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Thermodynamic characterization of Mexico City aerosol during MILAGRO 2006

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Abstract. Fast measurements of aerosol and gas-phase constituents coupled with the ISORROPIA-II thermodynamic equilibrium model are used to study the partitioning of semivolatile inorganic species and phase state of Mexico City aerosol sampled at the T1 site during the MILAGRO 2006 campaign. Overall, predicted semivolatile partitioning agrees well with measurements. $PM_{2.5}$ is insensitive to changes in ammonia but is to acidic semivolatile species. For particle sizes up to 1μm diameter, semi-volatile partitioning requires 15–30 min to equilibrate; longer time is typically required during the night and early morning hours. Aerosol and gas-phase speciation always exhibits substantial temporal variability, so that aerosol composition measurements (bulk or size-resolved) obtained over large integration periods are not reflective of its true state. When the aerosol sulfate-to-nitrate molar ratio is less than unity, predictions improve substantially if the aerosol is assumed to follow the deliquescent phase diagram. Treating crustal species as "equivalent sodium" (rather than explicitly) in the thermodynamic equilibrium calculations introduces important biases in predicted aerosol water uptake, nitrate and ammonium; neglecting crustals further increases errors dramatically. This suggests that explicitly considering crustals in the thermodynamic calculations is required to accurately predict the partitioning and phase state of aerosols.

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