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Parameterization of N₂O₅ reaction probabilities on the surface of particles containing ammonium, sulfate, and nitrate

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Abstract. A parameterization was developed for the heterogeneous reaction probability (γ) of N₂O₅ as a function of temperature, relative humidity (RH), particle composition, and phase state, for use in advanced air quality models. The reaction probabilities on aqueous NH₄HSO₄, (NH₄)₂SO₄, and NH₄NO₃ were modeled statistically using data and uncertainty values compiled from seven different laboratory studies. A separate regression model was fit to laboratory data for dry NH₄HSO₄ and (NH₄)₂SO₄ particles, yielding lower γ values than the corresponding aqueous parameterizations. The regression equations reproduced 80% of the laboratory data within a factor of two and 63% within a factor of 1.5. A fixed value was selected for γ on ice-containing particles based on a review of the literature. The combined parameterization was applied under atmospheric conditions representative of the eastern United States using 3-dimensional fields of temperature, RH, sulfate, nitrate, and ammonium. The resulting spatial distributions of γ were contrasted with three other parameterizations that have been applied in air quality models in the past and with atmospheric observational determinations of γ . Our equations lay the foundation for future research that will parameterize the suppression of γ when inorganic ammoniated particles are mixed or coated with organic material. Our analyses draw attention to a major uncertainty in the available laboratory data at high RH and highlight a critical need for future laboratory measurements of γ at low temperature and high RH to improve model simulations of N₂O₅ hydrolysis during wintertime conditions.

[Final Revised Paper](#) (PDF, 3398 KB) [Discussion Paper](#) (ACPD)

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