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Assessment of the reduction methods used to develop chemical schemes: building of a new chemical scheme for VOC oxidation suited to three-dimensional multiscale HO_x-NO_x-VOC chemistry simulations

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Abstract. The objective of this work was to develop and assess an automatic procedure to generate reduced chemical schemes for the atmospheric photooxidation of volatile organic carbon (VOC) compounds. The procedure is based on (i) the development of a tool for writing the fully explicit schemes for VOC oxidation (see companion paper Aumont et al., 2005), (ii) the application of several commonly used reduction methods to the fully explicit scheme, and (iii) the assessment of resulting errors based on direct comparison between the reduced and full schemes.
The reference scheme included seventy emitted VOCs chosen to be representative of both anthropogenic and biogenic emissions, and their atmospheric degradation chemistry required more than two million reactions among 350000 species. Three methods were applied to reduce the size of the reference chemical scheme: (i) use of operators, based on the redundancy of the reaction sequences involved in the VOC oxidation, (ii) grouping of primary species having similar reactivities into surrogate species and (iii) grouping of some secondary products into surrogate species. The number of species in the final reduced scheme is 147, this being small enough for practical inclusion in current three-dimensional models. Comparisons between the fully explicit and reduced schemes, carried out with a box model for several typical tropospheric conditions, showed that the reduced chemical scheme accurately predicts ozone concentrations and some other aspects of oxidant chemistry for both polluted and clean tropospheric conditions.

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