

## 2.003 An updated isoprene oxidation and deposition scheme in the IMAGES model.

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Abstract:

Our view of isoprene atmospheric degradation has dramatically changed in the last years, thanks to numerous laboratory and theoretical studies. We present a revised, thoroughly updated isoprene chemical mechanism relying on recent work, including the Caltech review (Wennberg et al., 2018). A special focus is the fate of hydroperoxy carbonyls generated at various instances in the oxidation of isoprene and other compounds, e.g. following the isomerisation of delta-hydroxyperoxys from isoprene+OH. We show that 1) the absorption cross sections of alpha- and beta-hydroperoxy carbonyls is considerably enhanced compared to monofunctional compounds; 2) the quantum yield of alpha-hydroperoxycarbonyl photolysis is of the order of 1; and 3) the reaction is shown to result for a large, likely dominant part, in the formation of an enol, whereas C-C scission is another viable channel. The pathway often believed to be dominant (O-OH bond breakup) is found to be negligible. The implications are important. The atmospheric fate of enols is still largely unexplored, except for a theoretical study (So et al., 2014) addressing vinyl alcohol. Based on their results, we propose updated chemical mechanisms for key hydroperoxycarbonyls formed in isoprene oxidation. An interesting aspect is a substantial production of formic and acetic acid, for which large missing sources have been reported over vegetated areas.

In addition, a new dry/wet scavenging scheme is presented, incorporating a new estimation method for the Henry's Law constants of oxygenated organic compounds (OVOCs). The dry deposition scheme is adjusted based on evidence of fast uptake of OVOCs by foliage. Extensive evaluation of the scheme against field measurements for O<sub>3</sub> and OVOC is presented. The impact of the updates in the chemical degradation and deposition schemes are assessed using a global model (IMAGES).