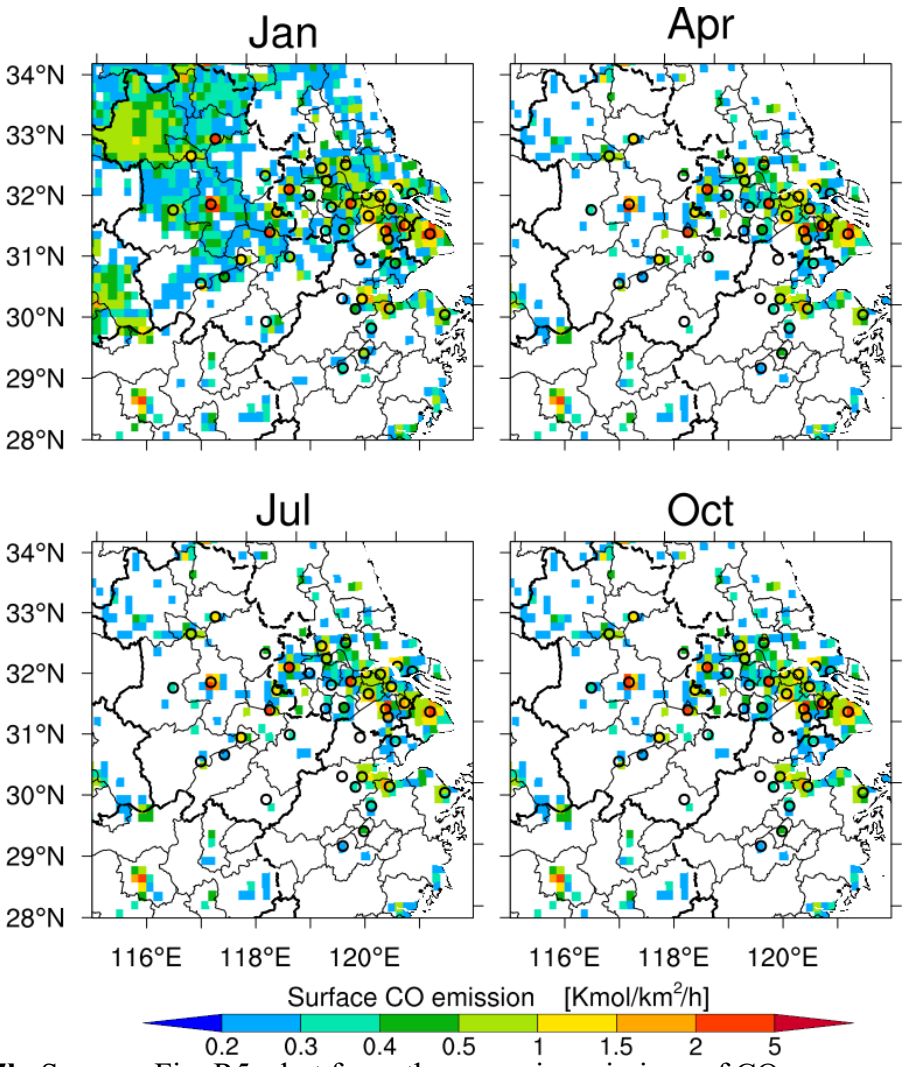

Figure R5b. Same as Fig. R5a, but for anthropogenic emissions of CO.

- ***There are discussions of the mismatch between the diagnosed planetary boundary layer (PBL) heights and ECs in WRF-CHEM. I want to remind that both the YSU and MYNN PBL schemes are non-local schemes. The non-local mixing is omitted in vertical mixing of chemicals as ECs from the PBL schemes are only used in the chemical mixing part of WRF-CHEM. Therefore, the vertical mixing of the chemicals isn't always consistent with the parameterization of PBLs in the WRF part of the model.***

According to Hong et al. (2006) and Nakanishi and Niino (2006), YSU and MYNN PBL schemes are non-local and local schemes, respectively. Therefore, both types of PBL schemes are examined in our study. The results show that two schemes lead to difference in surface $PM_{2.5}$ concentration, but are consistent in overestimating nighttime concentrations. For PBL mixing of chemical species, the scheme only needs the input of PBL mixing coefficient diagnosed from the PBL schemes. The non-local and local PBL schemes will diagnose different mixing coefficients that will affect the mixing of chemical

species. Therefore, in this sense, the mixing in chemistry part is consistent with the meteorological part in terms of the difference in local and non-local treatments. Now we add more details about the two PBL schemes and their estimation of PBL mixing coefficients in the revised manuscript as response to other reviewers.

- ***Another uncertainty in the PBL parameterization is that the PBL height is diagnosed differently in the individual PBL schemes of WRF. For consistency I suggest using the same diagnostics (e.g. based on bulk Richardson number) to determine the PBL height from the model cases with the YSU and MYNN schemes.***

The PBL height diagnosis is normally treated as the part of PBL scheme when use WRF or WRF-Chem, unless studies are investigating the difference between PBL parameterizations, which is beyond the scope of this study. This study focuses on the PBL mixing of pollutants, and the PBL mixing coefficient is the only input parameter into the chemical mixing scheme in WRF-Chem.

- ***The sensitivity of the diurnal variation of the simulated $PM_{2.5}$ to the model vertical resolution is presented here. The horizontal resolution of the nested model grid is 15km. This is quite coarse resolution, which makes harder to capture the effects of the urban island effect, inversions in the valleys, cold pool events and so forth. The authors are trying to improve the simulation of the PBL structure by refining the vertical resolution, while the horizontal grid remains the same. This shortcoming of the horizontal model grid needs to be discussed. I suggest moving the sensitivity case with the modified vertical resolution into SI.***

We agree that the modeling results of pollutant surface concentrations may vary with model horizontal resolution. However, many studies conducted the WRF-Chem simulations at horizontal resolutions of 10 km and coarser to investigate air pollution issue over China (e.g., Jiang et al., 2012; Tao et al., 2015; Gao et al., 2016; Zhang et al., 2016; Zhong et al., 2016; Zhao et al., 2017; Liu et al., 2018; Miao et al., 2018; Du et al., 2019; Wang et al., 2019). Specifically, Tao et al. (2015) examined the impacts of urbanization on meteorology and air quality during the month of July from 2008 to 2012 over East China at the comparable horizontal resolution (10 km) with this study, and found that urbanization tends to decrease surface concentration of $PM_{2.5}$ and increase it at higher altitudes. We believe the sensitivity experiments with varied vertical resolution at 15 km horizontal resolution are informative to readers and can provide useful reference for other researchers. Therefore, we decide to keep this part in the main text of manuscript.

In addition, although modeling studies at higher horizontal resolution may provide different values of pollutant surface concentration, we did one sensitivity experiment at 4 km and found it did not change the conclusion of this study. We add the discussion in the revised manuscript as "The model horizontal resolution may also affect the modeling results of PBL mixing and urbanization. However, one sensitivity experiment at 4 km horizontal resolution shows that the PBL mixing at the stations does not change

significantly (not shown). The modeling at higher resolution particularly down to large-eddy scale deserves further investigation."

- ***The authors consider the injection height of the anthropogenic emissions from the point sources in the model domain. This is advantageous as in many models (especially most of the global atmospheric chemistry models) all the anthropogenic emissions are released in the first model layer. However, it isn't clear how the injection heights for the emissions in East China are estimated in the study. Do the injection heights vary by weather and/or season? This will have a significant impact on the sulfate simulations, for example.***

This study uses the vertical variation profiles of power plant emissions following Wang et al., (2010). They derived the vertical profiles for East Asia based on the dataset of the U.S. and found that the profiles are comparable to those estimated in China and Japan (Woo et al., 2003; Wang et al., 2010). The injection heights are prescribed without temporal variations. Now we add the clarification in the revised manuscript as "Since diurnal variation of emissions and injection height of power plant emissions may have impacts on diurnal variation of surface pollutants, the experiments discussed above apply the diurnal profiles of anthropogenic emissions from five individual sector (i.e., agriculture, industry, transport, energy, and residential) following Olivier et al. (2003) and Wang et al. (2005) as shown in Fig. 1c and vertical distributions of anthropogenic power plant emissions following Wang et al. (2010) as shown in Table 2. Wang et al. (2010) derived the vertical profiles for East Asia based on the dataset of the U.S. and found that the profiles are comparable to those estimated in China and Japan (Woo et al., 2003; Wang et al., 2010)." and "Both diurnal and vertical variation profiles of anthropogenic emissions are prescribed without temporal variability."

- ***3.1. Why the model results are sampled on 3 hourly intervals, when the observations are available every hour?***

The outputs of pollutant concentrations in our experiments are every 3-hour to reduce the disk storage and increase the computational speed. This should not affect our investigation of diurnal variation. When comparing modeling results and observations, hourly observations are sampled at the model output frequency, i.e., 3-hourly.

- ***The uncertainties related to simulation of the biogenic VOC emissions aren't discussed in the paper. The modeled fluxes of the BVOC species will vary depending on the PBL scheme and model grid.***

The most significant impact of BVOC on surface $PM_{2.5}$ concentration may be through its impact on SOA. As we discussed, the SOA production is not considered in this study and its impact is mainly in summer. Therefore, we did not discuss the impact of BVOC in this study.

- ***How are the biomass burning emissions vertically distributed in the model? What diurnal cycle is applied to them?***

The biomass burning emissions in this study are from the global FINNv1.5 emission dataset, which was derived based on the MODIS Collection 6 (C6) fire detections. The FINN biomass burning dataset provides diurnal variations of emission fluxes following the Western Regional Air Partnership profile-WRAP (Freitas et al., 2009; Wiedinmyer et al., 2011; WRAP 2005). In this study, biomass burning emissions are vertically distributed following the injection heights suggested by Dentener et al. (2006) from the Aerosol Comparison between Observations and Models (AeroCom) project. Now, we add the clarification in the revised manuscript as "The biomass burning emissions follow the diurnal variation provided by WRAP (2005) and the injection heights suggested by Dentener et al. (2006) from the Aerosol Comparison between Observations and Models (AeroCom) project."

- ***The importance of accurate SOA simulations during summertime is discussed in the Summary. The simulation of the SOA contribution to the total $PM_{2.5}$ concentrations can help to capture the daytime maxima of the $PM_{2.5}$ concentrations in summer. This point has to be made clear in the main text, not in Summary. Why the authors didn't include the simulations with the SOA scheme in the main text?***

As we mentioned in the discussion section, we didn't consider the SOA production mechanism in this study because the current SOA mechanism in WRF-Chem is still highly uncertain. There is scarce observation for SOA evaluation over East China. We tend to avoid introducing another highly uncertain factor when focusing on studying the PBL mixing. As we discussed, it only affects significantly the diurnal variation of surface $PM_{2.5}$ concentration in summer. Therefore, we decide to just mention it in the discussion section and suggest future investigation.

Minor comments:

- ***Line 140: For WRF and WRF-Chem you can also cite this paper: Powers, J. G., et al. (2017), THE WEATHER RESEARCH AND FORECASTING MODEL Overview, System Efforts, and Future Directions, Bull. Amer. Meteorol. Soc., 98(8), 1717-1737, doi:10.1175/bams-d-15-00308.1.***

Thanks for your suggestion. Now this paper is cited.

- ***Throughout the text "s" is omitted in plural words: e.g. lines 386, 399, 419. There are other spelling errors as well.***

Thanks for checking. Now all of them are corrected.

- ***Line 199: I believe this reference is wrong: Lacono et al.. . .***

Now the reference is revised as "Iacono et al., 2000".

Reference

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