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Investigative modeling of new pathways for secondary organic aerosol formation

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Abstract. Recent advances in secondary organic aerosol (SOA) research are reviewed and the status of current understanding is investigated using a box model of SOA formation. Benzene and isoprene are newly identified precursors that are included in this SOA model; these precursors form SOA via secondary products. The model is also extended to include some representation of aqueous partitioning and the formation of high molecular weight products via oligomerization. Experimental data and empirical relationships are used where possible, because a detailed representation of SOA formation is not supported by the current state of information. Sensitivity studies are conducted with the SOA model and SOA predictions are found to be very sensitive to the treatment of the interactions between particulate water and organic compounds. While uncertainties due to model formulation are significant, influential model parameters include the aerosol partitioning ratios for several small products of isoprene and the partitioning constants for unidentified products (currently, the partitioning constants are derived by fitting experimental data). The pH value used as the reference for the activation of oligomerization is also a critical parameter. Recommendations for future work needed to improve SOA models include the elucidation of the water-organic relationship, the extent of phase separation, and laboratory experiments conducted under conditions more relevant to ambient studies (e.g., lower concentrations, higher relative humidity).

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