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Systematic reduction of complex tropospheric chemical mechanisms, Part II: Lumping using a time-scale based approach

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Abstract. This paper presents a formal method of species lumping that can be applied automatically to intermediate compounds within detailed and complex tropospheric chemical reaction schemes. The method is based on grouping species with reference to their chemical lifetimes and reactivity structures. A method for determining the forward and reverse transformations between individual and lumped compounds is developed. Preliminary application to the Leeds Master Chemical Mechanism (MCMv2.0) has led to the removal of 734 species and 1777 reactions from the scheme, with minimal degradation of accuracy across a wide range of test trajectories relevant to polluted tropospheric conditions. The lumped groups are seen to relate to groups of peroxy acyl nitrates, nitrates, carbonates, oxepins, substituted phenols, oxeacids and peracids with similar lifetimes and reaction rates with OH. In combination with other reduction techniques, such as sensitivity analysis and the application of the quasi-steady state approximation (QSSA), a reduced mechanism has been developed that contains 35% of the number of species and 40% of the number of reactions compared to the full mechanism. This has led to a speed up of a factor of 8 in terms of computer calculation time within box model simulations.

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