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Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part B): tropospheric degradation of aromatic volatile organic compounds

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Abstract. Kinetic and mechanistic data relevant to the tropospheric degradation of aromatic volatile organic compounds (VOC) have been used to define a mechanism development protocol, which has been used to construct degradation schemes for 18 aromatic VOC as part of version 3 of the Master Chemical Mechanism (MCM v3). This is complementary to the treatment of 107 non-aromatic VOC, presented in a companion paper. The protocol is divided into a series of subsections describing initiation reactions, the degradation chemistry to first generation products via a number of competitive routes, and the further degradation of first and subsequent generation products. Emphasis is placed on describing where the treatment differs from that applied to the non-aromatic VOC. The protocol is based on work available in the open literature up to the beginning of 2001, and some other studies known by the authors which were under review at the time. Photochemical Ozone Creation Potentials (POCP) have been calculated for the 18 aromatic VOC in MCM v3 for idealised conditions appropriate to north-west Europe, using a photochemical trajectory model. The POCP values provide a measure of the relative ozone forming abilities of the VOC. These show distinct differences from POCP values calculated previously for the aromatics, using earlier versions of the MCM, and reasons for these differences are discussed.

■ Final Revised Paper (PDF, 260 KB)
■ Discussion Paper (ACPD)

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