



Thermodynamics and Diagnostics of a Two-Dimensional Volatility Basis Set

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Organic Aerosol mixing can occur via the gas-phase exchange of semi-volatile vapors between particles. We believe this is a dominant mixing mechanism in the atmosphere. To probe and understand this process we must be able to represent the phase partitioning of organic compounds in the complex mixtures typical of ambient particles. A special challenge is that we typically cannot identify the molecular structures for more than a small fraction of the organic material in atmospheric particles. Phase partitioning means at least two things: the pure vapor pressure of compounds, and also whether condensed-phase mixtures will themselves phase separate. Both are critical in the atmosphere because they control not only the total amount of organic aerosol but also the stability of important particle distributions. An example is the traffic mode of primary aerosol. If the semi-volatile constituents in this mode (much of the mass) can mix with the more oxidized constituents of the accumulation mode, recondensation to the accumulation will be a major sink of traffic-mode mass. Working within the constraints of available observations, we develop a thermodynamic representation of organic aerosol phase behavior that is both consistent with vapor-pressure data and useful for both diagnostic analysis of ambient data and prediction of organic aerosol levels and evolution.