Fine Particle pH for Beijing Winter Haze as Inferred from Different Thermodynamic Equilibrium Models

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(ywang246@central.uh.edu) pH is an important property of aerosol particles but is

difficult to measure directly. Several studies have estimated the pH values for fine particles in North China winter haze using thermodynamic models (i.e., E-AIM and ISORROPIA) and ambient measurements. The reported pH values differ widely, ranging from close to 0 (highly acidic) to as high as 7 (neutral). In order to understand the reason for this discrepancy, we calculated pH values using these models with different assumptions with regard to model inputs and particle phase states. We find that the large discrepancy is due primarily to differences in the model assumptions adopted in previous studies. Calculations using only aerosol phase composition as inputs (i.e., reverse mode) are sensitive to the measurement errors of ionic species and inferred pH values exhibit a bimodal distribution with peaks between -2 and 2 and between 7 and 10, depending on whether anions or cations were in excess. Calculations using total (gas plus aerosol phase) measurements as inputs (i.e., forward mode) are affected much less by the measurement errors, and results are thus superior to those obtained from the reverse mode calculations. Forward mode calculations in this and previous studies collectively indicate a moderately acidic condition (pH from about 4 to about 5) for fine particles in North China winter haze, indicating further that ammonia plays an important role in determining this property. The phase state assumed, which can be either stable (solid plus liquid) or metastable (only liquid), does not significantly impact pH predictions of ISORROPIA.