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Modelling the evolution of organic carbon during its gas-phase tropospheric oxidation: development of an explicit model based on a self generating approach

B. Aumont[1], S. Szopa[1,*], and S. Madronich[2]
[1]Laboratoire Interuniversitaire des Systèmes Atmosphériques, UMR CNRS 7583, Universités Paris 7 et Paris 12, 94010 Créteil Cedex, France
[2]National Center for Atmospheric Res., Atmospheric Chemistry Division, P.O. Box 3000, Boulder, Colorado 80307, USA
[*] now at: Laboratoire des Sciences du Climat et de l'environnement, UMR CNRS CEA 1572, 91191 Gif-sur-Yvette, France

Abstract. Organic compounds emitted in the atmosphere are oxidized in complex reaction sequences that produce a myriad of intermediates. Although the cumulative importance of these organic intermediates is widely acknowledged, there is still a critical lack of information concerning the detailed composition of the highly functionalized secondary organics in the gas and condensed phases. The evaluation of their impacts on pollution episodes, climate, and the tropospheric oxidizing capacity requires modelling tools that track the identity and reactivity of organic carbon in the various phases down to the ultimate oxidation products, CO and CO_2. However, a fully detailed representation of the atmospheric transformations of organic compounds involves a very large number of intermediate species, far in excess of the number that can be reasonably written manually. This paper describes (1) the development of a data processing tool to generate the explicit gas-phase oxidation schemes of acyclic hydrocarbons and their oxidation products under tropospheric conditions and (2) the protocol used to select the reaction products and the rate constants. Results are presented using the fully explicit oxidation schemes generated for two test species: n-heptane and isoprene. Comparisons with well-established mechanisms were performed to evaluate these generated schemes. Some preliminary results describing the gradual change of organic carbon during the oxidation of a given parent compound are presented.

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