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Comment

Interactive comment on “Comparisons of WRF/Chem simulations in Mexico City with ground-based RAMA measurements during the MILAGRO-2006 period” by Y. Zhang et al.

Y. Zhang et al.

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Response to Reviewer #2:

We greatly appreciate the reviewer's very critical comments about our manuscript. Here are our point-to-point responses to the reviewer's comments.

Major comments: 1) The methodology employed by this study is similar to many other meteorological and air quality modeling studies. The authors do not put their model results into context of previous CTM simulations of Mexico City or those obtained for other urban areas. Therefore, it is not clear how the quantification of model performance can be used by others or for what purposes.

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Response: We seem to disagree with the reviewer on this. This study examines the WRF/Chem simulated meteorological variables and criteria pollutants simultaneously for different times of the day, under different PBL and LSM schemes, and under different weather episodes for the entire period of the MILAGRO campaign. This is a necessary step for the application of WRF/Chem in Mexico City as it poses to be the next-generation meteorological and air quality modeling system. We think that without an extensive evaluation of a meteorological and air quality model over a particular area, the further application of the model for that area is rather questionable.

2) A major problem in this paper is that it does not utilize other surface and aircraft data to evaluate and interpret the model predictions. There are numerous trace gas measurements made at other surface sites and from several research aircraft. At the end of the paper, the authors state that additional comparisons are underway using those data, but those comparisons are needed in this study. To predict ozone correctly for the right reasons requires not only a reasonable emission inventory and a good prediction of the meteorology, but also a good prediction of NO_x and VOCs in the region. NO_x is evaluated to some extent, but VOCs are totally ignored.

Response: As stated in the title of the manuscript, this work presents comparisons of the WRF/Chem simulations with the ground-based RAMA measurements during the MILAGRO period. The main purpose of doing this is to get focused with tackling one issue at one time. Once we get an idea of the model performance in terms of surface variables, it would be easier to interpret the model simulations at vertical levels using measurements made from several research aircrafts.

There are indeed numerous trace gas measurements made at other surface sites; however, getting these measurements for model validation is not as easy as one would expect. I have been keeping checking on the NCAR Community Data Portal for MILAGRO data since early 2007 and downloaded some measurements at T0 for model validation. However, using these data for model validation is not easy since they tend to be fragmented and in some cases poorly explained and not quality controlled. This

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is the only reason why comparisons of VOCs are not included in the manuscript.

In the revised version, we included comparisons between the observed and model simulated VOC species at the T0 supersite during MILAGRO. The VOC species were measured by the PTR-MS (proton transfer reaction - mass spectrometry) instrument (Fortner et al., 2009, Atmospheric Chemistry and Physics).

3) Because the field campaign data are largely ignored, this type of modeling study could have been done for any period and for many large cities with an air-quality monitoring network. While the terrain in Mexico City is a challenge for CTMs, there is little evaluation on how the model simulates the thermally-driven circulations other than a direct comparison of observed and simulated surface winds.

Response: Please see our response to 1) and 2). Apparently, we have to focus on what the title suggests and cannot include too many things in one paper.

4) A discussion of the impact of the chosen model configuration on the predicted air quality parameters is needed. A limited domain is chosen with fixed boundary conditions; therefore, multiday variations in the background ozone and CO mixing ratios would affect the local results to some extent. This could have been quantified given the available data during the field campaign. Emissions outside of the MCMA also seem to be ignored. So sources from other large cities in central Mexico are ignored as well that could contribute to background values observed in Mexico City.

Response: The impact of the model configuration (model domain, model resolution, spin-up time, model initialization, et al.) on the predicted air quality parameters as well as on meteorological variables merits extensive analysis and should be addressed in a separate work.

The emissions inventory used in this work uses the gridded emissions inventory for the MCMA compiled by the Molina Center for Energy and the Environment (MCE2). Emissions outside of the MCMA are not included as mentioned in the manuscript.

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Other Comments: 1. Page 1333, lines 18-27 through page 1334, lines 1-19: Much of this material is more appropriate for the WRF Users guide than in this study. It lists options in WRF, that are not even used in this study and it is not apparent how this discussion contributes to the paper.

Response: We agree. This section is re-written in the revised version.

2. Page 1333, starting on line 20: The authors now describe which options are used in this study, but provide no reason why these are used as opposed to others available in WRF/Chem.

Response: We choose options to use in this study based on our experiences with WRF and WRF/Chem as well as model stability and computing time. We also performed sensitivity studies initially to see which options gave the best simulations for these particular runs. We included some of the information in the revised version.

3. Page 1335: No discussion is included on the emissions employed for areas outside of Mexico City. While emissions from Mexico City are the dominant factor contributing to photochemical production of ozone in the area, there are several large nearby cities that could contribute to regional background values of ozone and other trace gases. Were emissions outside of MCMA set to zero?

Response: Yes, emissions outside of MCMA were set to zero.

4. Page 1336, line 22: The authors need to include a brief description or table on the initial and boundary conditions for trace gases. I would expect temporal variations in longer-lived species, such as ozone and CO, that would affect local mixing ratios on the order of 10-20 - which is not small. Instead of using default values, why not use profiles of trace gases obtained from aircraft measurements or ozonesondes to provide more appropriate boundary conditions that vary from day to day. The authors state that the results were insensitive to choice of initial and boundary conditions, but do not describe how that conclusion was reached.

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Response: This is a very good point. Currently the WRF/Chem model does not have the capability (i.e., data assimilation for trace gases) to incorporate measurements from research aircraft or ozonesondes for initialization but this is something that would surely improve the model simulations.

We performed sensitivity studies by using different spin-up time (i.e., 6-hour, 12-hour and 24-hour) as well as using the chemistry data from the previous day simulations. We did not notice large differences in terms of concentrations at surface for trace gases, which is consistent with what other researchers have obtained.

We included a brief description on the initial and boundary conditions for trace gases in the revised version.

5. Page 1338, line 9: Please provide more specific references that are available, than just a reference to an entire workshop. There are also numerous papers from a variety of mesoscale models on this topic as well.

Response: Revised as suggested.

6. Page 1338, line 17: I suspect that a 3-km grid spacing is sufficient to resolve most of the circulations influenced by terrain in the region, especially when one is evaluating basin-averaged meteorology, ozone, and CO. But mesoscale model predictions still contain errors in the timing and structure of those circulations at individual stations that are not necessarily due to urban effects. Although the RAMA stations are located in an urban environment, observed winds at those stations are largely influenced by the thermally-driven flows associated with heating/cooling of the terrain and larger-scale synoptic forcing.

Response: We agree. We looked at the performance of the WRF/Chem model in simulating surface meteorological variables at individual stations (I have the table but the table did not appear nicely here so I did not include it). There are large variations in terms of correlation coefficients and root-mean-square-errors from station to station.

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One thing we are not sure whether the variations are caused by urban effects (buildings, roads, underlying surface, et al.) or by insufficient horizontal resolutions or both.

7. Page 1338, line 23: The authors first mention the problem with the YSU scheme of predicting a boundary layer depth at night that is the height of the lowest model level. This is a well-known problem in the WRF community and a recent paper (Hong et al., Monthly Weather Review, 2006) has described a more up-to-date version that attempts to improve the representation of the stable boundary layer. The text should mention this somewhere. It would be useful for the authors to re-run the simulations with the newer scheme that has been available to the community since June 2008, since the version of the YSU scheme used in this study is out of date.

Response: We re-ran all the simulations using the new version of WRF/Chem (V3.0.1) which includes the updated version of the YSU scheme. Except for nocturnal PBL heights, the two versions produce rather similar results. The analyses and discussions in the revised version are based on the model simulations from the new version of WRF/Chem. It turns out that the new version of WRF/Chem with the updated PBL scheme does not necessarily improve the model simulations when compared to the previous version.

8. Page 1339, lines 1-18: The authors should also describe how predicted surface winds (presumably at the lowest model level) are compared to observations (which are most made at a lower height). If the model level is higher than the observation height, then the simulated winds should be higher than observed (unless the simulated winds were extrapolated to the observed height). As stated by the authors, the biggest factor contributing to the over-prediction in wind speed is likely the omission of an urban canopy parameterization. WRF/Chem does have an urban canopy parameterization, but there may not be sufficient information to define building information needed for this parameterization.

Response: In addition to winds at different vertical levels, the model also outputs the

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winds at 10-m height which is the standard height for measuring surface winds. We used the modeled 10-m winds as the surface winds.

Yes, the new version of WRF/Chem does have an urban canopy parameterization but there is no sufficient information in terms of buildings and surface conditions. We believe that accounting for urban effect would significantly improve the model simulated surface and low-level winds in the urban environment.

9. Page 1340, line 14: While it is probably correct that the positive bias in ozone is related to NO emissions being too small, the PBL also plays a role. Since the predicted PBL is too low it should have led to ozone lower than observed if the emissions were correct. So, the underestimation in ozone is exacerbated by errors in the PBL depth. There could be other plausible contributing factors as well.

Response: The nocturnal PBL height simulated by the updated version of YSU scheme appears to be comparable to that determined from radiosonde measurements at the headquarters of the Mexican National Weather Service but positive bias in ozone is still outstanding at night. It appears that the overestimation in ozone concentrations at night is primarily related to NO emissions being too small.

10. Page 1341, line 15: The authors note two important sources of SO₂ that could affect the under-prediction of SO₂; however, these plumes would be transported into the basin periodically. Was SO₂ consistently lower than observed? Or was SO₂ just too low when the observations indicated large peaks associated with the Tula and volcano plumes? If SO₂ was always lower, then that would point to local sources in the city rather than the two point sources. Estimates for SO₂ are available for these sources; why not employ them in the model?

Response: This is a very good point. Yes, SO₂ was consistently lower in the model simulations than the observed regardless of the stations and time of the day, which means that local sources must play a role in the underestimation of the simulated SO₂.

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In the revised version, discussions on SO₂ are removed as suggested by other reviewers.

11. Page 1342, line 1-12: There is a recent paper (Stephens et al., ACP, 2008) on weekend/weekday effect in Mexico City that should be cited. There may be some information in that paper useful for interpreting the findings of this paper.

Response: Thanks for this suggestion. Yes, the paper is cited and some discussions are provided in the revised version.

12. Page 1342, line 18: I do not understand the author's speculation of SO₂ sources outside of Mexico City to explain the observed weekend/weekday variations.

Response: It is assumed and is largely justified to say that the emissions in Mexico City are more or less lower on weekend than on weekday. The observed concentrations show decreases for CO, NO, NO₂ and NO_x or little change to slight increases for O₃ from weekday to weekend, which is consistent with the decreased emissions in the MCMA from weekday to weekend. Only SO₂ concentrations show a large increase from weekday to weekend, which is not consistent with the decreased emissions from weekday to weekend. This seems to suggest that the large increase in SO₂ concentrations from weekday to weekend are not related to local sources in the MCMA.

In the revised version, discussions on SO₂ are removed as suggested by other reviewers.

13. Page 1342, line 25: The authors correctly state the importance of PBL height for predicting trace gas concentrations. There have been numerous studies in the literature that already have performed sensitivity simulations using CTMs (e.g., CMAQ) similar to those presented in this section. Some need to be cited as well as how the present sensitivity compares with previous findings.

Response: Revised as suggested.

14. Page 1343, lines 23-24: The authors state that the PBL height compares favorably

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with Shaw et al. (2007), but do not provide any evidence. Why not utilized those data in this study?

Response: We have contact Dr. William Shaw and have asked Dr. Shaw for their data for the purpose of model validation but we have not got response, yet.

15. Page 1346, line 15: I agree with the author's statement that more extensive analysis is needed. The authors perform a relatively straight-forward analysis that has been routinely performed by other investigators. Little new insight regarding photochemical processes in the urban area has been achieved. Given the extensive data collected during MILAGRO, there could have been interesting analyses to provide new contributions to science.

Response: Please see our response 1 and 2 under Major comments.

16. Section 5.4: Three episodes are examined in more detail whether air quality predictions are better for some meteorological conditions than others. The time series and statistics indicate similar levels of performance, although a longer time period with multiple days for each type of meteorological conditions would have been useful. I am not sure much is gained by presentation of this material than what is stated in Section 5.4.4. While they conclude that it would be useful to include wet deposition, the lack of a treatment of wet deposition did not seem to make the performance of that period any worse than the other periods.

Response: The statistics for each type of meteorological conditions are done for multiple days during the MILAGRO period.

It is only our speculation to say that the inclusion of wet deposition might improve the model performance since the model consistently performs poorly in terms of chemical species during the El Norte events.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 1329, 2009.

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