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Geoscientific Model Development Discussions

Interactive comment on "Identifying the causes of differences in ozone production from the CB05 and CBMIV chemical mechanisms" *by* R. D. Saylor and A. F. Stein

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This paper addresses the important scientific issue of mechanistic differences between two versions of the carbon bond gas-phase chemical mechanism as they are implemented in the NAQFC model. The trial update in the chemical module of this model is relevant for the air quality modeling community, assessing model performance, in particular for the ozone concentrations. The idea to explore the differences between the both versions of chemical mechanism (carbon bond) is not totally new, the authors cite previous studies that have been made. In contrast, this paper provides new contributions studying with some care the chemical discrepancies that lead to overestimation of

ozone concentrations in the NAQFC model. The manuscript is well written and address relevant scientific modelling questions within the scope of GMD.

Therefore, I found this manuscript suitable for publication if you manage to adequately resolve some points outlined below.

Major Comments

1. It is important that authors address with more emphasis the interest in considering the update of carbon bond mechanism (CB05) in the simulations performed with the NAQFC model. Also, add information about the more recent version of the carbon bond mechanism (CB06, CB06-TUV).
2. The discrepancies obtained between the operational mechanism and the trial mechanisms for ozone concentration are clearly seen on figure 1, this figure shows the mean bias ground level ozone for a one-year period. Otherwise, when you perform the sensitivity test you consider a different time period in a box model, 10-day simulation. Then is not obvious that the ozone concentrations are overestimated in the NAQFC model for a 10-day period (air quality forecast over a week or diurnal episodes should be interesting). Assuming that the ozone concentrations are overestimated when the trial mechanism is used in an Air Quality Model. On this case the ozone maximum will occur at the same time of day for both mechanisms?
3. It is also very important to indicate the main differences between both chemical mechanisms as they were included in the model NAQFC. There must be notable changes in some reactions of the two chemical mechanism versions. For example, in a comparison between CB05 and CB06 mechanisms, you could make emphasis in some reactions:
    - $OH + NO2 => HNO3$ increased by 5%, then greater radical sink,

- $NO2 + hv => NO + O$ increased by 7% then more ozone,
- $N2O5 + H2O => 2HNO3$ decreased by approximately 80%. Implies less NOx removal at night.

The features of both chemical mechanisms (CBIV and CB05) itself may help to highlight your results and conclusions. Therefore, I suggest to show a summary of the main features CBIV and CB05 mechanisms, previous showing the results. In addition, is not clear from section 1 (14-20) and section 2 (5-9) if both mechanisms are somehow modified for their inclusion in the NAQFC model. For example both 63 and 64 reactions from the original CB05 mechanism are the same as you present in the appendix.

4. The ozone overestimation for the June to October period showed in figure 2 needs some discussion. This behavior is quite similar to that showed in Sarwar et al., 2008. It is possible to relate the discovered reactions that cause the over estimation in ozone concentrations within the period of time with bigger discrepancies?

5. On figure 2 the ozone concentrations from CB05 are greater than CBIV except for the scenario s37. Do you have any comments?

6. To better represent de overestimation of ozone concentrations from CB05 with respect to CBIV would be helpful to bring the percentage of O3 overestimation and put on your consideration to add a plot of the sensitivity analysis of an ozone precursor species.

7. Yarwood et al., 2005, shows that the CB05 mechanism overestimates the concentrations for O3, HNO3, H2O species when doing 24 hours simulations in a box model. There are really important changes in your chemical mechanisms that account to different results?

Minor Comments

1. Suggestion. Figure 1 shows mean bias ozone from CB05 in color black, while in Figure 2 the ozone mixing ratio is in red.

2. In some places the word “reactions” is written with R, and some equation labels are with an extra coma.

Interactive comment on Geosci. Model Dev. Discuss., 4, 2687, 2011.