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Simulating the detailed chemical composition of secondary organic aerosol formed on a regional scale during the TORCH 2003 campaign in the southern UK

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Abstract. Following on from the companion study (Johnson et al., 2006), a photochemical trajectory model (PTM) has been used to simulate the chemical composition of organic aerosol for selected events during the 2003 TORCH (Tropospheric Organic Chemistry Experiment) field campaign. The PTM incorporates the speciated emissions of 124 non-methane anthropogenic volatile organic compounds (VOC) and three representative biogenic VOC, a highly-detailed representation of the atmospheric degradation of these VOC, the emission of primary organic aerosol (POA) material and the formation of secondary organic aerosol (SOA) material. SOA formation was represented by the transfer of semi- and non-volatile oxidation products from the gas-phase to a condensed organic aerosol-phase, according to estimated thermodynamic equilibrium phase-partitioning characteristics for around 2000 reaction products. After significantly scaling all phase-partitioning coefficients, and assuming a persistent background organic aerosol (both required in order to match the observed organic aerosol loadings), the detailed chemical composition of the simulated SOA has been investigated in terms of intermediate oxygenated species in the Master Chemical Mechanism, version 3.1 (MCM v3.1). For the various case studies considered, 90% of the simulated SOA mass comprises between ca. 70 and 100 multifunctional oxygenated species derived, in varying amounts, from the photooxidation of VOC of anthropogenic and biogenic origin. The anthropogenic contribution is dominated by aromatic hydrocarbons and the biogenic contribution by α - and β -pinene (which also constitute surrogates for other emitted monoterpene species). Sensitivity in the simulated mass of SOA to changes in the emission rates of anthropogenic and biogenic VOC has also been investigated for 11 case study events, and the results have been compared to the detailed chemical composition data. The role of accretion chemistry in SOA formation, and its implications for the results of the present investigation, is discussed.

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