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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Model for acid-base chemistry in nanoparticle growth (MABNAG)" *by* T. Yli-Juuti et al.

T. Yli-Juuti et al.

taina.yli-juuti@helsinki.fi

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Reply to the comments from Anonymous Referee 1. Comments from the referee are written on italics and our reply on normal font.

This manuscript presents a new, size-resolved particle growth model that couples the extended Aerosol Inorganics Model (e-AIM) to dynamic condensation calculations. Several scenarios are modeled using measured or estimated gas phase ammonia, amine, sulfuric acid, organic acid, temperature, relative humidity, and nanoparticle growth rates in Hyytiälä, Finland, a remote boreal forest environment. Salt formation is found to be an important contributor to nanoparticle growth under conditions where the base concentrations are high, but this pathway is not as important under conditions

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more typical to the remote boreal forest. Under most conditions relevant to the boreal forest, organic acid salts are unlikely to be observed in substantial abundance. Condensed organics are found to have an average vapor pressure on the order of 10-6 Pa. This manuscript has great relevance, is within the scope of Atmospheric Chemistry and Physics, and should be published once the very minor comments below are addressed.

We would like to thank Anonymous referee 1 for the constructive and encouraging comments. Please find below our detailed reply to each of the comments.

Comments: 1. Page 7186, line 22: The only time the authors describe the Hyytiälä site is in the Appendix. The authors should at least mention here (the first occurrence of the site in the manuscript) that it is a remote boreal forest environment in Finland.

Thank you for pointing this out. We have now added following line in the revised manuscript: '...which is a boreal forest background site situated in southern Finland (Hari and Kulmala, 2005)'.

2. Section 4: It would enhance clarity to the reader if, for each section discussing a particular simulation, the authors included an introductory sentence to the effect of: "In this simulation, X and Y were varied while A, B, and C were held constant in order to determine the effect of..." to remind the reader more explicitly of the purpose of each simulation.

In the revised manuscript we have modified the text to introduce the simulation sets in the first paragraphs of the subsections 4.1-4.5.

3. Page 7190, lines 25-26: Be more explicit. The fraction of bases in the particle dry mass decreased as particle size was increased.

In the revised manuscript we replaced 'as a function of particle size' with 'as the particle size increased'.

4. Page 7191, lines 4-6: The authors state that under the high base conditions, the

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acid-base chemistry is driven by the bases (as opposed to the acids). Is this because there is no correlation between sulfuric acid content and base content? The authors should make this point clearer.

Yes, because there is no correlation between mass fractions of sulfuric acid and bases (mass fraction of sulfuric acid decreases as the particle grows, while mass fractions of the bases staying approximately constant) at high gas phase concentrations of the bases it seems evident that neutralization of sulfuric acid is not driving the condensation of the bases at these conditions. To clarify, we have modified the text in the revised manuscript to say following:

'However, at the highest amine and ammonia concentrations, 10^{10} cm^{-3} and 10^{11} cm^{-3} respectively, there was little change in the mass fractions of base compounds during particle growth although sulfuric acid mass fraction decreased as the particle size increased. This lead to lack of correlation between the mass fractions of sulfuric acid and the bases. Therefore, at these conditions the controlling factor for the partitioning of the bases to the particle phase seems to be their high gas phase concentrations and the acid-base chemistry in the particle phase is driven by the bases.'

5. Page 7194: On this page, the authors compare MABNAG to a conceptual growth model. The authors state that qualitatively similar results are obtained for both models and then provide a somewhat vague comparison of the two. This discussion could be enhanced by inclusion of a table that explicitly compares the calculated composition using each model.

In the revised manuscript we have included a figure (Fig. 8) to illustrate the comparison of the two models. We have also extended the discussion on this topic within the text by stating now the following:

'The two models, MABNAG and the conceptual model (Riipinen et al., 2012) give qualitatively similar results on the particle growth with the same gas phase concentrations and initial composition of the particle: mass fraction of organic acid increases while

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mass fractions of sulfuric acid and bases decrease as the particle grows (Fig. 8). However, MABNAG predicts less amine and more ammonia, and in total less bases, in the particle compared to the conceptual model.'

6. Page 7198, lines 23-27: Validation of this model could also be achieved by comparing to nanoparticle composition measurements. Obviously, those measurements are hard to make, but this should be mentioned.

We agree with the referee and have added following sentence at the end of the paragraph in the revised manuscript:

'Measuring the evolution of nanoparticle composition during the growth is challenging, but as the experimental techniques on this area develop, such measurements will serve as an important comparison point in validating the growth model.'

7. The manuscript would benefit from a more thorough proofreading for grammar and typographical errors. Below are a list of some of them:

a. Page 7182, line 10: The reference to Eq. (7) actually refers to Eq. (6).

b. Page 7178, line 13: Change "is" to "are"

c. Page 7188, line 16: Change "in" to "is".

d. Page 7191, lines 17-19: "As the underlying assumption...." This is not a sentence. Please revise.

e. Page 7191, lines 24 and 27: Should "of the bases" be "for the bases"?

Thank you for noting these. We have corrected these in the revised manuscript. We have also carefully checked the spelling of the rest of the manuscript and made the corrections in the revised manuscript.

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 7175, 2013.