Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2019-819-RC2, 2020

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Treatment of non-ideality in the multiphase model SPACCIM-Part2: Impacts on the multiphase chemical processing in deliquesced aerosol particles" *by* Ahmad J. Rusumdar et al.

Anonymous Referee #2

Received and published: 22 January 2020

The authors present a sensitivity study of the impact of considering nonideal solution effects on predictions of aqueous aerosol chemistry using the SPACCIM-SpactMod model. The study is well-conceived, and the results highlight the potential significance of nonideal solution effects in multiphase atmospheric chemistry, something that is generally ignored in atmospheric models due in part to computational expense but also because of a lack of data. I think the manuscript will be suitable for publication in ACP after a few clarifications.

- The aqueous chemical kinetic data in CAPRAM, which the multiphase chemical ki-

netic simulations in this study were based on, for the most part was not originally measured/reported as a function of activity but rather of concentration. The measurements that form the basis of that data were also mostly performed under much more dilute and closer to ideal conditions than the aqueous aerosol conditions considered here. How accurate is it to use those rate laws but plug in the activities calculated here - which are in many cases very different from the activities where the rates were originally measured both because of the high concentrations of atmospheric aerosols but also because of the nonideality? Is it even possible to evaluate this?

- I agree with the other referee's comment that the uncertainty in the MR parameterizations for Fe and Mn are a significant weakness, especially given the likely importance of those two ions in multiphase atmospheric chemistry. Could the authors estimate those parameters, perhaps from available lab data, to at least constrain the effect?

- Considerable uncertainty exists in the measured and reported rate data for much TMI chemistry, especially when it comes to ionic strength and pH dependence. Can the authors comment on the relative significance of these uncertainties to the nonideal solution effects calculated here?

- How often in the simulation are the activity coefficients recalculated, i.e. as concentrations change in the aqueous phase? Does it happen at every timestep?

- Since much depends in this study on the model chosen for activity coefficients, it would have been nice to see a sensitivity study of other popular approaches that could have been used instead. This is done somewhat in Table 3 and page, last paragraph. Given the sharp criticism presented, the discussion of Mao et al (2013) in this paragraph needs more elaboration (how do you know the implementation was 'incorrect'?), perhaps in the SI.

Interactive comment on Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2019-819, 2019.