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Atmospheric Chemistry and Physics Discussions

Interactive comment on "HULIS in nanoaerosol clusters; investigations of surface tension and aggregate formation using molecular dynamics simulations" *by* T. Hede et al.

Anonymous Referee #1

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This manuscript addresses questions of high relevance for atmospheric science, namely the issue of morphology of multicomponent aqueous/organic aerosol particles, and provides important molecular level insight into the structural properties of aqueous nanodroplets containing HULIS. I recommend its publication subject to minor changes and corrections as noted below. In my review, I will focus only on the molecular dynamics part of the work, as this is my area of expertise. I don't feel competent to comment on the aspects of the paper concerning the theory of nucleation/condensation.

1. In the abstract, the term 'Humic-like substances of larger systems' is unclear and should be rephrased.

2. Details on computational cost of the simulations would be of interest (typical total CPU time per one trajectory).

3. MD simulations were performed for systems containing 3 different HULIS species, however, results of only two of them (CPA and PAL) are discussed in section 4.1 (Aggregate formation). Results for PAD should also be provided and discussed, unless they are very similar to one of those shown (in which case it should be stated).

4. In the radial number density (RND) plots, RND of water should be included to show the position of the water/vapor interface of the cluster and to provide a frame of reference regarding the location of the various features occurring on the radial density profile of the HULIS species.

5. Regarding the surface tension calculations (section 4.2), in the paragraph below Table 2, please provide the experimental value and also the value obtained for the extended liquid/vapor interface using the SPC/E model explicitly. Please discuss possible effects of a deviation of the surface tension of a water cluster of 10 000 water molecules from that of an extended liquid/vapor interface.

Technical issues: - Replace 'solvatisation shell' with 'solvation shell'. - The term 'molecular dynamics' is usually written in lower case. - Replace 'nosé-Hoover' with 'Nosé-Hoover'.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 6957, 2011.