2.160 1-Octanol Water Partition Coefficient as a Predictor of Liquid-Liquid Phase Separation in Mixed Organic/Inorganic Particles.

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Abstract:

Aerosol particles interact with water vapor in the atmosphere, undergoing phase transitions and separations. One example is liquid-liquid phase separation (LLPS), which could impact the hygroscopicity and heterogeneous chemical reactivity of aerosol particles. Here, we propose to predict LLPS of mixed organic/inorganic particles using 1-octanol water partition coefficient (K_{OW}). LLPS data of single inorganic–single organic systems, including separation relative humidities (SRH), were compiled from literature. LLPS is found to occur for organic compounds with log K_{OW}> 0, while it is inhibited for other cases (i.e., log K_{OW}< 0). The threshold could be rationalized by change in the Gibbs free energy associated with partitioning. The positive correlation between K_{OW} and Setchenov coefficient (k_S) indicates that LLPS is driven by salting-out effect. K_{OW} explains the occurrence and suppression of LLPS for α-pinene and isoprene secondary organic aerosol (SOA). K_{OW} also implies that formation of organosulfates and organonitrates may potentially alter LLPS of SOA. Our data analysis further suggested the usefulness of solid phase extraction (SPE) in investigating LLPS of complex organic mixtures. As compared to the current predictor O:C, K_{OW} may introduce additional information on functional groups to facilitate LLPS prediction based on chemical composition. Experiments are conducted to examine the feasibility of this idea. To validate the rigorousness of *Kow* as a LLPS predictor, deliquescence and efflorescence relative humidities (DRH and ERH) of organic mixtures after SPE are measured using Hygroscopic Tandem Differential Mobility Analyser (HTDMA).