

Interactive comment on “Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions: Part 1 – general equations, parameters, and terminology” by U. Pöschl et al.

Anonymous Referee #1

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The paper together with another paper “Part 2” tends to provide a general model framework for gas-particle interactions including chemistry. The concept is based on layered model with a sorption layer and quasi-static surface layer beside gas phase and bulk layers. The model comprises a set of rate equations to be solved in quasi-steady manner. Honestly, I cannot say whether the model is universally thorough and provides a general basis for future works and experiment planning. I could say that the model is at least a good step towards a comprehensive model framework which is certainly

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needed. The problem with the paper is its length and style of presentation. I would not like to publish as long paper in regular journal without any specific reason. I criticised the length already in the first phase of submission but the comment was ignored. I feel that I am forced to accept the cumbersome form of the paper, but it is not clear why.

I suggest the acceptance for the paper after I have got clear answers for the following:

1. Many phase transition processes may include significant release/absorption of heat. The paper does not say anything on coupling between mass and heat transfer.
2. The model includes a plenitude of different parameters, coefficients etc.; it would be good to have some hints for most important of them how to find values for them or possibly how to estimate their values using other known parameters and thermodynamical relations
3. the paper makes a reader's position difficult with some long sentences and long concepts, for example "pseudo-first-order quasi-static surface transformation rate coefficient" or sentence "Again the transfer. . . ." below Eq. 61; the paper must be polished from these
4. The concept of "kinetic theory of condensed phases" is used in several places; what is it exactly, is there some certain well-established kinetic theory?
5. Quasi-steady approximation (QSA) is used for coping with time dependence, some criteria should be given when QSA is acceptable when not, the question is not just reducing the time increment but of the ratio of the characteristic time scales of modelled processes vs. the time scales of governing processes; it is not always clear what are the most important governing physical process in each cases.

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6. The model is 1-dimensional but deals with, for example, spherical particles; how is the geometry taken into account for example if the bulk diffusion is important; I am not satisfied with the answer that the model reduces to some resistance/conductance formulation with “semi-theoretical” geometry corrections and terms; if the model carry the label “comprehensive” it should be more rigorous as regard the treatment of geometries; on the other hand some models with a detailed geometrical framework may have only gas phase “layers” and bulk, omitting sorption layer, quasi-static surface layer and near-surface bulk, it would good to know under what conditions or for which systems the extra layers are important

Detailed/Technical comments:

1. To orientate the reader, each sub-section in Sections 2 and 3 could shortly tell what are well-known things and what are possibly novel items to be presented in the section; that could be said in the beginning of each section
2. Section 2.2. Gas phase diffusion: “flow regime” and “transport flow”, I would replace “flow” by “flux”
3. In Eqs. 16 and 17, should α appear there?
4. In the beginning of Page 2125: “F-S is most appropriate under isothermal conditions”; the works by Paul Wagner and Markku Kulmala and their co-workers have shown that F-S works well also under non-isothermal conditions.
5. In the beginning of p. 2130: “. . . or thermal accommodation coefficient.”; thermal accommodation is really different thing from mass accommodation
6. before Eq. 31, I suppose inserting Eq. 2 and not 3?

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7. below Eq. 50, “rapid surface bulk-mass transport (low-viscosity liquid droplets”;
how is viscosity related to bulk transport, due to some flow processes, circulation
etc. or just due to relationship with diffusivity?
8. Eq. 28 has some “–“ signs but Eq. 83 has only “+” signs, should they be consis-
tent?
9. P. 2165: why is Henry’s law coefficient proportional to S_{X_i} , by the classical def-
inition, the coefficient should be temperature dependent constant; the so called
effective Henry’s law coefficient may depend also on pH
10. Conclusions and outlook: “multiple condensed phases (solid/liquid, surface/bulk,
homogeneous/heterogenous...)”, solid and liquid are phases but others men-
tioned are not
11. Conclusions, item (i); what is meant by “flexible convolution/deconvolution”?

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