Geophysical Research Abstracts, Vol. 8, 04260, 2006
SRef-ID: 1607-7962/gra/EGU06-A-04260

Importance of mineral cations and organics in gas-aerosol partitioning of reactive nitrogen compounds: case study based on MINOS results

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The partitioning of reactive nitrogen compounds between the gas and the aerosol phase, as observed during the MINOS (Mediterranean INtensive Oxidant Study) campaign in Crete, Greece, in July and August 2001, has been studied with three thermodynamic gas-aerosol equilibrium models (EQMs) of different chemical complexity: ISORROPIA, which is limited to the ammonium sulfate-nitrate-sodium-chloride-water-system, SCAPE2, which also includes mineral elements (calcium, magnesium and potassium), and EQSAM2, which additionally accounts for organic acids. The different EQMs, as applied at the same level of complexity, generally produce comparable results within the range of measurement uncertainties (on average within ˜10%), although they differ considerably in particular aspects. Model simulations of three distinct air pollution episodes during MINOS show that organic acids (lumped) and soluble mineral cations need to be included in EQMs to accurately simulate the gas-aerosol partitioning of ammonia and nitric acid.

ACPD, 2005, Vol.5, pp. 12857-12893, SRef-ID: 1680-7375/acpd/2005-5-12857, http://direct.sref.org/1680-7375/acpd/2005-5-12857