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Impact of C_1-C_5 alkyl nitrate chemistry on tropospheric ozone - a box modelling study

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Alkyl nitrates ($RONO_2$) are organic trace gases that are emitted from oceanic and biomass burning sources and produced photochemically from the oxidation of hydrocarbons (RH) in the presence of nitrogen oxides (NO_x). Their formation terminates the catalytic tropospheric ozone production by temporarily storing the active form of nitrogen. Due to a relatively long lifetime of a few days to a few months they can be destroyed far away their sources by photolysis or OH radical oxidation, releasing NO_2 back to the local atmosphere. Given the right circumstances, this might change ozone concentrations on regional levels and alter the oxidative capacity of the atmosphere.

The chemistry of alkyl nitrates is currently under-represent in global chemistry-climate models. If present, they appear in a lumped from or only short-chained nitrates are considered explicitly. Here we extend the tropospheric chemical mechanism (CheT) of the UK Chemistry and Aerosols (UKCA) model to include the chemistry of C_2-C_5 alkyl nitrates (and C_4-C_5 alkanes). The new mechanism is tested in a box model in a range of NO_x and RH conditions using the Master Chemical Mechanism (MCM) as a benchmark. Prior to addition of the new chemistry the original CheT mechanism has been revised and updated, revealing that the differences in the reaction rate coefficients (especially in inorganic chemistry) between the CheT and the MCM sometimes had a greater impact on species concentrations than the level of mechanism reduction.

We estimate the impact of $RONO_2$ on concentrations of the major oxidants (O_3, OH and HO_2) at steady state under constant NO_x and RH forcing, as well as in initial pulse of NO_x and RH pollution by analysing the fluxes through individual reactions.