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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A comparison of atmospheric composition using the Carbon Bond and Regional Atmospheric Chemistry Mechanisms" *by* G. Sarwar et al.

Anonymous Referee #2

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Chemical mechanisms are needed to simulate atmospheric chemistry in 3-D chemical transport models (CTMs) and this manuscript compares a newly developed mechanism (RACM2) to another mechanism (CB05TU) that is widely used. Mechanism comparisons are useful in providing information to guide mechanism selection for particular model applications, providing context for interpreting model results, and assessing overall uncertainties in atmospheric chemistry by comparing results from two independently derived mechanisms. RACM2 is a larger mechanism than CB05TU containing roughly twice the numbers of reactions and chemical species. Both mechanisms produce predict similar concentrations for chemical species of concern in air quality

management, with average differences of: ozone (6%); nitrate (6%); sulfate (10%); ammonium (10%); PM2.5 (7%). These differences are comparable to or smaller than uncertainties expected from other CTM components such as emissions and meteorological input data, deposition algorithms or modeling grid resolution. Both mechanisms provide nearly identical responses to anthropogenic emission reductions.

Comments

1. On page 6931, line 20, modeled OH concentrations are compared to measurements for an urban location in Houston. The authors do not explain whether the median model predictions are for the 12 x 12 km grid cell containing the monitor – I assume this is the case. Later in the manuscript (page 6941, line 20) the authors point out substantial model under-predictions of VOCs in Houston which will strongly influence OH production. Realistically, the authors lack an objective basis for concluding whether one mechanism matches the observed OH concentrations better than the other.

2. On page 6932, line 16, modeled H2O2 concentrations for 2006 are compared to observed concentrations from 2001. The RACM2 and CB05TU predictions differ one from another by 10% but are less than half the observed concentration. The authors invoke a scaling factor of 2.5 from another modeling study to conclude that RACM2 agrees better than CB05TU with the observations. The uncertainties in this comparison are so great that it is unreasonable to conclude that one mechanism matches the observed H2O2 concentrations better than the other.

3. On page 6933, line 12, modeled peroxyacyl acid concentrations for the US are compared to measured peroxyacetic acid concentrations from China with the stated assumption (on line 25) that concentrations will be similar for the US and China. How can this assumption be justified and then used to support a conclusion that RACM2 agrees better than CB05TU with the observations?

4. On page 6934, line 14, modeled CH3OOH concentrations for 2006 are compared to observed concentrations from 2001. The RACM2 and CB05TU predictions differ one

from another by 25% (0.20 vs. 0.15 ppb) but are half of the observations (0.4 ppb). The authors invoke a scaling factor of 1.96 from another modeling study to conclude that RACM2 agrees better than CB05TU with the observations. The uncertainties in this comparison are so great that it is unreasonable to conclude that one mechanism matches the observed CH3OOH concentrations better than the other.

5. On page 6940, modeled O3 concentrations are compared to observed concentrations in four cities and then by selecting some days with high O3 the authors conclude that RACM2 is "improving the comparison at high observed O3" (line 28) compared to CB05TU. In reviewing the underlying data presented in Figures 7a-d it seemed that a systematic comparison could lead to a different conclusion. Selecting the 3 days that appear to have the highest observed O3 in each city (Los Angeles, September 3, 4, 10; Houston, September 1, 7, 14; Atlanta, September 16, 15, 27; New York, September 9, 8, 18 and 27) reveals that in Los Angeles RACM2 over-predicts by more than CB05TU, in Houston RACM2 improves upon under-prediction by CB05TU, in Atlanta both mechanisms over and under-predict, and in New York RACM2 over-predicts consistently whereas CB05TU over and under-predicts. In summary, RACM2 improved performance in one city (Houston) but degraded performance in two cities (Los Angeles and New York). Reliance upon the Houston result is questionable because the authors point out substantial model under-predictions of VOCs in Houston (page 6941, line 20). The authors should revise their conclusion.

6. Page 6941. I found Section 3.3.3 difficult to follow because several concepts are combined in a single long paragraph. I suggest re-writing this paragraph to focus on vertical O3 distributions in the mid to upper troposphere.

7. Page 6943. Section 3.5.2 discusses SOA. Table 3 shows RACM2 producing 42% higher anthropogenic SOA concentrations than CB05TU which is opposite a 22% decrease reported by a comparison for Europe (page 6926, line 1). Some discussion of this difference needs to be added.

8. Page 6946, line 9. Conclusions about the accuracy of predictions for H2O2, MEPX and PACD cannot be supported due to uncertainties in the comparisons (discussed in points 2-4 above) and should be removed.

9. Page 6946, line 16. Data presented by the authors contradict a conclusion that RACM2 improves O3 predictions when observed O3 is high (point 5 above) and this conclusion should be modified or deleted.

10. Page 6946, line 20. A summary statement is made that "the two mechanisms produce relatively large differences in the predictions of O3 and secondary particles" when the differences range from 6% to 10%. These are small differences in the context of other uncertainties in the modeling such as the emissions and meteorological input data. The statement should be revised to the mechanism predictions are similar.

11. Page 6924, line 9. The statement "RACM2 predictions generally agree better with the observed data than the CB05TU predictions" is broad and unqualified and should be deleted.

12. Page 6946, line 11. Data presented by the authors contradict a conclusion that RACM2 improves O3 predictions when observed O3 is high (point 5 above) and this conclusion should be modified or deleted.

13. Page 6946, line 20. A summary statement is made that "RACM2 enhances ozone and secondary aerosols by relatively large margins" when the differences range from 6% to 10%. These differences are small in the context of other uncertainties in the modeling such as the emissions and meteorological input data. I suggest changing this statement to "RACM2 and CB05TU predict similar concentrations for ozone and secondary aerosols" which would then help to explain why the mechanisms produce similar responses to emission reductions.

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