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

Anonymous Referee #2

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In the manuscript, the authors presented a “Model for Acid-Base chemistry in Nanoparticle growth (MABNAG)” to investigate the dynamics of condensational growth and its coupling with the particle phase chemistry. The systems with sulfuric acid, one kind of organic acid, ammonia, one kind of amine, and water were studied. In the MABNAG model, it was assumed that the growth rate is limited by condensation of sulfuric acid and organic acid, with a fast (instantaneous) equilibrium between the particle and the gaseous water, ammonia, and amine. Because of this assumption, their derived growth rate of nanoparticles corresponded to the upper limit of the actual growth rate. In reality, the assumption is only reasonable for water but not for ammonia and amine, since in the atmosphere the concentration of water is typically 10⁸-9 times higher than those of ammonia and amine. A more accurate model also needs to treat the conden-

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sation of ammonia/amine dynamically. In the current study, the assumption is accurate enough for an upper limit estimation. Based on the assumption, at each step, (1) the equilibrium of water, ammonia, and amine with the particle is maintained, while the equilibrium saturation vapors of sulfuric acid and organic acid are calculated (Peq,i). (2) Using equation (1), a new composition is obtained, which is used for calculating the new equilibrium. Performing (1) and (2) iteratively, the growth rate of nanoparticles can be obtained. According to their simulations, the authors claimed that the amine concentration affected the growth rate less than organic acid concentration, which is obvious according to their assumption. Overall, the material presented in the manuscript is interesting and may be publishable, pending revisions as outlined below. (1) On page 7190 line 27, the authors claimed that “the mass fractions of the bases decreased simultaneously with the mass fraction of sulfuric acid during particle growth suggesting that the condensation of the bases on the particle was driven by the neutralization of sulfuric acid instead of organic acid”. This statement was wrong. The decrease of basic species percentage was because of the basic species was limited (Figure 4 panel d->e->f). If the basic species were not limited, the mass percentage of basic species would not decrease (Figure 4 panel g->h->i). Figure 4 panel i clearly shows that the basic species also react with organic acid in the particle phase. Also, the topic of the base-organic acid reaction on nanoparticle growth has been suggested previously (Chem. Rev. 112, 1957, 2012; Phys. Chem. Chem. Phys. 15, 5738, 2013), but those relevant literatures were largely ignored here. (2) For Figure 4, it would be better if the mass percentage was presented in mole percentage, which would make it easier to compare the relative abundance of basic to acidic species. For example, in Figure 4 panel i, it appears that basic species are less than acidic species. However, if the mole percentage is used, the percentage of basic and acidic species may be equal. (3) From Figure 7(c), it is even evident that organic acid reacts with ammonia. At size of 40 nm, the mole fraction of organic acid²⁻ is close to the half of NH₄⁺. This half coefficient is a result of charge conservation. I suggest that the authors replot all the mass percentage in mole percentage or at least present both.

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

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