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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Molecular Dynamics Simulation of the Surface Tension of Aqueous Sodium Chloride: from Dilute to Highly Supersaturated Solutions and Molten Salt" *by* Xiaoxiang Wang et al.

Anonymous Referee #1

Received and published: 11 December 2017

This succinct paper uses molecular dynamics to probe the concentration dependent variation in surface tension of aqueous sodium chloride solutions, and to demonstrate/support the general concept of a previous semi-empirical model by Dutcher et al (2010).

I support the presentation of supporting evidence from molecular dynamics simulations in ACP generally. These tools, whilst often not overly reliable for absolute values such as saturation vapour pressures, are useful in determining trends at least. I am not an expert in MD simulations but, without providing a detailed critique of model configura-

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Discussion paper

tions, I suggest the paper is accepted for publication in ACP after some minor issues are addressed, and the paper better reshaped for the audience of this journal.

General comments:

In section 2.1, the authors note how simulations from 1000K to 1700K are used and extrapolated down to 298.15K. Is this a requirement from the simulation over simulations at lower temperatures? It is not clear whether any extrapolation would need to account for specific non-linearities that change over such a large temperature range. One might imagine any error in this process might impact on the offset presented in figure 3a?

It would be nice to see some quantitative analysis of potential impact of this work. Whilst the impact of cloud activation processes should be small, where do the authors suggest this new dependency needs to be taken into account? For example given the below cloud focus, would it potentially influence the efflorescence transition RH according to the energy differential between a solid and saturated state? Would it affect growth rates in varying humidity environments? Could you perform some quantitative analysis on this? If not, please make it clear why.

How applicable would the model be to other salts, particularly mixed salts that might arise in non-marine environments? The increased interest in bulk to surface partitioning studies require more thorough supporting studies on systems with surfactant organics. Where do MD simulations have a role here? Please guide the reader on some broad issues as to where you might demonstrate these tools in more obviously pressing issues.

Minor comments:

Page 2, line 10: I would suggest - size-effects at ‘the’ nanoscale.

Page 2, line 38: Suggest - based on the ‘following’ concept

Page 2, line 40: “solute” (t)hat

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