



## **Simulating the speciation of organic oxidised nitrogen compounds and their relative contributions to total oxidised nitrogen (NO<sub>y</sub>) in the boundary layer**

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It has been suggested that organic oxidised nitrogen compounds may account for a significant part, if not all, of the well documented problem of 'missing NO<sub>y</sub>'. It is estimated that there are as many as 100 alkyl nitrates in polluted tropospheric air masses, although their relative contribution to total NO<sub>y</sub> has not been well defined. In this presentation, the speciation of about 700 alkyl and multifunctional organic nitrates, peroxy nitrates and nitroaromatic compounds has been simulated using a Photochemical Trajectory Model (PTM) which makes use of the Master Chemical Mechanism (MCM), a chemistry scheme of 124 volatile organic compounds (VOCs) involving a total of ca. 5900 chemical species in ca. 14000 reactions. Because of its near-explicit nature, the MCM is ideal for studies of speciation of various classes of organic compounds observed in the polluted troposphere. In this presentation, the speciation and relative contributions (to total simulated NO<sub>y</sub>) of the above organic oxidised nitrogen compounds and inorganic oxidised nitrogen compounds are investigated using the PTM operating on 4-day back trajectories arriving at a site near Chelmsford in the southern UK during the Tropospheric ORganic CHEMistry experiment (TORCH) in August 2003.