Atmospheric Chemistry and Physics
An Interactive Open Access Journal of the European Geosciences Union

Atmos. Chem. Phys., 6, 4889-4904, 2006
www.atmos-chem-phys.net/6/4889/2006/
© Author(s) 2006. This work is licensed
under a Creative Commons License.

Implementation of a Markov Chain Monte Carlo method to inorganic aerosol modeling of observations from the MCMA-2003 campaign – Part II: Model application to the CENICA, Pedregal and Santa Ana sites

F. M. San Martini[1,*], E. J. Dunlea[2], R. Volkamer[1,**], T. B. Onasch[3], J. T. Jayne[3], M. R. Canagaratna[3], D. R. Worsnop[3], C. E. Kolb[3], J. H. Shorter[3], S. C. Herndon[3], M. S. Zahniser[3], D. Salcedo[4], K. Dzepina[2,6], J. L. Jimenez[2,6], J. M. Ortega[1,***], K. S. Johnson[1], G. J. McRae[5], L. T. Molina[1,7], and M. J. Molina[1,**]

[1]Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA, USA

[2]Cooperative Institute for Research in the Environmental Sciences (CIRES), Univ. of Colorado at Boulder, Boulder, CO, USA

[3]Aerodyne Research Inc., Billerica, MA, USA

[4]Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos, Cuernevaca, Morelos, México

[5]Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA

[6]Department of Chemistry and Biochemistry, University of Colorado-Boulder, Boulder, CO, USA

[7]Molina Center on Energy and the Environment, La Jolla, CA, USA

[*]now at: the Board on Chemical Sciences and Technology, National Academies, Washington, D.C., USA

[**]now at: University of California San Diego, La Jolla, CA, USA

[***]now at: Sandia National Laboratory, Livermore, CA, USA

Abstract. A Markov Chain Monte Carlo model for integrating the observations of inorganic species with a thermodynamic equilibrium model was presented in Part I of this series. Using observations taken at three ground sites, i.e. a residential, industrial and rural site, during the MCMA-2003 campaign in Mexico City, the model is used to analyze the inorganic particle and ammonia data and to predict gas phase concentrations of nitric and hydrochloric acid. In general, the model is able to accurately predict the observed inorganic particle concentrations at all three sites. The agreement between the predicted and observed gas phase ammonia concentration is excellent. The NO_z concentration calculated from the NO_y, NO and NO_2 observations is of limited use in constraining the gas phase nitric acid concentration given the large uncertainties in this measure of nitric acid and additional reactive nitrogen species. Focusing on the acidic period of 9–11 April identified by Salcedo et al. (2006), the model accurately predicts the particle phase observations during this period with the exception of the nitrate predictions after 10:00 a.m. (Central Daylight Time, CDT) on 9 April, where the model underpredicts the observations by, on average, 20%. This period had a low planetary boundary layer, very high particle concentrations, and higher than expected nitrogen dioxide concentrations. For periods when the particle chloride observations are consistently above the detection limit, the model is able to both accurately

predict the particle chloride mass concentrations and provide well-constrained HCl (g) concentrations. The availability of gas-phase ammonia observations helps constrain the predicted HCl (g) concentrations. When the particles are aqueous, the most likely concentrations of HCl (g) are in the sub-ppbv range. The most likely predicted concentration of HCl (g) was found to reach concentrations of order 10 ppbv if the particles are dry. Finally, the atmospheric relevance of HCl (g) is discussed in terms of its indicator properties for the possible influence of chlorine-mediated photochemistry in Mexico City.

Final Revised Paper (PDF, 1400 KB) Discussion Paper (ACPD)

Citation: San Martini, F. M., Dunlea, E. J., Volkamer, R., Onasch, T. B., Jayne, J. T., Canagaratna, M. R., Worsnop, D. R., Kolb, C. E., Shorter, J. H., Herndon, S. C., Zahniser, M. S., Salcedo, D., Dzepina, K., Jimenez, J. L., Ortega, J. M., Johnson, K. S., McRae, G. J., Molina, L. T., and Molina, M. J.: Implementation of a Markov Chain Monte Carlo method to inorganic aerosol modeling of observations from the MCMA-2003 campaign – Part II: Model application to the CENICA, Pedregal and Santa Ana sites, Atmos. Chem. Phys., 6, 4889-4904, 2006. Bibtex EndNote Reference Manager