

# ***Interactive comment on “Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: Part 2 – exemplary practical applications and numerical simulations” by M. Ammann and U. Pöschl***

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We highly appreciate the referee’s readiness to review our two companion papers presenting a kinetic model framework for aerosol and cloud surface chemistry and gas particle interactions (Pöschl et al., 2005a, Ammann and Pöschl, 2005), because we are aware that the papers are rather long and comprehensive, which implies a lot of work for referees. In this comment, we respond to the specific comments regarding part 2 of our presentation of the kinetic model framework, in which exemplary practical numerical simulations of a few model systems are presented. A detailed response to

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the general comments regarding part I has been given in the discussion section of that paper (Pöschl et al., 2005b).

In our detailed response we will retrace along the comments made by the referee.

1. Abstract and Introduction and Summary and Conclusions recycle the same blocks of text, for example 2nd and 3rd paragraphs in Abstract have many sentences which are reproduced in first 2 paras in Introduction; Intro and Summary must be completely rewritten.

We believe that within a manuscript of this size it is important to refer to overall goals and detailed aims at a number of places to facilitate the orientation of the reader. Therefore, a few repetitions between introduction and summary are hardly avoidable. Nevertheless, we will try to minimize redundancies in the revised manuscript.

2. Section 3, 2nd para: It is said that the plateaus illustrate the occurrence of quasisteady- conditions in real time-dependent systems, however, the plateaus are calculated by the quasi-steady model, I feel that it is circular reasoning; see also Comment 5 in the review of the Part 1

In this paragraph in section 3, we are referring to section 2, in which we are presenting explicit numerical simulations of time dependent systems. In these simulations (within section 2) we are explicitly treating all fluxes without any steady-state approximations at all. In this respect, if explicit simulations reveal 'plateaus' (periods of a constant net rate of uptake), during these periods quasi-steady state approximations could be applied as presented in section 3. We will make sure that this point will be clarified even more in the revised manuscript.

Detailed/Technical comments:

1. Section 2.2.1: it is assumed that bulk diffusion is fast; since Table 1 also lists scenarios 2 with slower bulk diffusion, the difference between scenarios 1 and 2 should be clarified already in 2.2.1

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This comment is well taken, and we will add a sentence, where the first reference to Table 1 appears.

2. Eq. 21 is quite self-explaining, that is fluxes (normalised by surface area) should be multiplied by the surface area and then divide by the volume to get volume based concentration changes, but it could be explained explicitly

We have given the surface to volume ratio to indicate this conversion. Nevertheless, we will give an explicit explanation of how the flux based mass balance has been converted to the volume based balance for clarity.

3. Fig. 15: the text (section 3.6, 2nd para) refers to Tables 1 and 3, but Fig. caption refers to Tables 2 and 3

The comment is appreciated, the Figure captions will be corrected, the reference in the text is correct.

4. Fig. 1: different curves should be explained in the caption, although they are labelled by the symbols

This comment has been well taken, and the individual curves will be explained in the caption

5. Fig. 3: it said that particle surface composition and gas uptake coefficient are presented, although there is only one quantity (two curves for two scenarios)

Indeed, in this figure, only the gas uptake coefficient is plotted. The caption will be changed accordingly.

6. Fig. 4: explain also in the caption the difference between Figs. 4-9, that is refer to Table 1

In response to this remark, we will add a sentence describing the organization of the plots in the figures in Figures 4 and 7, in which a series of three scenarios start.

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7. Figs. 11-13: refer to Table 2 in the caption

We will add a reference to Table 2 in these captions, but also that the model systems SS2 to SS4 only refer to the scenario SS1-1, the first line in Table 2.

8. Fig. 14: Figs. a and b: the curves fill only small fraction of the Fig. area, rescale Y-axis

We have made sure that within all Figures in all plots of the surface accommodation coefficient, the bulk accommodation coefficient and the gas uptake coefficient are scaled on the same y-axis with the same range to facilitate comparison among the plots within one figure, but also from figure to figure. We are aware, that the very small deviations from 1.0 in the case of Fig. 14 b, make the figure look a little empty, however it strongly contrasts the deviations in alpha and gamma in the same figure, which we consider an important message.

9. Table 1: replace “bulk diffusion” by “surface-bulk transport”, right?; explain in the caption different scenarios and the symbols

No, the term ‘bulk diffusion’ is correct in this context: during the time scale of the simulations presented, the complete system reaches solubility saturation in model system L1 (small particles, bulk saturation), whereas in L2 solubility saturation is established only near the surface, while the net uptake flux is limited by bulk diffusion in large droplets. We will change the defining term for L1 to bulk saturation and for L2 to bulk diffusion to make the distinction more clear. The explanations of the symbols will be added to the caption.

10. Tables 2 and 3: explain in the captions those symbols which are not explained in Table 1, refer to Table 1 for others

We will add explanations of the symbols used in the caption to each table, and also a short explanation of how the scenarios in Table 1 are organized.

References

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Comment

Ammann, M. and U. Pöschl, Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: Part 2 - exemplary practical applications and numerical simulations, Atmospheric Chemistry and Physics Discussions, 5, 2191-2246, 2005.

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