

## ***Interactive comment on “On the implications of aerosol liquid water and phase separation for organic aerosol mass” by Havala O. T. Pye et al.***

### **Anonymous Referee #1**

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This study investigated aerosol water interactions with semi-volatile SOA species and uptake of water onto OA with a focus on simulating conditions during the SOAS campaign. They have developed a method to take into account effects of non-ideality and phase separation on SOA formation and partitioning. They found that inclusion of water in an organic phase led to increased SOA concentrations, particularly at night. Aerosol properties, such as the OM/OC and hygroscopicity parameter were captured well, but additional improvements in daytime organic aerosol are needed to close the model-measurement gap. I found this modeling study is conducted very well making use of comprehensive measurements conducted in the SOAS campaign. The authors made great efforts in implementing state-of-the-art knowledge of aerosol water and phase separation into the regional model. I appreciate this study very much and recommend for publication in ACP after the following comments are addressed.

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#### Specific comments:

- P4, L10: Have you actually implemented eq(1) into the model? Terpene and toluene SOA have higher viscosity and lower bulk diffusivity compared to isoprene SOA (e.g., Renbaum-Wolff et al., 2013; Song et al., ACP, 2016). Were SOA particles in SOAS totally dominated by isoprene SOA and only little influence by terpene or anthropogenic emissions? Please clarify and justify.
- P4, L21: “SOA from cloud processing is relatively minor in terms of average SOA concentrations.”: Please justify this sentence by adding some explanations or reference(s). Have you investigated this by modeling or is this implied by measurements? Was aqueous phase processing (particle-phase chemistry in deliquesced particles) also minor?
- P5, L13: Just to draw your attention, the recent study (Li et al., 16, 3327, ACP, 2016) has extended eq(2) by including number of N and S per molecule to estimate volatility.
- P5, eq(2): This should be  $C_0$ , but not  $C^*$ . As you discuss in this manuscript,  $C^*$  (effective saturation mass concentration) includes the effect of non-ideality, but I believe eq(2) can be only used to estimate pure compounds saturation mass concentration.
- Figure 4: I wonder why  $C^*$  of glyoxal is  $1e02 \text{ ug m}^{-2}$ . I believe  $C_0$  of glyoxal is much higher based on eq(2). Is this because glyoxal is very water soluble so that  $C^*$  is lowered?
- Figure 4: It seems that high molar mass and low volatility compounds (i.e., particle-phase products such as dimers, peroxyhemiacetals, oligomers, etc. that would locate close to the alkane line) were not considered in CMAQ. Do you have reason? Were such compounds not detected by measurements in SOAS?
- P13, L12, P14, L2: All IEPOX-derived species were assumed to be non-volatile and I suppose that the model also assumed that such product formation is irreversible. Have you evaluated this assumption by sensitivity simulations? Is it possible that such product

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formation is actually reversible and might evaporate under certain conditions?

- P15, Figure 7: Model reproduced OC well, while overestimating POC and underestimating SOC. Is it possible actually this may suggest that measurements might have overestimated SOC? I suppose that SOC was assumed to be equivalent to OOA based on AMS-PMF analysis (correct?). What are uncertainties of the measurements? I wonder this, as AMS measures chemical composition and estimate secondary formation processes by post numerical analysis, while the model simulates secondary processes directly.

- P21, L8: Could gas-phase ELVOC formation or particle-phase chemistry help to close the measurement-model gap?

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