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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulation of Mexico City plumes during the MIRAGE-Mex field campaign using the WRF-Chem model" *by* X. Tie et al.

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Responses to Reviewers:

Reviewer 2:

We thank the reviewer for the careful reading of the manuscript and helpful comments. We have revised the manuscript following their suggestions as is described below.

This paper describes the performance of a chemical transport model in simulating ozone and its precursors over central Mexico during the March 2006. The model is then used to examine ozone production efficiency and the role of different ozone precursors on ozone production. There are a number issues that need to be addressed before the paper is suitable for publication. While the material in the paper is presented reasonably well, there are numerous awkward phrases and some descriptions are too generic and lack specificity. I have noted some of the awkward phrases and generic descriptions in my comments below, but I may have not found all of them and I encourage the authors to re-check the rest of the manuscript as well.

Major comments:

1) The lack of a description of the emissions, initial conditions, and boundary conditions that were used for the model simulation is a major omission in this study. Emissions are an important input, which should not merely be cited in another paper. Also describing how emissions are prescribed outside of Mexico City would be useful to understand how they contribute to background concentrations. The authors should also include a list of meteorological physics options used, particularly the PBL parameterization. There is description regarding the performance of the PBL, but no description on how it is represented in the model. Nor do the authors provide any direct evidence regarding the performance of the PBL.

According to the suggestion by the reviewer, we add text to give more detailed description for emissions and boundary conditions. We also add a Table to describe the emission inventory for SO2, CO, NO, and VOCs used for this study, and also for other previous studies. The PBL scheme (YSU scheme) used in the model is described. The performance of the PBL in the WRF-Chem model is evaluated by Zhang et al [2009]. In the revised manuscript, we briefly described the general result from the study of Zhang et al.

2) The adjustment factor was not applied to all quantities in Fig. 6. Why not? It would seem that dispersion errors would affect all species. Also, some of the hydrocarbons are already overestimated and applying the adjustment factors would push the model in the wrong direction (assuming a linear relationship, but of course it is not that simple).

We realize that there is a large uncertainty related to the adjustment factor. Therefore, this factor is only used for giving a very preliminary estimate for the uncertainty of the

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dispersion factor in the model. In this calculation, only long chemical-lived species, which is more suitable to be adjusted by the dispersion errors, such as CO, NOy, NOz, and O3 are applied in the calculation. We add text to clarify this issue in the revised manuscript.

3) Section 4 presents an analysis of ozone production efficiency and the role of different ozone precursors in on ozone production. They use March 22 for this analysis. Given that transport to the northeast occurred on other days during March, have the authors analyzed the results to determine whether their conclusions occurred on other days? It would be useful to include some text whether the behavior of the model on March 22 is similar to other transport periods. For example, would varying meteorological conditions either increase or decreased ozone production efficiency? What about cloudiness, its impact on photochemistry in the region, and whether the model adequately simulated cloudiness? I would also encourage some inclusion of aircraft data in this section to show how the model performed both close to Mexico City and further downwind where the secondary ozone maxima was produced in the model. For example, were OH and HO2 observations made on the C-130 that could be used to verify the behavior seen in Fig. 13?

In the revised manuscript, we describe the ozone and ozone production efficiency in another flight (Mar/18-flight 6). The results (not shown) are similar to Figures 11 and 12, which is consistent to our current conclusions. The cloud simulation in the model is always a big challenge for regional model, especially for small or regional scale cloud. I believe there are some validation works which have been done by the WRF group. This evaluation is beyond the scope of this paper. For the point of usage of more aircraft data, we compare the model OH values with the measured data (see the figure in supplement). These figures are not included in the model, and will be used for another separated study.

4) My impression from reading this manuscript is that ozone chemistry is reasonably simulated, since the authors seem to attribute most of the errors to uncertainties in

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Discussion Paper

dispersion. If that is the case, does that mean that simple photochemical mechanism such as RADM are all that is needed to understand oxidant chemistry in a megacity plume? Are details of hydrocarbon chemistry not included the lumped approaches significant? Some discussion is warranted in the paper.

At present, due to limitation of the computation capability, the chemical scheme used in regional models are all simplified in some degrees. Several different models with different chemical schemes have been applied in ozone studies in Mexico City, for example, WRF-Chem (RADM scheme) and CAMx (SAPRC-99 scheme). Even both the models use simplified chemical schemes, the basic ozone chemistry is well represented compared to the surface measured ozone values. For example, the model results show that the in Mexico, the ozone chemical production are in VOC-limited regime, while in the rural area, the ozone chemical production are in NOx-limited regime. These results suggest that the uncertainty related to the ozone chemistry scheme is less than other physical/chemical processes in the model, such as transport, dispersion, etc. The above discussion is included in the revised manuscript.

Minor comments:

Page 9222, line 1: “in the Mexico City outflow” is awkward and should be rephrased.

Changed to “in the downwind of Mexico City plume”

Page 9222, line 9: Suggest changing “enhancement of” to “increase in”.

Changed.

Page 9222, line 12: Suggest changing “pollution levels” to “ozone mixing ratios”, unless the 0-25% underestimation refers to all pollutants in addition to ozone.

Changed.

Page 9223, line 13: I’m not sure the sentence starting “The campaign coordinated : : :” is entirely correct. Were the coordination with satellite measurements part of

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MIRAGEMex, or was that for the INTEX-B campaign?

Change to “The campaign integrated”

Page 9223, line 18: Change “The city is at” to “The city is located at”.

Changed.

Page 9224, line 12: Suggest making “In addition to : : :” a start of a new paragraph, and further down on line 19 make “Lei et al. : : :” a new paragraph. It was difficult to follow the lines of thought in this long paragraph. It would help if it were re-phrased to provide a better motivation for the present work.

Changed.

Page 9224, line 26: The previous paragraph mentions a few, of the many, photochemistry simulations performed for central Mexico over the years. The authors should include some statements that differentiate the present work from previous studies.

The text regarding some differences in different models is added in the revised version.

Page 9225, line 26: “cycling pattern” is awkward and should be rephrased.

Changed to “a regional cycle pattern”

Page 9226, line 3: What do you mean by “city plume” that was measured by the aircraft. It would be useful to be specific at first, and then use this term later. There are phrases later in the paragraph referring to where the aircraft intersected the “city plume” but provides no rationale for determining that the measured values originated from Mexico City. Although not as likely, the higher concentrations could arise from other large urban areas in the region.

The “city plume” is defined.

Page 9227, line 28: Suggest making “In this study, : : :” a new paragraph.

Changed.

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Page 9227, line 29: Suggest changing “The model ran from ” to “The model simulation period was from”.

Changed.

Page 9228, line 5: “measurement” should be “measurements”. But perhaps a more specific statement would be that the model was compared to “ground measurements from operational monitors”.

Change to “ground measurements from operational monitors”

Page 9228, line 11: Change “field campaign” to “field campaign measurements”. Perhaps one could be more specific to mention that in this study the model is compared with aircraft observations collected downwind of the city, which were not done in the previous studies mentioned in this paragraph. This sort of discussion would have been better at the end of the introduction.

Text is revised according to the reviewer’s suggestion.

Page 9229, line 5: Averaging both the observations and the model results in Fig. 2 (and in Fig. 3) is a useful method of summarizing model performance. But it also hides many errors in the predicted timing of CO plumes and in the spatial distribution of CO plumes. I think some discussion regarding the variability of model performance is warranted.

The text regarding the variability of model performance is added in the revised manuscript.

Page 9230, line 3: The authors state that the calculated BL height during the evening is better on March 18, but provide no evidence that it is. Just because the surface CO is closer to the observations does not imply the PBL is necessarily correct. Have the authors actually evaluated the predicted PBL depths? While I’m not suggesting that an in depth presentation of the PBL predictions be given, at least some comparisons with the available data should be made in light of the discussion for Fig. 3. Similarly,

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the model discussion needs to include a description of which PBL treatment is used in WRF.

The paper by Zhang et al. [2009; in ACP] has discussed a detailed evaluation of the predict PBL. Because the Zhang et al. [2009] also use the WRF model to calculate PBL height, their result is consistent with this calculation. Some of their major founding regarding the PBL evaluation is added in the revised manuscript.

Page 9231, line 1: The authors state that the March 28 flight for CO is shown to provide some insights into the background atmosphere, but they present no such insights. What do they mean by this? Also, the scale of the plot is such that one cannot tell the difference between the observed and predicted. There does seem to be some differences suggesting errors on the predicted background concentrations (which also seem to be evident on other flights). Again, having a description on how boundary conditions were handled would be useful.

In the revised text, we add the description to clarify that the background condition refers to the aircraft measurements without large impacts by the Mexico City pollutions. The description of the boundary conditions used in this study is stated in the revised paper. The scale of plot is chosen to be consistent with other flights in order to clearly compare the Mexico City pollution to non- MC plume case.

Page 9231, line 10: A criterion is described for the "city plume", but it would seem that an increase in CO could arise from other urban plumes the aircraft encounters – not just the Mexico City plume.

Other effects include the other small city emissions. As we described (in revised manuscript), the non Mexico City emissions are smaller than the Mexico City emissions, and are located in outside of the MC. As a result, the large increase of the air pollutants in plumes nearby the MC region is mainly due to the effect of MC emissions.

Page 9231, line 22: Change "transport processes" to " dispersion processes" since transport is usually thought of as transport by the mean winds (and included in the parentheses already) and diffusion is a turbulent mixing process. Dispersion represents both mean and turbulent processes. But I'm not sure I agree with the reason for the underestimation stated in this sentence. The errors associated with dispersion are just speculation since an evaluation of transport and mixing has not been presented in this paper. Another plausible explanation is uncertainties in emission rates.

The "transport processes" is changed to "dispersion processes". We also state that other errors also can be introduced in the model simulations, such as the uncertainties related to emissions, PBL height etc. The above correction factor can only provide an estimate of the errors related to the dispersion process, instead of an accurate calculation.

Page 9232, line 2: I understand why one would want to create an adjustment factor based on CO, that could be applied to other species to 'correct' for transport errors. However, the differences between observed and simulated CO are not solely due to dispersion processes. As stated earlier, part of the problem could be due to emissions that vary from day to day. And the uncertainties in the emissions of other species are not likely to be the same as CO (which is probably the specie with the best emissions estimate). The authors should include some text to note the assumptions regarding their correction factor in Eq. (1).

The text is included to description regarding their correction factor.

Page 9237, line 23: "during outflow" is awkward and should be rephrased.

Change to "in the downwind of Mexico City plume"

Page 9283, line 6: Is there a reference(s) that can be provided on the use of Eq. (2) for photochemical age? Page 9239, line 6: "lower in nearby city" is awkward and should be rephrased.

The chemical age is defined by Kleinman et al., ACP (2008), and is added in the revised

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paper. The word of “lower in nearby city’ is changed to “lower in the areas nearby city”.

Page 9240, Section 4.4: The O3 to NOz comparison is similar to the model predictions in Mena et al. (2009) along the C-130 flight tracks. What does this mean in terms of different chemical mechanisms employed by the two models?

The similarity between two independent models indicates that the transport and chemical processes in the 2 models are similar. In the revised manuscript, Mena et al. [2009] is added in text.

Page 9241, line 14: I assume that the secondary ozone maximum downwind of the city is from previous days emissions? Why not use the model results to say something about this history of this air mass?

In the revised manuscript, text is added to describe the history of the air mass.

Figure 4: The blue and green are difficult to distinguish. Suggest changing to other colors. Same comment for Figure 5.

Change “black” to “red”

Figure 6: The black and blue are difficult to distinguish. Same comment for Figures 8-10.

Change “blue” to “green”

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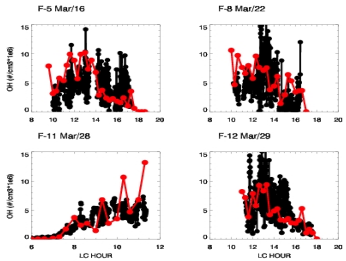

The comparison between calculated OH (red) and measured OH (black).

Fig. 1.

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