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Estimation of secondary organic aerosol formation parameters for the Volatility Basis Set combining thermodenuder, isothermal dilution and yields measurements

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Secondary organic aerosol (SOA) constitutes a major fraction of the total organic aerosol (OA) in the atmosphere. SOA is formed by the partitioning onto pre-existent particles of low vapor pressure products of the oxidation of volatile, intermediate volatility, and semivolatile organic compounds. Oxidation of the precursor molecules results a myriad of organic products making the detailed analysis of smog chamber experiments difficult and the incorporation of the corresponding results into chemical transport models (CTMs) challenging. The volatility basis set (VBS) is a framework that has been designed to help bridge the gap between laboratory measurements and CTMs. It describes the volatility distribution of the OA and the SOA. The parametrization of SOA formation for the VBS has been traditionally based on fitting yield measurements of smog chamber experiments. To reduce the uncertainty of this approach we developed an algorithm to estimate parameters such as volatility product distribution, effective vaporization enthalpy, and accommodation coefficient combining SOA yield measurements with thermograms (from thermodenuders) and areograms (from isothermal dilution chambers) from different experiments and laboratories. The algorithm was first evaluated with “pseudo-data” produced from the simulation of the corresponding processes assuming SOA with known properties. The results showed excellent agreement and low uncertainties when the volatility range and the mass loadings range of the yield measurements coincide. One of the major features of our approach is that it estimates the uncertainty of the resulting parameterization for different atmospheric conditions (temperature, concentration levels, etc.). In the last step of the work, the use of the algorithm with realistic smog laboratory data is demonstrated.