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HOx regeneration in isoprene oxidation: global model evaluation of newly-proposed reaction sequences

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There is now overwhelming evidence that the traditional isoprene chemical oxidation mechanism used in CTMs requires substantial revision. Lelieveld et al. ($Nature$, 2008) showed that strong OH regeneration must be invoked in order to explain observed HOx levels in isoprene-rich, pristine conditions, and suggested that it occurs through the reactions of isoprene peroxy radicals with HO_2. Paulot et al. ($Science$, 2009) showed in a laboratory study that the OH-reaction of isoprene hydroperoxides generates OH along with dihydroxy epoxides possibly contributing to secondary organic aerosol formation. However, measurement campaigns at mid-latitudes indicate that HOx regeneration occurs even at mid-latitudes (Hofzumahaus et al., $Science$, 2009; Ren et al., $J.Geophys.Res.$, 2008) where isoprene peroxy radicals are expected to react mostly with NO. A likely explanation is provided by the theoretical study of Peeters et al. ($Phys.Chem.Chem.Phys.$, 2009), which showed that isomerization reactions of specific isomer/conformer peroxy radicals from isoprene lead to the formation of HO_x radicals and photolabile hydroperoxy aldehydes (denoted HPALDs), at rates such that the traditional reactions of the isoprene peroxy radicals (with NO and HO_2) are outrun in most non-urban atmospheric conditions. We present a detailed global modelling study aiming at quantifying the impact of the new reactions proposed by Paulot et al. and Peeters et al. on the global tropospheric composition. The calculated concentrations of key compounds will be evaluated against measurement campaigns at Tropical (e.g. GABRIEL) and mid-latitudes (INTEX-A, PROPHET), and sensitivity simulations wil be performed to estimate the remaining uncertainties.