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Atmospheric Chemistry and Physics Discussions

Interactive comment on “Internal mixing of the organic aerosol by gas phase diffusion of semivolatile organic compounds” *by* C. Marcolli et al.

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The manuscript deals with a very important and relevant topic: thermodynamic properties of semi volatile organic compounds in aerosol particles and state of mixing. The definition of semi volatile organic compounds (SVOCc) is linked to relevant atmospheric properties as particle size and ambient temperature as well as to the main chemical characteristics, as molecular weight and polarity. The subject is within the scope of Atmospheric Chemistry and Physics and contains new and interesting results. I have some minor points to address a) The gas diffusion process described in this paper is shown to be very sensitive to the temperature. Frequently, continental areas experience strong diurnal variation of the temperature. Does it make sense to consider an isothermal equilibration of the organic species during time scales of 1 week (or even 1 day) in these areas? Conceptually, in the afternoon most SVOCs will evaporate to re-condense after midnight to give a completely internally mixed aerosol population, therefore the time scale would be of ca.12 h for a large number of species irrespectively of their specific Henry's law constant. b) It must be stated that chemical reactions of SVOCs are not taken into account by the present study. The most simple reaction is the neutralization of volatile carboxylic acids by ammonia. This would impact the partition of species like oxalic acid which, indeed, is found in the aerosol phase in significant concentrations (see Figure 3 of the paper) despite of its high vapour pressure. c) In section 3.3, the predictions of the model are compared with the observations by Mochida et al. (2003) who found that the size-distribution of oxalic acid in a marine polluted environment may reflect its redistribution in the aerosol population by gas-phase diffusion. However, a different case is provided by Neususs et al. (J.Geophys.Res. 105, D4, 4513-45-27, 2000) who found in a similar environment that dicarboxylic acids and hydroxyacids exhibit different size-distributions, despite of only limited differences in volatility. d) pg. 5796, line 15 the authors sustain that the treatment used by Meng and Seinfeld (1996) is too simple to describe the behaviour of species concentration in the gas and aerosol phase in Fig1. Can the authors explain better this concept? An explicit intercomparison between the two approaches will be very helpful in showing the differences. e) Another not clear topic is the influence of aerosol polydispersity. Do the results presented in Fig. 1 remain the same if the model is shifted from ultrafine (present data) to accumulation? f) It is also no clear how the equilibration time constants calculated in Fig. 2 for molecular weights of 100 and different vapour pressures can be extrapolated to different molecular weights: please discuss this briefly g) It should be helpful for the readers to add on the right axis of Fig. 3 the corresponding molecular weights

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