

Interactive comment on “Effects of Water-soluble Organic Carbon on Aerosol pH” by Michael A. Battaglia Jr. et al.

Anonymous Referee #2

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In “Effects of Water-soluble Organic Carbon on Aerosol pH”, the authors examine changes in pH due to water solute organic acid with inorganic-organic single-phase aerosol systems, at conditions from two locations: Baltimore (more acidic) and Beijing (less acidic). In the manuscript, the authors detail use of three widely used thermodynamic models: E-AIM, ISORROPIA, and AIOMFAC for calculations of water content, activity coefficients, and pH. The results should that the impact of the organic content explored here on pH was minimal, and continues to support the role of the inorganic compounds in determining pH. However, there are some unanswered questions regarding the calculation methods, and in particular the role of dissociation equilibria of the organic acids, that should be clarified or handled in more depth. The paper would be of interest to the Atmospheric Chemistry and Physics readership, and should be

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considered for publications after the following are addressed.

1. Organic acids and dissociation:

It was stated that “non-acidic WSOC were found to have a larger effect. . . than organic acids” due to their larger impact on H⁺ activity. However, it is not clear how the models used handle the concentration and the concentration, ionic strength, and pH dependent dissociation of the weak organic acids. Clarify how AIOMFAC treats the organic acids. Selection of organic acids can be put into E-AIM, both with an UNIFAC treatment, and a fitted treatment, which, I believe, treats the organic acid as non-dissociating and partially-dissociating. It would be helpful to see the impact of the two treatments in the pH results. It may be that different treatment of the dissociation equilibrium may result in more significant changes in pH by the organic acid.

2. Effects due to selected method/models:

There remains an underlying question of if the results (e.g., the minimal impact of WSOC on aerosol pH) is due to the method and models used, versus being representative of the true pH in the Baltimore and Beijing conditions. It would be helpful to compare results with various treatments of organic acid dissociation equilibrium (see above comment) as well as organic-inorganic mixtures. For the later, one can add organic compounds to E-AIM, by way of using UNIFAC functional groups – how do the results from this method compare to the that with a combined E-AIM for the inorganic, AIOMFAC for the organic method used here? E-AIM was used for the Baltimore data, and ISORROPIA for the Beijing data – how do the results vary if this was switched? For example, a model-based impact likely explains the isolated group of points in Fig 4 (page 16 line 21 – page 17 line 11) – is that same group of points found with oxalic acid is treated using a different model?

3. Effects of the inorganic salts and the model organics chosen:

How much impact did the choice of method to go from individual ions to salts (page

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11) have on the results? How does this compare to results if the ions were evenly distributed into all the possible salt combinations? For the organics, more information on why the three particular non-acids were chosen. (line 22, page 8) Also, why were organic acids and non-organic acids not considered together? (line 5, page 9). Is it expected that having the mixture would impact the results?

4. Minor comments:

- Define what is meant by "... the thermodynamic equilibrium problem..." (line 2, page 4).
- What are the typical organic to inorganic mass ratios of the two region (line 1, page 9)
- How much H^+ was typically added for electroneutrality (line 19-20, page 9), compared to the other cations? Was it significant? Please comment.
- "AIOFAC" typo, line 9, page 13

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