Interactive comment on “Eta-CMAQ air quality forecasts for \( \text{O}_3 \) and related species using three different photochemical mechanisms (CB4, CB05, SAPRC-99): comparisons with measurements during the 2004 ICARTT study” by S. Yu et al.

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We thank the anonymous referee #2 for the constructive and helpful comments, and the incorporation of which has led to a substantially improved manuscript.

Reviewer #2(Comments):

The paper describes a very comprehensive and thorough evaluation of Eta-CMAQ predictions, using three different gas-phase chemistry mechanisms, with surface, aircraft and ship observations. The overall model evaluation results are generally well-presented, but additional details to support some of the authors’ conclusions or explanations would be helpful.

Response: We thank the reviewer for the overall positive assessment of the manuscript.

Major comments: 1) Although not directly relevant to this paper, it would be useful for the authors to provide a brief discussion of how differences between the meteorological model (NOAA Eta) used in the forecast version of CMAQ versus those (MM5 or WRF) used in the hindcast versions of CMAQ can influence model performance. In particular, the authors refer to the previous evaluation of the three mechanisms in CMAQ by Luecken et al. (2008) using the MM5-CMAQ combination and it would be useful for the authors to qualitatively compare that evaluation with the evaluation in this paper.

Response: We thank the reviewer for this suggestion. We actually just finish a draft of a manuscript entitled “Comparative evaluation of the impact of WRF-NMM and WRF-ARW meteorology on CMAQ simulations during the 2006 TexAQS/GoMACCS study—Part I: Ozone (O3)” (Yu et al. to be submitted to ACP, 2010) in which the meteorological effects from WRF-NMM (successor of NOAA Eta) and WRF-ARW (successor of MM5) on the CMAQ simulation are studied. The primary conclusion is that at the AIRNow surface sites ARW-CMAQ and NMM-CMAQ have a very similar good performance for the high max 8-hr O3 concentration portion (>40 ppbv) with slightly better performance for ARW-CMAQ (the NMB values of ARW-CMAQ and NMM-CMAQ for the data with max 8-hr O3>40 ppbv are 8.1% and 9.4%, respectively) and both ARW-CMAQ and NMM-CMAQ consistently overestimate the observations in the low O3 concentration range (<40 ppbv) with NMB values of 38.9% for ARW-CMAQ and 48.3% for NMM-CMAQ, respectively, during the 2006 TexAQS/GoMACCS study. Since this work will be submitted in another manuscript, we will not put it here to avoid redundancy because it is not directly relevant to this paper. Regarding the work of Luecken et al. (2008) which showed the results for different year (2001), qualitative comparison of our work for 2004 with Luecken et al. (2008) is not fair or reasonable because different year may
have different situations (meteorology and emissions).

2) In Section 3.1 (page 22964), the authors comment that one reason for the overestimation of O3 mixing ratios less than 75 ppb is that the model does not correctly treat the titration of O3 by NO in urban plumes. How would accounting for this titration change the relative performance with the three mechanisms? Would CB4, which exhibits the least overestimation, now under-estimate the lower O3 mixing ratios? Conversely, would CB05 and SAPRC-99 predictions be closer to the observed values? While these are not easy questions to answer, my point is that determining which mechanism gives better performance is very difficult since the "right" answer with one mechanism could be due to a combination of "wrong" reasons.

Response: We agree with the reviewer that it is difficult to determine which mechanism gives better performance for the right reasons. On the basis of NO simulation results on the ground (ship and AIRMAP, see Tables 4 and 5), CB4 has less underestimation of NO than CB05 and SAPRC-99, leading to more titration of O3 and less overestimation of O3.

3) In Section 3.2 (page 22965), the underestimations of CO concentrations are attributed to inadequate representation of pollution associated with biomass burning from outside the domain. Did the authors conduct a sensitivity study with CO boundary conditions to confirm this hypothesis?

Response: Yes, Mathur (2008, JGR) had following sentences to describe these “In Figure 4d, significant enhancements in measured CO mixing ratios are noted along the flight segments between 1700–1800 GMT between altitudes of 2–4 km and also between 2000–2100 GMT coincident with enhancements in measured acetonitrile mixing ratios (not shown) suggesting that the aircraft sampled the biomass burning plume associated with the Alaskan fires. These enhancements were not captured in the base case simulation which used the default static lateral boundary conditions, but are more accurately represented in the assimilation simulation.”

4) In Section 3.2 (page 22967), the authors do not provide an explanation of why the simulated terpene mixing ratios in layer 3 are significantly higher than in other layers. Do they see the same vertical behavior for other species that are emitted from surface sources?

Response: Yes, as shown in Figure 4, isoprene concentrations are also high for this case when observations took place over the northeastern part of USA on 7/22. We think that VOC emission inventory over this area create high emissions of terpenes and isoprene. Obviously, more study is needed about the VOC emission inventory.

Minor comments: 1) Page 22957, line 5: Remove "the" before "observations".
Response: Done.

2) Page 22957, lines 9 and 12: Remove "the" before "observed".
Response: Done.

3) Page 22958, line 25: Insert "the" before "lumped structure".
Response: Done.

4) Page 22958, line 26: Insert "the" before "SAPRC" and "the" before "lumped molecule"
Response: Done.

5) Page 22959, line 2: Change "formulation" to "formulations".
Response: Done.

6) Page 22959, line 4: Consider changing "different chemical mechanisms" to "they" and removing "prediction" before "results".
Response: Done.

7) Page 22959, lines 18-19: Change "by 30-45 pph" to "that are 30-45 ppb".
8). Page 22960, lines 10, 13 and 20: Add "the" before "three photochemical".
Response: Done.
9). Page 22960, line 11: Add "the" before "2004 ICARTT period".
Response: Done.
10) Page 22960, line 16: Remove "the" before "observations".
Response: Done.
11) Page 22960, line 15: Change "description of CB4" to "descriptions of the CB4".
Response: Done.
12) Page 22961, line 11: Change "species is used to represent similar organic compound" to "species are used to represent similar organic compounds".
Response: Done.
13) Page 22961, line 11: Change "compares" to "compare".
Response: Done.
14) Page 22961, line 27: Add comma after "radical".
Response: Done.
15) Page 22961, line 29: Add comma after "ALDX".
Response: Done.
16) Page 22962, line 13: Change "alkenes which allowed to" to "alkenes, which are allowed to".
Response: Done.

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17) Page 22963, line 26 and Page 22964, lines 5 and 18: Add "the" before "three mechanisms".
Response: Done.
18) Page 22964, line 6: Remove "the" before "O3 mixing ratios".
Response: Done.
19) Page 22964, line 9: Consider removing "at the low mixing ratio ranges".
Response: Done.
20) Page 22964, line 10: Consider changing "more O3 for all O3 mixing ratio ranges than CB4" to "more O3 than CB4 for all O3 mixing ratio ranges".
Response: Done.
21) Page 22964, line 21: Change "except" to "exception".
Response: Done.
22) Page 22965, line 23: Change "somehow" to "somewhat".
Response: Done.
23) Page 22966, lines 2 & 3: Consider changing "the relative better" to "relatively better".
Response: Done.
24) Page 22966, line 3: Change "on" to "for".
Response: Done.
25) Page 22966, line 4: Add "the" before "different mechanisms".
Response: Done.
26) Page 22966, line 13: Remove "the" before "consistent".
Response: Done.

27) Page 22966, line 18: Change "Three mechanisms" to "The three mechanisms".
Response: Done.

28) Page 22966, line 20: Add "the" before "reasons".
Response: Done.

29) Page 22966, line 21: Add "in" before "Fig. 2".
Response: Done.

30) Page 22966, line 22: Consider changing "CB05 has relative better performance for H2O2 and CO compared to those of" to "CB05 performs relatively better for H2O2 and CO than".
Response: Done.

31) Page 22967, line 6: Consider changing "Comparing" to "Compared".
Response: Done.

32) Page 22967, line 15: Consider changing "relative" to "relatively".
Response: Done.

33) Page 22967, lines 17, 25 and 27: Add "the" before "three".
Response: Done.

34) Page 22968, line 6: Consider changing "models" to "model predictions" or "modeled values".
Response: Done.

35) Page 22968, line 10: Change "offshore flow from the southwest and west where are" to "offshore flows from the west and southwest that are".
Response: Done.

36) Page 22968, line 13: Change "flow from" to "flows from the".
Response: Done.

37) Page 22968, line 24 and Page 22969, lines 5 and 11: Add "the" before "three".
Response: Done.

38) Page 22969, line 1: Add "in" before "Table 4".
Response: Done.

39) Page 22969, line 12: Remove "the" before "slightly better performance".
Response: Done.

40) Page 22969, lines 15 to 17: Need to rephrase: emissions are estimated by SMOKE not CMAQ. Maybe change "model" to "the SMOKE/Eta/CMAQ modeling system"??
Response: Done. It is BEIS model.

41) Page 22969, line 22: Add "the" before "three".
Response: Done.

42) Page 22969, line 25: Change "observation" to "observations" or "observed values".
Response: Done.

43) Page 22969, line 26: Consider changing "indicating too high background O3 mixing ratios in the model" to "indicating that background O3 mixing ratios in the model are too high".
Response: Done.
44) Page 22969, line 27: The values for ozone production efficiency are redundant since they are already provided three lines above.
Response: Done. The values have been removed in the revise manuscript.
45) Page 22969, line 28: Consider changing "analyzed" to "discussed".
Response: Done.
46) Page 22969, lines 29 and 30: Consider changing "Too high NOz mixing ratios in the model indicate" to "The overpredictions of NOz mixing ratios indicate".
Response: Done.
47) Page 22970, line 4: Add "the" before "three".
Response: Done.
48) Page 22970, line 8: Consider changing "of three mechanism model configurations" to "with the three different mechanisms".
Response: Done.
49) Page 22971, line 6: Consider rephrasing "On the basis of vertical results"
Response: Done.
50) Page 22971, lines 11 and 14: Add "the" before "three".
Response: Done.
51) Page 22971, line 12: Change "somehow" to "somewhat".
Response: Done.
52) Page 22971, line 13: Consider changing "relative better performance on" to "relatively better performance for".
Response: Done.
53) Page 22971, line 14: Remove "the" before "CB4".
Response: Done.
54) Page 22971, line 22: Consider changing "observed pollutants" to "observed pollutant concentrations" or "observed pollutant mixing ratios".
Response: Done.
55) Page 22972, lines 3 to 5: Consider changing "Too high NOz mixing ratios in the model also contribute" to "The overpredictions of NOz mixing ratios also contribute".
Response: Done.
56) Page 22972, lines 8 and 10: Add "the" before "three".
Response: Done.

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