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Interactive comment on "Comparison of tropospheric chemistry schemes for use within global models" *by* K. M. Emmerson and M. J. Evans

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We would like to make some comments regarding the version of the CBM-IV mechanism used in the box-modelling study of Emmerson and Evans entitled 'Comparison of tropospheric chemistry schemes for use within global models'. Moreover, we also wish to comment on our experience of the online performance of the modified CBM-IV scheme of Houweling et al (1998) when applied in a large-scale global model, especially concerning PAN.

The version of CBM-IV mechanism used by global models is a modified version of the original scheme given by Gery et al (1989), as published by Houweling et al.

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(1998). The main modifications are the elimination of aromatics (TOL, CRES and XYL), propane, modifications to the product distribution for the oxidation of OLE and ISOP and the addition of two extra trace species, these being a higher peroxy species (ROOH) and a lumped organic nitrate (ORGNTR). The motivation for this modification was that the scheme of Gery et al (1989) was tuned for polluted urban simulations, whereas the modified scheme improves the performance for background conditions by extending the methane oxidation chemistry and updating the product distribution for the isoprene oxidation reactions (which has been assessed online by von Kuhlmann et al, 2004). Moreover, some of these modifications were subsequently incorporated into CBM-IV during a later update documented by Jeffries et al (2002). This modified CBM-IV scheme is currently used in TM3 (Houweling et al., 1998), TM4 (van Noije et al, 2006), TM5 (Krol et al, 2005) and GISS model E (Shindell et al., 2003) resulting in 64 reactions and 24 transported tracer species, rather than the full scheme of Gery et al (1989). Recent updates to the rate coefficients have also been performed which result in improved agreement for CO in remote locations (Williams and van Noije, 2008).

Recently, this scheme has been involved in a number of assessments (e.g. Stevenson et al, 2006) and multi-model intercomparisons as part of several EU research projects, namely AMMA-EU (https://www.amma-eu.org/) and the GEMS project (http://gems.ecmwf.int/). Direct comparisons have been made with many different models, including both p-TOMCAT and MOZART-3. For PAN the concentrations over West Africa typically exceed those exhibited by p-TOMCAT for such tropical conditions using identical emission inventories. For Europe, we also see PAN at the surface which is at least ˜50% that simulated in MOZART-3. Houweling et al (1998) also include a plot of PAN at the surface versus measurements at remote locations which shows that the mechanism may have the tendency to produce too much PAN for such locations. This is not in agreement with the evolution of PAN shown for the pre-defined scenarios in Figure 3 (plots b and d) of Emmerson and Evans (2008). A possible reason for this difference is that the precursor radical (C2O3) is also formed during the oxidation of ISOP by O3 and MGLY by OH in the scheme of Houweling et al (1998). Moreover, MGLY

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and PAR are emitted in polluted conditions to account for a fraction of the missing aromatics (using the stiochiometry given in Gery et al. (1989)). This further increases the formation of PAN under urban conditions. In light of these findings we feel that the conclusion concerning PAN formation of Emmerson and Evans should be treated with caution concerning the performance of the CBM mechanism as applied in large-scale models.

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