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Modelling the impact of multiphase chemistry on processing of oxygenated aromatic compounds

In the present study, we have developed and applied a detailed aqueous-phase oxidation mechanism of substituted aromatic compounds. The mechanism considers the oxidation of phenol, cresol, benzyl alcohol, benzaldehyde, and benzoic acid by different oxidants leading to formation of non-cyclic compounds. The developed mechanism has been coupled to the existing multiphase mechanism MCMv3.2 (Master Chemical Mechanism version 3.2) linked with CAPRAM4.0 (Chemical Aqueous Phase Radical Mechanism 4.0). Detailed model studies were carried out using the air parcel model SPACCIM (Spectral Aerosol Cloud Chemistry Interaction Model). The simulations revealed the high importance of cloud as well as aerosol chemistry for oxidation of the substituted aromatics. For instance, aqueous-phase chemistry leads to a substantial increase in organic aerosol mass, significant amounts of benzoic acid, and reduced concentrations of 2-nitrophenol.

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