Simulating the Partitioning of Semivolatile Inorganic Aerosol during the MILAGRO 2006 Campaign

Christos Fountoukis[1], Amy Sullivan[2], Rodney Weber[2], Timothy Vanreken[3,7], Marc Fischer[4], Edith Matías[5], Mireya Moya[5], Delphine Farmer[6], Ronald Cohen[6] and Athanasios Nenes[1,2]

[1]School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA.
[2]School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, GA.
[3]National Center for Atmospheric Research, Boulder, CO.
[4]Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, CA.
[5]Centro de Ciencias de la Atmosfera, Universidad Nacional Autonoma de Mexico, Mexico City, Mexico.
[6]Department of Chemistry, University of California Berkeley, Berkeley, CA.
[7]Now at Laboratory for Atmospheric Research, Department of Civil & Environmental Engineering, Washington State University, Pullman, Washington.

ABSTRACT

The partitioning of semivolatile inorganic species between the gas and particulate phase was studied using a) high time resolution (5-minute) measurements from the MILAGRO 2006 campaign in Mexico City and b) a state-of-the-art aerosol equilibrium model, ISORROPIA-II, which explicitly treats the thermodynamics of the K^+-Ca^{2+}-Mg^{2+}-NH_4^+-Na^+-SO_4^{2-}-HSO_4^--NO_3^--Cl^--H_2O aerosol system. Overall, a very good agreement between predictions and observations was found for particulate ammonium, nitrate, chloride and gas phase ammonia. Below 50% RH, best agreement was found when considering the stable state solution of ISORROPIA-II indicating the potential existence of deliquescence branch aerosols. In the ammonia-rich environment of Mexico City, $PM_{2.5}$ is not very sensitive to changes in ammonia; instead, a combined reduction in total sulfate and total nitrate appears to be a more promising strategy for $PM_{2.5}$ control. The importance of including crustal species in predicting aerosol nitrate and ammonium is also investigated.