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

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Abstract. 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 are constrained by measured gas (g) and aerosol (a) concentrations: Total ammonia ($NH_{3(g)}$ and $NH_{4(a)}^+$), total nitrate ($HNO_{3(g)}$ and $NO_{3(a)}^-$), total sulfate ($H_2SO_{4(g)}$ and $SO_{4(a)}^{2-}$), total chloride ($HCl_{(g)}$ and $Cl^-_{(a)}$), sodium ($Na^+_{(a)}$), calcium ($Ca^{2+}_{(a)}$), magnesium ($Mg^{2+}_{(a)}$), potassium ($K^+_{(a)}$) and organic acids (a). Although the three EQMs differ considerably in particular aspects, their application at the same level of complexity yields comparable results for the equilibrium composition and phase partitioning of ammonia and nitric acid, i.e. within the range of measurement uncertainties (~10%). Their application at different levels of complexity, however, gives rise to substantial differences for the gas-aerosol partitioning of reactive nitrogen compounds. Our results show that only if (soluble) mineral components and (lumped) organic acids are accounted for, the observed gas-aerosol partitioning of ammonia and nitric acid can be accurately reproduced for air pollution episodes characterized by a complex chemical mixture, typical for the Mediterranean lower atmosphere.

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