Response to Interactive comment from Referee #1

We thank the referee#1 for taking the time to read the manuscript and offer helpful comments and suggestions. We have modified the manuscript according to the referee's comments. The detailed changes can be found in the word-tracking in the manuscript. The point-to-point responses to the referee's comments are listed below. The referee's comment is repeated with our response in bold.

This article coupled mesoscale and large eddy scale models to simulate air quality in a densely populated city, shows the effect of spatial resolution on the model results and identifies the effect of turbulence on atmospheric chemistry. The content of the whole article is integrated and the model built in this study will effectively promote the air quality forecast to reach the large eddy scale. It is suggested to accept this manuscript with a minor revision. But I still have the following suggestions and questions about the article:

1. The simulation period in this article is short. Although it is difficult for CFD and LES models to run a longer simulation, but as a state-of-art study, could the authors try to simulate or give some discussion about the simulation of the pollution processes, for instance, the pollution for several consecutive days and its elimination?

Response: We agree with the reviewer that a longer simulation period covering a full pollution process could provide more insight on the LES simulations. However, due to the long computing time, we cannot quickly extend the runs in the current paper. Additionally, the simulation date was chosen based on the sample time of the ozone sounding observations (one measurement per week), as well as the convective boundary layer type. So that the pollution event is not considered in the current work. After this general evaluation, we will investigate more on the pollution processes under different weather conditions in the next steps.

2. How is the urban canopy scheme and its parameters set up in this study? It is suggested to clarify in the method section.

Response: The urban canopy scheme is not used in this study, so the urban's effects are only reflected through multiple constant surface parameters (e.g., albedo, roughness, heat capacity, thermal conductivity, etc.) combined with the urban fraction in the land-use data. We have clarified it in the method section. One may expect that urban canopy model is important for the simulations in highly urbanized area, since it may improve the accuracy of the surface and boundary layer properties (Chin et al., 2005; Ching 2013). However, there are great uncertainties in the applications of the urban parameters and urban canopy parameterizations. First, different resolutions and urban morphological descriptions may be required for different urban areas to be "fit" for the purpose (e.g., Baklanov et al., 2009; Ching, 2013), because each city has its own unique degree and characteristic of urban metabolism. This requires many tests, validations and adjustments of urban parameters based on target observations. Second, the accuracy of derived urban properties is sensitive to the resolution of land-use data used (e.g.,

Chin et al., 2005), as well as the definitions and processing methods (Ching, 2013; Cai et al., 2016). Third, urban canopy parameterizations are sensitive to the urban canopy parameters that define the urban morphology (Salamanca et al., 2011). More importantly, there is also great uncertainty in the simulation results when using urban canopy models. Many studies have shown that the model's performance is sensitive to the urban parameters and urban canopy models, different meteorological conditions, and different variables (e.g., Salamanca et al., 2011; Oleson et al., 2008). Therefore, to avoid additional uncertainties caused by the urban parameters, the urban canopy scheme is turned off for both mesoscale and LES runs for consistency. In the next step, we will investigate the impact of urban parameters and the different urban canopy models (single layer model and multi-layer model) on the simulations of both physical and chemical variables.

3. There is no verification result of simulated and observed meteorological data in the article, and it is impossible to explain the phenomenon well in terms of meteorological factors. Will it be added or explained in the supplement?

Response: In this paper, we compared the simulations with the vertical profiles of the potential temperature, water vapor mixing ratio, wind speed and wind direction measured by the ozone sounding. The result shows that the LES simulations obtained similar meteorological fields to the mesoscale simulations, and confirms that the LES can reasonably capture the boundary layer development. As for the surface stations, there is no co-measured meteorological data at the EPD surface stations. However, Hong Kong Observatory (HKO) operates the standard meteorological observations at separated stations (see Figure R1). We compared the simulated temperature (T), wind speed (WS), and wind direction(WD) with HKO measurements. The time series averaged from the stations covered by D06 and D07 are shown in Figure R2. It shows that the mesoscale and LES simulations obtained similar trends and can generally match the observations, which is consistent with the sounding comparison. The LES shows some improvements in the wind simulations, while the simulated temperature is a bit worse. This meteorological evaluation has been added into the supplement.

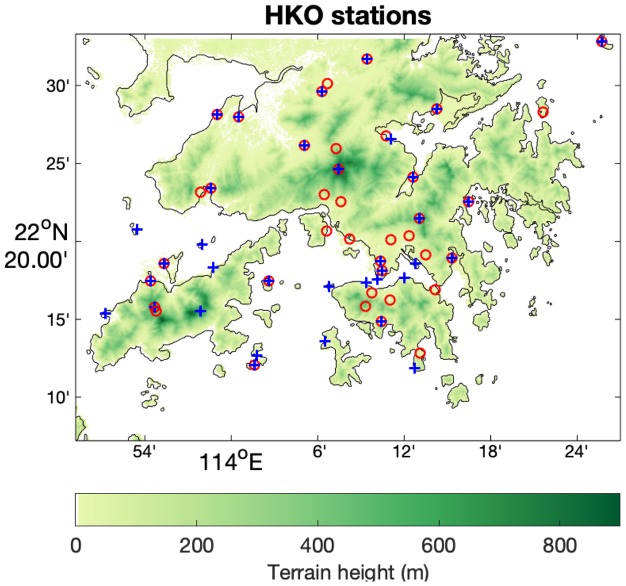

Figure R1. Map of the HKO stations covering the simulated period. Red circles are the sites with temperature observations; blue crosses are the sites with wind observations.

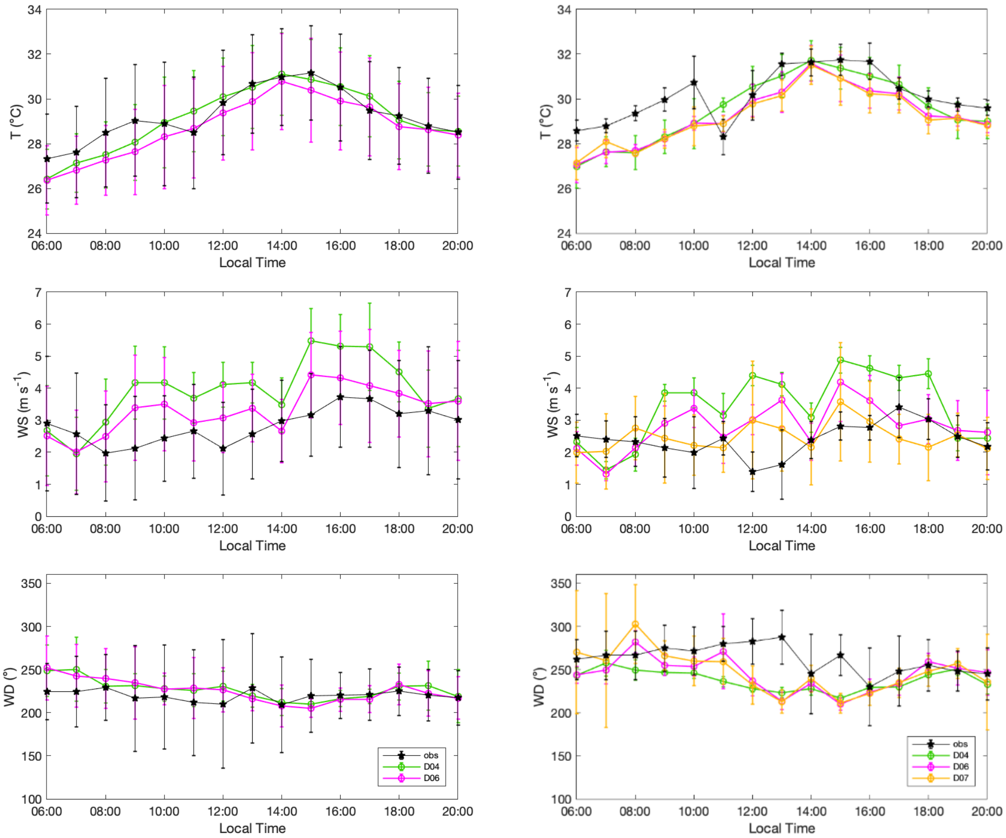

Figure R2. Time series of temperature (T), wind speed (WS), and wind direction (WD) averaged from stations covered by D06 (left) and D07 (right). The black pentagrams are the observations; the circles with different colors are the simulations with different resolutions (green: D04, 900 m; magenta: D06, 100 m; yellow: D07, 33.3 m). Error bars refer to the standard deviations.

4. The article introduces the simulation results of roadside stations and ordinary stations, but it is not intuitive enough. Could the authors add time series diagrams for comparative analysis?

Response: We have further categorized the general stations into urban, suburban, and rural stations. The station types are listed in Table 1. To make it clearer in the time series comparison in Figures 7 & 8, we have marked the station types with different colors for the station names.

5. Regarding the overestimation of NOx simulation and the underestimation of O_3 simulation at some sites, could the authors further analyze it from the aspect of VOCs and explain it in combination with the actual industrial distribution?

Response: Since the VOCs are not measured at the surface stations, it would be difficult to explain the NO_X and O_3 mismatches from the aspect of VOCs, because we do not know if the VOCs are right. We think the overestimation of the NO_X at some stations is not related to the industry, because the industries are with a distance to those stations (see Figure 2b). One possible reason for the overestimation of the NO_X is that the road

emission is overestimated at the surface, because all the roads (including the roads above ground) emissions are added into the first layer and some stations are lower than the overpass. We added this explanation to the revised manuscript.

6. The vertical profiles in Fig 5 do not show a significant difference between mesoscale WRF and LES-WRF. In other words, the simulation accuracy of LES-WRF is not higher enough as we expected. Could the authors further show some comparison of potential temperature, water vapor mixing ratio, wind speed, wind direction, ozone mixing ratio, etc. inside the PBL or city surface layer?

Response: The vertical structure of the meteorological and chemical fields is determined by both the large scale transportation and the local variation. In the mesoscale models, the large scale motions are resolved while the turbulent eddies are parameterized. In the LES, the large scale structures are constrained by the mesoscale model, and the turbulent mixing is resolved. Therefore, the vertical profiles above the boundary layer are expected to be consistent between the mesoscale and LES simulations. As for the boundary layer, the similarity between the mesoscale and LES does not mean that the accuracy of LES is not enough. It indicates that the YSU scheme and the LES produced similar vertical mixing in this case. We plotted the same figure with Fig. 5 but below 800 m to show clearer comparison in the boundary. It is added into the supplement.

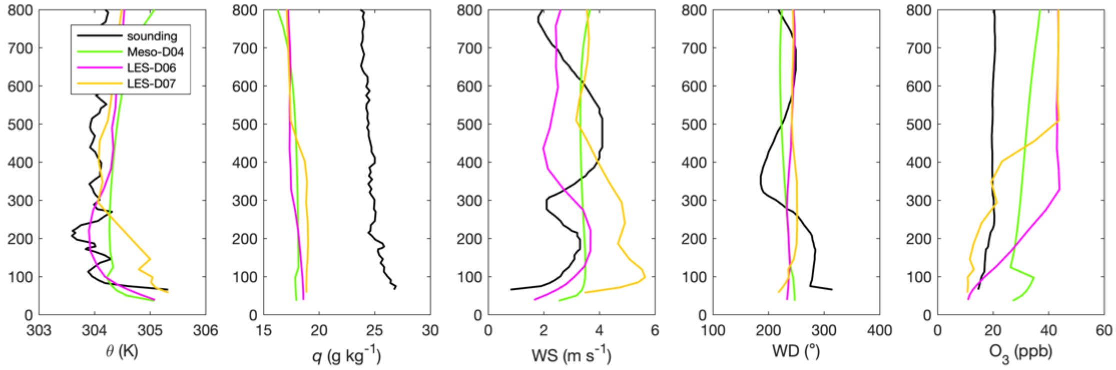

Figure R3. Comparison between ozone sounding measurements and model simulations in the boundary layer at 13:55 LT. The variables are the potential temperature (θ; a), the water vapor mixing ratio (q; b), wind speed (WS; c), wind direction (WD; d), and ozone mixing ratio (O3; e). The black lines represent observations; the green lines the simulations from D04 with resolution of 900 m; the magenta lines the simulations from D06 with resolution of 100 m; and the yellow lines the simulations from D07 with resolution of 33.3 m.

7. Could the authors discuss some potential bottlenecks for the use of WRF-LES-Chem in future air quality predictions?

Response: One bottleneck of using WRF-LES-Chem in future air quality prediction is that the original WRF based on terrain-following coordinates with a resolution of more than several ten meters (for high-resolution LES mode) cannot resolve buildings, which is becoming important if the resolution further increases to 10 m or less. To solve it, an alternative meshing technique, which is called immersed boundary method (IBM) is adopted (Lundquist et al., 2010; Lundquist et al., 2012). Another disadvantage is the

huge amount of computing time, which makes it difficult to apply it in the real-time forecast. This may be improved by accelerating WRF by leveraging GPUs. Some work has been done by different groups, e.g., WRFg, https://wrfg.net/wrfg-description/. With such further developments of the model system, opportunities exist for optimizing the WRF-LES-Chem in future air quality prediction. This has been added in the discussion in the revised manuscript.

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