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Simulation of peroxyacetyl nitrate (PAN) in EMAC in comparison with aircraft and satellite measurements

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The tropospheric trace gas peroxyacetyl nitrate (PAN, $CH_3C(O)OONO_2$) is an important reservoir gas for tropospheric nitrogen oxides (NO_x=NO+NO_2). It is formed due to photochemical oxidation of non-methane hydrocarbons (NMVOC) with binding of NO_x. The destruction of PAN is primarily thermal and releases NO_x again. Because of the long lifetime of PAN at low temperatures, as in the free upper troposphere, the distribution of NO_x depends on the long-range transport of PAN and the global distributions of ozone and OH in the lower atmosphere are also strongly influenced. In addition to ozone, PAN is an important component of photochemical smog and has a negative effect on humans and plants in high concentrations.

The simulation of PAN is challenging, because a very large number of chemical trace gases (many precursors, especially NMVOC) are involved in the formation of PAN and therefore a comprehensive chemistry has to be considered in the simulation. In addition, the distribution of PAN strongly depends on the vertical transport, the exact sources and emissions of NMVOC are often uncertain and the thermal destruction of PAN is difficult to determine.

We present new model simulations of the Earth system model ECHAM/MESSy Atmospheric Chemistry (EMAC) (Version 2.53), in which we have optimized the used chemistry and emissions with the goal of a more realistic PAN distribution. Results of these simulations are compared with an older EMAC simulation (with standard chemistry) as well as with measurement data. Results from the Gimballed Limb Observer for Radiance Imaging of the Atmosphere (GLORIA) on the HALO research aircraft and the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on the ESA ENVISAT satellite are used.