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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Kinetic multi-layer model of aerosol surface and bulk chemistry (KM-SUB): the influence of interfacial transport and bulk diffusion on the oxidation of oleic acid by ozone" *by* M. Shiraiwa et al.

Anonymous Referee #2

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The manuscript under review presents KM-SUB, a benchmark model framework that explicitly treats interfacial and bulk transport as well as chemical reactions at the surface and in the bulk of aerosol particles. It is another paper in a series of recent papers by the authors that apply the modeling framework suggested by Poeschl, Rudich, and Ammann (2007) to different systems, and shows once more how versatile this framework is.

The unique contribution of KM-SUB is that it resolves concentration profiles on the particle surface throughout the bulk of the particle and does not require a-priori as-

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sumptions about radial mixing or steady state. The model is applied to the ozonolysis of oleic acid particles, and three scenarios are investigated representing different regimes (kinetic limitation by interfacial transport, kinetic limitation by bulk reaction, kinetic limitation by bulk diffusion).

The paper fits well within the scope of ACP, is clearly written and addresses an important topic. I recommend it for publication with some minor modifications.

1. Kinetic parameters for base cases 1-3: The results of three base cases are instructive, however references for the choice of kinetic parameters are missing and should be added.

2. Regarding BC1 and BC2: Both model simulations appear to fit the lab experiment. I assume that one of them is more realistic than the other? Please include a statement that clarifies this.

3. Nothing is mentioned regarding the assumption on what species are formed by the oleic acid degradation. Please add some clarification. Could these species react further?

4. Atmospheric implications: What might be a potential impact of having multiple species reacting/adsorbing on the particle? Calculations that include these processes are clearly beyond the scope of this paper, but it would be helpful for modelers who work on larger scale models to include a statement if that's possible.

5. Page 301, line 1-5: In addition to the possible explanations given by the authors, I am wondering if the existence of oleic acid in aged atmospheric particles can be simply explained by the fact that other species (inorganic and organic) can condense on the particles and coat them, hence shutting off the ozonolysis as described in this paper.

6. Conclusions: The comparison with K2-SUB is briefly mentioned ("fairly good agreement"). It would be helpful if this comparison was expanded, i.e. for the three scenarios, state more clearly and more quantitatively when high resolution of the bulk is needed

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and when a simpler two layer approach does just as well.

7. Typos: Page 302, line 2: Verb is missing in this sentence. Caption for figure 10: Should read “loss rate”. Page 313, line 15: Should read “Gäggeler”.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 281, 2010.