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Atmospheric
Chemistry
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Discussions

# *Interactive comment on* "Megacity impacts on regional ozone formation: observations and WRF-Chem modeling for the MIRAGE-Shanghai field campaign" *by* X. Tie et al.

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More clear response can be seen in the supplement pdf file

Anonymous Referee #2

We thank the reviewer for his/her careful reading of the manuscript and the helpful comments. The comments of the Reviewer are addressed below and in the revised manuscript. We believe that the paper is significantly improved with these changes. The manuscript presented a study of ozone chemistry in Shanghai region by field measurement and WRF-Chem model simulation. This work gave a quite comprehensive overview from a number of aspects of ozone formation. The highlight of the MS was

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the model capacity in computing simultaneously the variation of VOCs, nitrogen compounds and ozone. I agree with the acceptance of the MS for publication on ACP with consideration of several issues listed below: (1) One big problem was the correlations of pollutants with CO. It presented the results but did not address much about the reason for the correlations. As the authors mentioned, CO was considered as a tracer from primary emissions, and in the MS the authors correlated it to PM2.5, NOx and VOCs. It was a surprise to see the correlation between CO and PM2.5. As we knew that a large portion of PM2.5 came from secondary production. The CO-NOx showed good correlation at lower levels while poor at higher NOx levels, I had difficulty to understand this because the local sources causing higher NOx could also led to high CO. The correlation between CO and VOC were, very unfortunately, only done for VOCs groups (alkanes, alkenes, and aromatics) instead of species, it was very hard to know better for sources. I would suggest to perform such analysis for typical VOC species which were used for tracers for specific sources.

We thank the Reviewer for the suggestions. Combined with the comments of Reviewer 2 (he/she suggested that since there were not too much information in the CO ratio figures, Figure 8-10 should be removed from the paper), accordingly, we have removed Figures 8-10 in the revised paper.

(2) The authors stated in the MS that their model could well simulated O3, VOCs, and NOx at the same time. However, section 3.2 for model evaluation was generally descriptive, As the species discussed in this section covered fresh emitted ones (NO, and HCs), inter-mediate compounds (HCHO, and other OVOCs), products O3, and PM2.5 which came from both primary emissions and secondary processes. It would be very interesting if the authors could add some discussion about the key processes or mechanisms causing the discrepancies. And as the NOx/VOCs ratios from emissions to ambient air were the key for the work, the authors could also gave the comparison of simulated ratio with measured ones. According to the reviewer's suggestions, we have added some discussions regarding some discrepancies. For

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example, the largest inconsistency between modeled and measured results is the HONO concentration. We add a diurnal variation of HONO to show that the maximum concentration of HONO occurs in the early morning at 6 am, corresponding to high concentration of soot. This result suggests that the heterogeneous reactions on the surface of soot may contribute the large concentration of HONO (Hauglustaine, et al., 1996). However, this is a very complicated process, and need a detailed study for this issue. We intend to conduct a separate study for this heterogeneous process. These statements have added in the revised paper. The bias of background concentrations of CO is also analyzed and stated in the revised paper. We also clarified that the NOx/VOC ratio of 0.4 is used in our default model study, and all comparisons between model calculation and measurement are based on this emission ratio. (3) Again, the manuscript needs to address the VOCs to species-specified discussion. As the ozone formation was modeled to be largely VOC control regime, and HCHO/NOy was used for the diagnostic analysis for ozone formation. It would be interesting to know what VOC species were measured, how they were computed. In the revised paper, we described in more details regarding the VOC species in the field experiments. At the PD site, there are 2 online VOC instruments. One instrument (Apel et al. 2010) is the Trace Organic Gas Analyzer (TOGA), an in- situ gas chromatograph/mass spectrometer (GC-MS). The TOGA instrument continuously measured every 2.8 min 32 species including select NMHCs, halogenated compounds, and mono functional non-acid OVOCs. The detailed species measured by TAGO are listed in Table 1 of Apel et al. (2010). Another instrument is the GC-MS/NCAR-ACD (Greenberg et al., 2004) for continuously measuring light hydrocarbons (including C2H6, C2H4, C3H8, C3H6, C2H2, iC4H10, nC4H10) with time resolution of 45 minuets. This information has been included in the revised paper. References; Apel, E.C., T. Karl, F. Flocke, A.J. Hills, L. Emmons, S. Madronich, A. Fried, X. Tie, L. Mauldin, T. Campos, B. Sive, L. Kleinman, S. Springston, J. Ortega, D. Blake, A. Baker, C. Warneke, D. Welsh-Bon, J. de Gouw, Z. Zheng , R. Zhang, J. Rudolph, W. Junkermann, and D.D. Riemer, Characterization of volatile organic compounds in the Mexico City Metropolitan area and in the outflow

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from the city, Atmos. Chem Phys. 10, 2353-2375, 2010. Hauglustaine, D. A., B. A. Ridley, S. Solomon, P.G. Hess, and S. Madronich, HNO3/NOx ratio in the remote troposphere during MLOPEX 2; Evidence for nitric acid reductions on carbonacess aerosols? Geophys. Res. Lett., 23, 2609-2612, 1996.

Please also note the supplement to this comment:
http://www.atmos-chem-phys-discuss.net/13/C1435/2013/acpd-13-C1435-2013-supplement.pdf

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Interactive comment on Atmos. Chem. Phys. Discuss., 13, 1673, 2013.