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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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General comments

The present manuscript presents an analysis aimed at understanding the differences in ozone production between two versions of the Carbon Bond mechanism used in air quality models. The study is motivated by the fact that the air quality forecast system NAQFC has greater model-measurement bias for ground-level ozone with the more recent version of the chemical mechanism, CB05, than with the previous one, CBMIV. The analysis is performed by grouping reactions that are either removed or substituted in order to get back to the CBMIV representation. The manuscript is well structured

and written. It falls whithin the scope of the journal and I recommend its publication. However, the manuscript would profit from a short discussion on future model developments of the chemistry that would reduce the model-measurements bias (see comment below).

Main comment

The authors successfully identify the part of the mechanisms that is critical for the prediction of NO_x and O_3 but do not point to any potential improvement of both CB05 mechanism and NAQFC system that future work could focus on. For example, the present study identifies the species NTR as critical for modeling O_3. One way to proceed may be to split NTR in two or more alkyl nitrate species like saturated and unsaturated. For instance, the nitrates from isoprene are quite reactive and recycle some NOx upon reaction with OH (Paulot et al, 2009). Moreover, their reaction with O_3 may be a significant sink (Horowitz et al., 2007) although partly recycling NO_x. On the other hand, the nitrates from NMHC and TERP are less reactive (mostly saturated) and likely recycle less NO_x upon reaction with OH. Finally, recent data on the $NO + HO_2$ reaction (Butkovskaya et al., 2005 and 2009) suggest a significant HNO_3-channel that leads to significantly lower O_3 production in the lower troposphere (Cariolle et al., 2008; Søvde et al., 2011).

Minor comments

p. 2691, l. 5-7: a short description of how the mechanism were altered in the NAQFC implementation would be helpful for the reader.

Supplement: could you add the expressions for all the kinetic functions used in the mechanisms (ARR2, TERM, KTYP2, KTYP3 and SUN).

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