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A parameterization of the heterogeneous hydrolysis of N_2O_5 for mass-based aerosol models: improvement of particulate nitrate prediction

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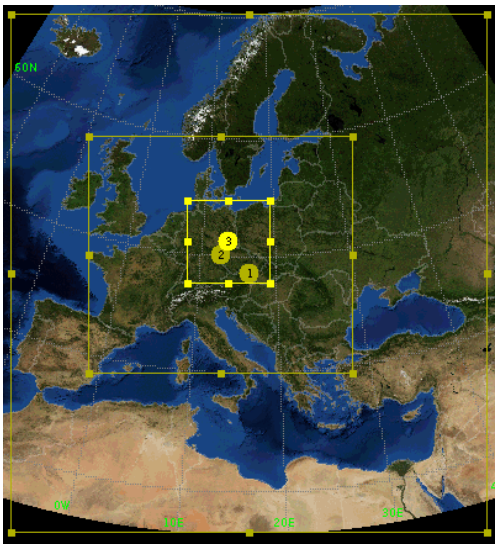


Figure S1. Domain setting of WRF-Chem simulation.

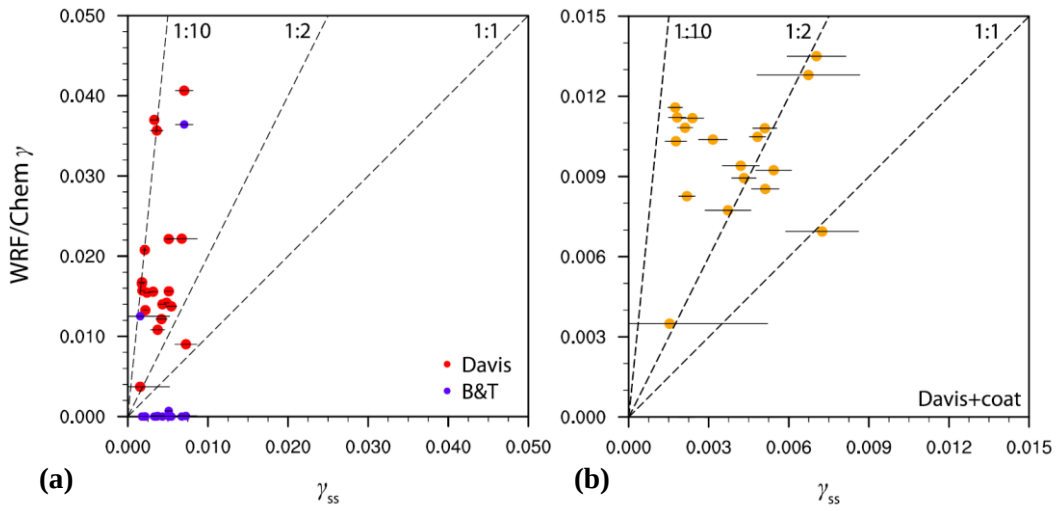


Figure S2. Modelled γ (Chang et al., 2016) versus calculated γ_{ss} (reaction probability in steady state) using aircraft observations from the 31 May flight of CalNex 2010 campaign. (a) Davis (Davis et al., 2008, namely Ch&Davis) and B&T (Bertram and Thornton, 2009) parameterization; (b) Davis+coat (Anttila06).

Source: Figure 10 of Chang et al. (2016).

S1. Temporal evolutions of NOx and N_2O_5

The concentration of gaseous precursor (NOx) was observed under the frame of HOPE-Melpitz campaign with 1h temporal resolution. As shown in Fig. S3 (newly added), the modelled NOx concentration was in line with the measurement, with a factor of 0.9 for both OldN2O5 and NewN2O5 cases. Therefore, the high overestimation of particulate nitrate should not be resulted from the uncertainty of NOx.

The N_2O_5 concentration was accumulated during nighttime in NewN2O5 case, and was totally dissociated into NO_2 and NO_3 during daytime (Fig. S3b). However, the N_2O_5 could not accumulate during nighttime in OldN2O5 case, due to its highly overestimated reaction constant.

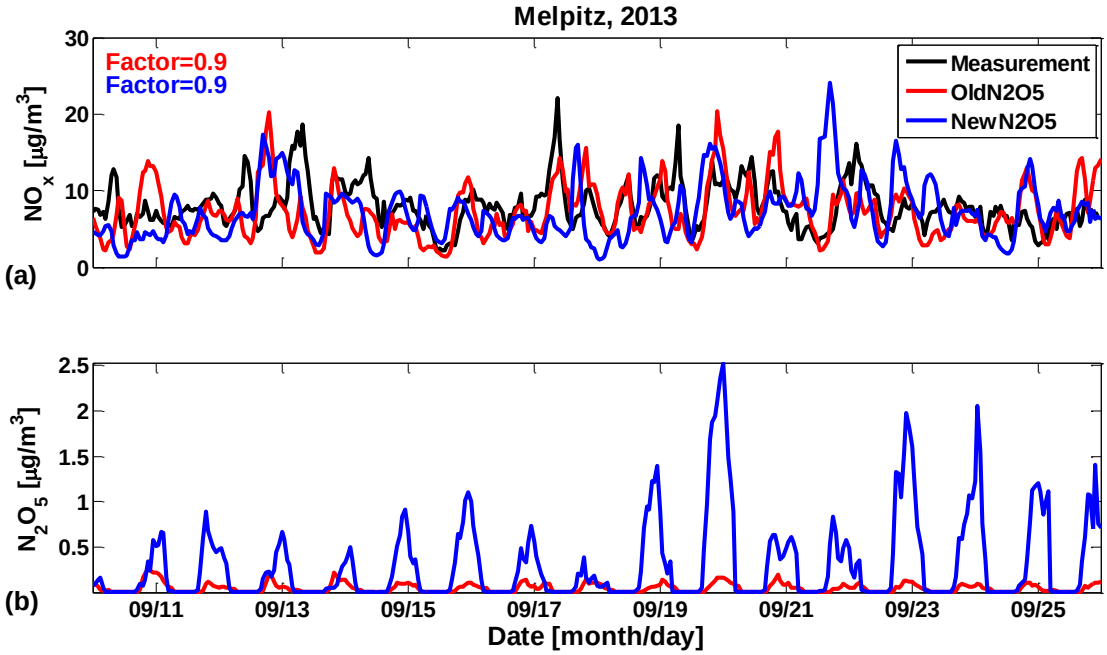


Figure S3. Time series of NOx (a) and N_2O_5 (b) at Melpitz.

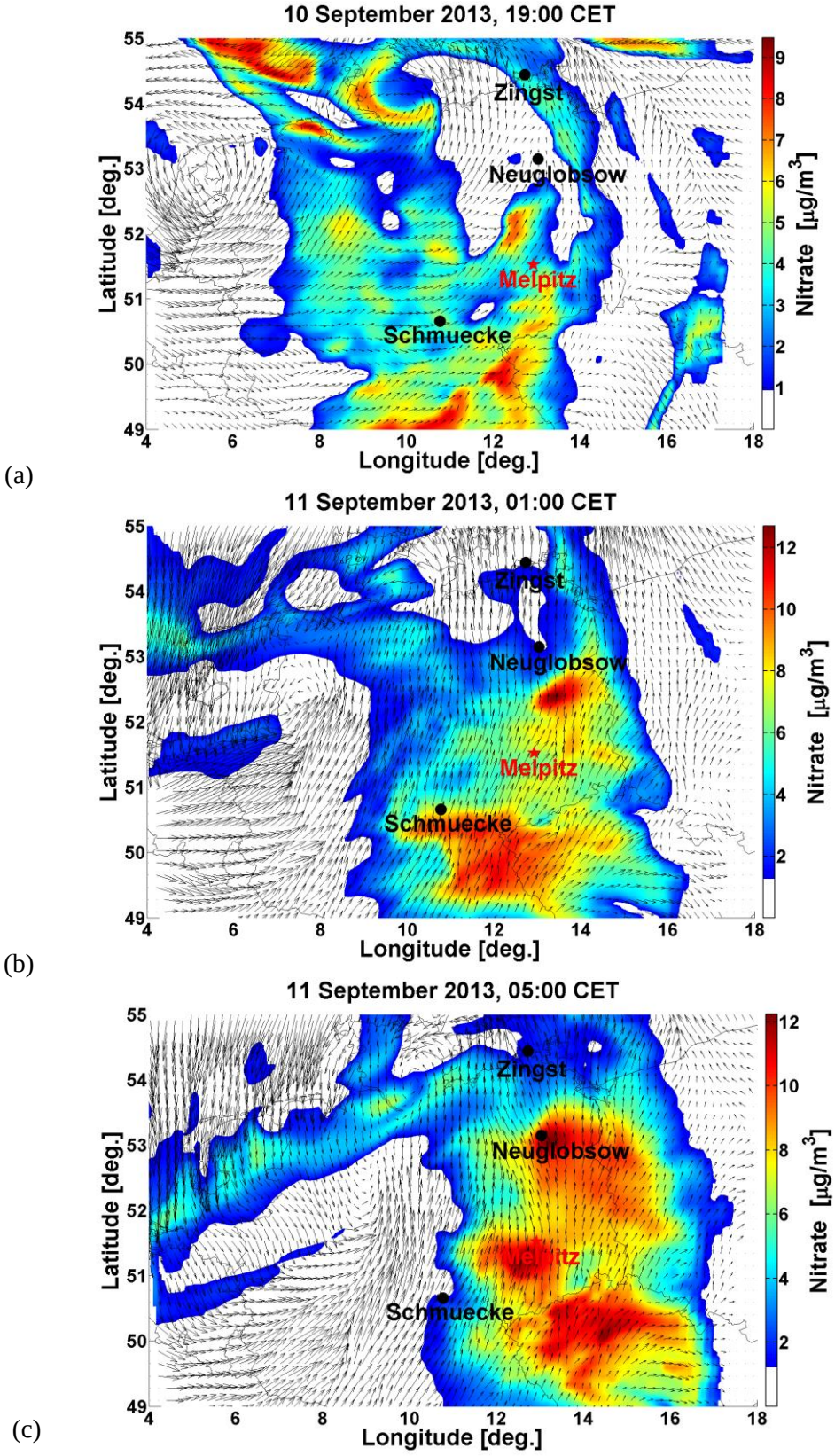
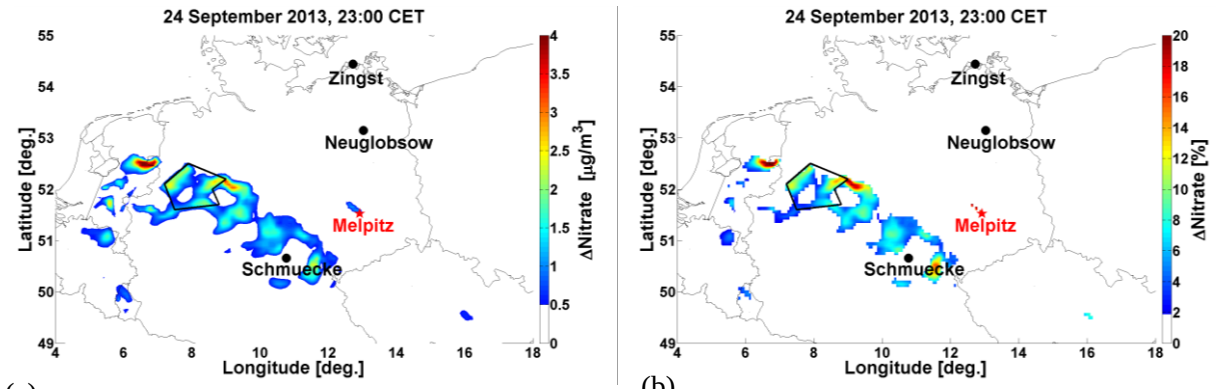


Figure S4. Spatial distribution of particulate nitrate mass concentration and wind pattern, modelled results of NewN2O5 case. (a) 2013-09-10, 19:00 CET; (b) 2013-09-11, 01:00 CET; (c) 2013-09-11, 05:00 CET.



(a) (b)

Figure S5. Horizontal distribution of modelled results at 24 September 23:00 CET, based on NewN2O5. (a) Difference of particulate nitrate mass concentration between with and without organic coating effect; (b) difference of particulate nitrate mass concentration in percentage between with and without organic coating effect, where with differences less than 2% or 0.5 µg/m^3 are indicated by white colour.

References:

Chang, W. L., Brown, S. S., Stutz, J., Middlebrook, A. M., Bahreini, R., Wagner, N. L., Dubé, W. P., Pollack, I. B., Ryerson, T. B., and Riemer, N.: Evaluating N2O5 heterogeneous hydrolysis parameterizations for CalNex 2010, Journal of Geophysical Research: Atmospheres, 121, 5051-5070, 10.1002/2015JD024737, 2016.