Atmos. Chem. Phys. Discuss., 9, C11629–C11630, 2010
www.atmos-chem-phys-discuss.net/9/C11629/2010/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Coupling aerosol surface and bulk chemistry with a kinetic double layer model (K2-SUB): oxidation of oleic acid by ozone" *by* C. Pfrang et al.

Anonymous Referee #2

Received and published: 19 March 2010

The authors present a model that couples aerosol surface and bulk chemistry, based on a framework presented earlier by Poschl et al.(2007). This model is then applied to the reaction between ozone and oleic acid - a system that has studied many times in the laboratory. In short the model is used to fit the laboratory experiments from Ziemann et al. (2005), using best estimates of kinetic parameters (such as bulk and surface reaction rates, diffusion coefficients, solubilities, etc.). From this analysis the authors demonstrate that the bulk reaction plays an important role, although the exact contribution of the surface and bulk is not possible due to the uncertainties in the kinetic parameters. The calculations also help constrain the mass accommodation coefficient and demonstrate the sensitivity to this parameter. Suggestions for future laboratory

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studies also result from the calculations. The paper is clearly written and addresses an important area of atmospheric chemistry. The scientific approach is valid, and the resulting tool (the model) should be especially helpful when applied to multicomponent systems and when surface and bulk reactions are comparable. As a result, I support this publication after the following comments are adequately addressed:

Figures 3 and 4: In Figures 2 and 7 the authors included a plot that compares the experimental data with the calculations (see for example Figures 2a, 7a and 7c). But in others figures this comparison is left out (see for example Figures 3 and 4). I would prefer to see the comparison of the experimental data with the calculations in all the figures. I realize that this information is included in the supplemental data, but it makes for easier reading if it is included in the main text. Since this is more of a personal preference I will leave it to the authors to decide.

Page 26984, line 16-17. The authors suggest that studies covering a longer reaction time would be beneficial. In this case a large fraction of the particles will be oxidized, and the matrix may be very different from the starting matrix (pure oleic acid). In this case fundamental parameters such as diffusion coefficients, solubilities, etc. may change. Please comment on this point and discuss any possible uncertainty these changes may have on the calculations.

Similar to reviewer 1, I wondered if some of the conclusions in this paper could be obtained with the traditional "resistor" modelling formulations (for example the equations in Worsnop et al. GRL, 2002). I think it would be useful if this was briefly discussed and also highlight in more detail examples were the traditional "resistor" formulations will fail and K2-SUB is needed. This comment doesn't impact my support of this paper. Regardless, the analysis in this paper is strong and important and does highlight a new and more comprehensive modelling approach.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 26969, 2009.

ACPD

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